Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 10:04 PM EDT

PDB ID	:	2KNC
BMRB ID	:	16496
Title	:	Platelet integrin ALFAIIB-BETA3 transmembrane-cytoplasmic heterocomplex
Authors	:	Yang, J.; Ma, Y.; Page, R.C.; Misra, S.; Plow, E.F.; Qin, J.
Deposited on	:	2009-08-20

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

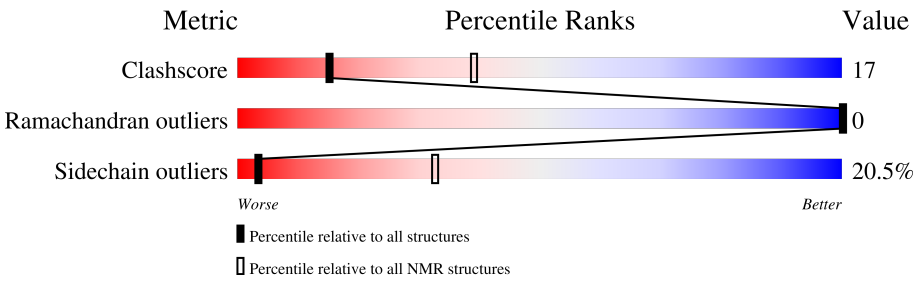
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 86%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	54	28% • • 65%
2	B	79	19% 6% • 73%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:970-A:988, B:700-B:720 (40)	0.34	5

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

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

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

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2128 atoms, of which 1083 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Integrin alpha-IIb.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	54	862	280	435	69	76	2	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	955	GLY	-	expression tag	UNP P08514
A	956	ALA	-	expression tag	UNP P08514
A	957	MET	-	expression tag	UNP P08514
A	958	GLY	-	expression tag	UNP P08514
A	959	SER	-	expression tag	UNP P08514

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	79	1266	401	648	104	111	2	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	684	GLY	-	expression tag	UNP P05106
B	685	ALA	-	expression tag	UNP P05106
B	686	MET	-	expression tag	UNP P05106
B	687	GLY	-	expression tag	UNP P05106
B	688	SER	-	expression tag	UNP P05106

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Integrin alpha-IIb

Chain A: 28% • • 65%

G955 A956 M957 G958 S959 E960 E961 R962 A963 I964 P965 I966 W967 W968 V969 L970 L974 M987 W988 K989 V990 G991 F992 F993 K994 R995 N996 R997 P998 P999 L1000 E1001 E1002 D1003 D1004 E1005 E1006 G1007 E1008

• Molecule 2: Integrin beta-3

Chain B: 19% 6% • 73%

G684 A685 M686 G687 S688 K689 G690 P691 D692 I693 L694 V695 V696 L697 L698 S699 V700 M701 L705 L709 K716 L717 L718 I719 T720 I721 H722 D723 R724 K725 E726 F727 A728 K729 F730 E731 E732 E733 R734 A735 R736 A737 K738 W739 D740 T741 A742 N743 N744 P745 L746 Y747 K748 E749 A750 T751 S752

T753 F754 T755 N756 I757 T758 Y759 R760 G761 T762

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

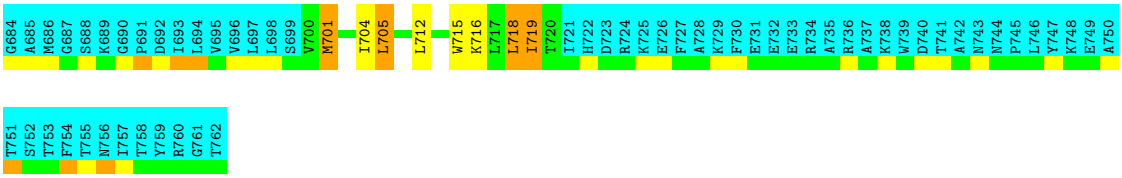
• Molecule 1: Integrin alpha-IIb

Chain A: 22% 7% 6% 65%

G955 A956 M957 G958 S959 E960 E961 R962 A963 I964 P965 I966 W967 W968 V969 L970 V971 G972 V973 L974 L978 L979 M987 W988 K989 V990 G991 F992 F993 K994 R995 N996 R997 P998 P999 L1000 E1001 E1002 D1003 D1004 E1005 E1006 G1007 E1008

• Molecule 2: Integrin beta-3

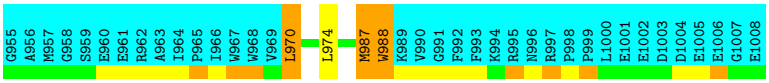
Chain B: 16% 5% 5% 73%



4.2.2 Score per residue for model 2

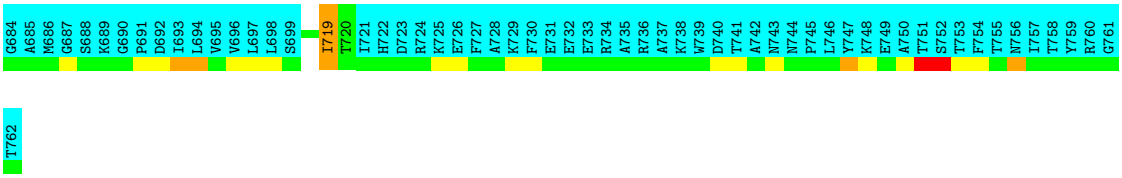
- Molecule 1: Integrin alpha-IIb

Chain A:



- Molecule 2: Integrin beta-3

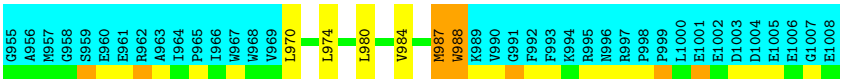
Chain B:



4.2.3 Score per residue for model 3

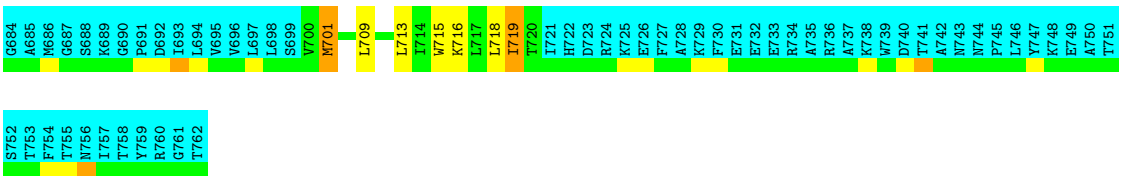
- Molecule 1: Integrin alpha-IIb

Chain A:



- Molecule 2: Integrin beta-3

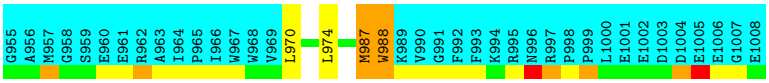
Chain B:



4.2.4 Score per residue for model 4

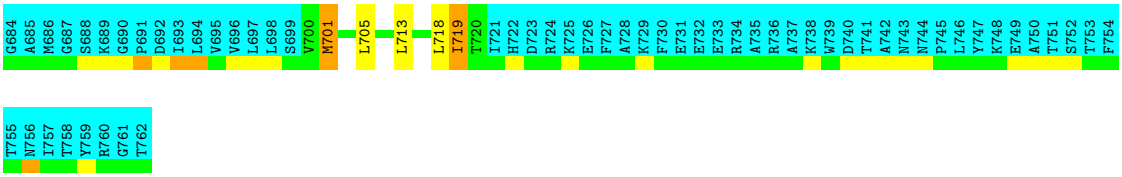
- Molecule 1: Integrin alpha-IIb

Chain A:



- Molecule 2: Integrin beta-3

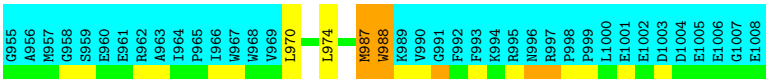
Chain B:



4.2.5 Score per residue for model 5 (medoid)

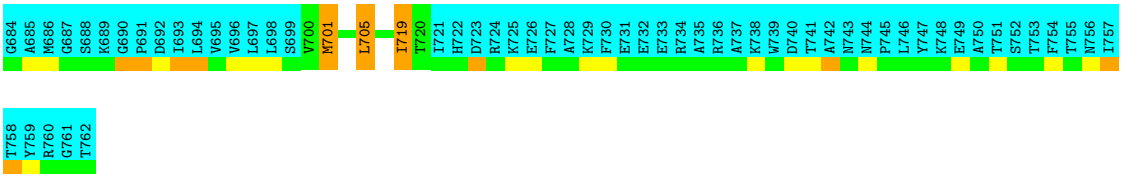
- Molecule 1: Integrin alpha-IIb

Chain A:



- Molecule 2: Integrin beta-3

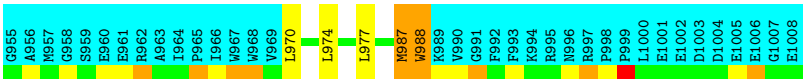
Chain B:



4.2.6 Score per residue for model 6

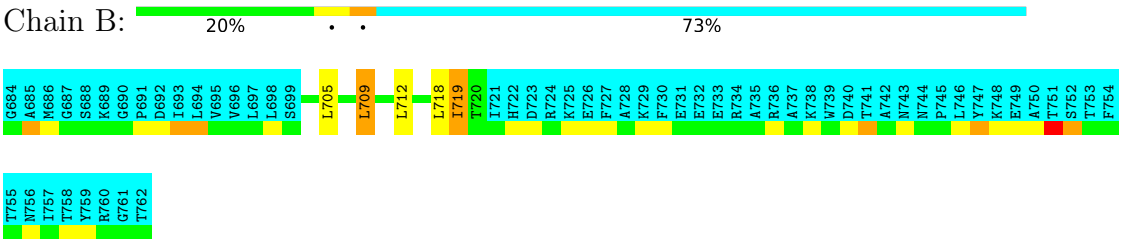
- Molecule 1: Integrin alpha-IIb

Chain A:



• Molecule 2: Integrin beta-3

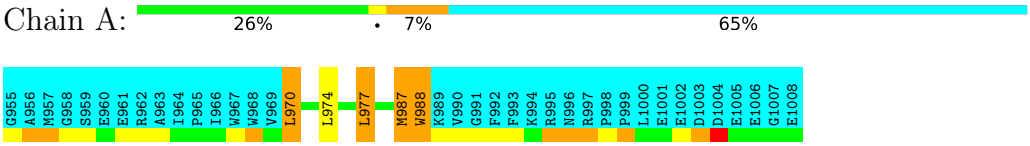
Chain B:



4.2.7 Score per residue for model 7

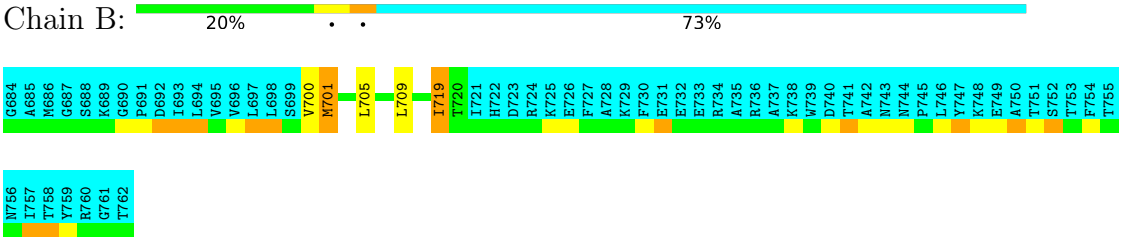
• Molecule 1: Integrin alpha-IIb

Chain A:



• Molecule 2: Integrin beta-3

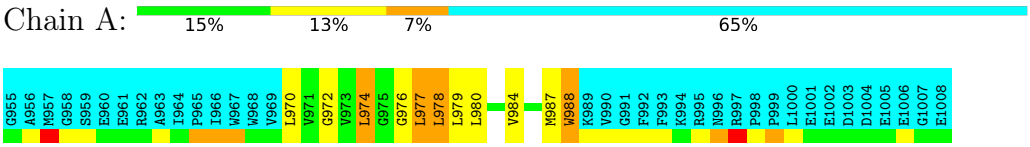
Chain B:



4.2.8 Score per residue for model 8

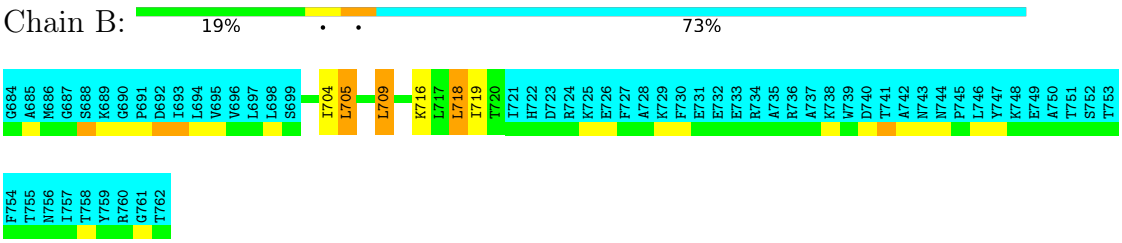
• Molecule 1: Integrin alpha-IIb

Chain A:



• Molecule 2: Integrin beta-3

Chain B:



4.2.9 Score per residue for model 9

- Molecule 1: Integrin alpha-IIb

Chain A: 20% 11% • 65%

G955 A956 M957 G958 S959 E960 E961 R962 A963 I964 P965 I966 W967 W968 V969 L970 L974 G975 G976 L979 L983 V984 M987 W988 K989 V990 G991 F992 F993 K994 R995 N996 R997 P998 P999 L1000 E1001 E1002 D1003 D1004 E1005 E1006 G1007 E1008

- Molecule 2: Integrin beta-3

Chain B: 22% 5% 73%

G684 A685 M686 G687 S688 K689 G690 P691 D692 I693 L694 V695 V696 L697 L698 S699 I704 L712 K716 I719 T720 I721 H722 D723 R724 K725 E726 F727 A728 K729 F730 E731 E732 E733 R734 A735 R736 A737 K738 W739 D740 T741 A742 N743 N744 P745 L746 Y747 K748 E749 A750 T751 S752 T753 F754 T755

N756 I757 T758 Y759 R760 G761 T762

4.2.10 Score per residue for model 10

- Molecule 1: Integrin alpha-IIb

Chain A: 22% 9% • 65%

G955 A956 M957 G958 S959 E960 E961 R962 A963 I964 P965 I966 W967 W968 V969 L970 V971 G972 V973 L974 L979 V984 M987 W988 K989 V990 G991 F992 F993 K994 R995 N996 R997 P998 P999 L1000 E1001 E1002 D1003 D1004 E1005 E1006 G1007 E1008

- Molecule 2: Integrin beta-3

Chain B: 16% 8% • 73%

G684 A685 M686 G687 S688 K689 G690 P691 D692 I693 L694 V695 V696 L697 L698 S699 V700 M701 I704 L709 L712 L713 I714 L717 L718 I719 T720 I721 H722 D723 R724 K725 E726 F727 A728 K729 F730 E731 E732 E733 R734 A735 R736 A737 K738 W739 D740 T741 A742 N743 N744 P745 L746 Y747 K748 E749

A750 T751 S752 T753 F754 T755 N756 I757 T758 Y759 R760 G761 T762

4.2.11 Score per residue for model 11

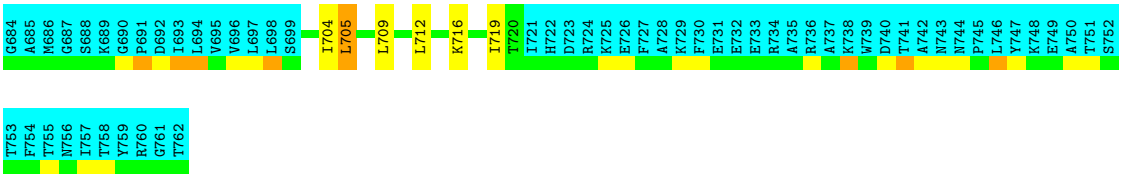
- Molecule 1: Integrin alpha-IIb

Chain A: 22% 11% • 65%

G955 A956 M957 G958 S959 E960 E961 R962 A963 I964 P965 I966 W967 W968 V969 G972 G976 L979 V984 L985 A986 M987 W988 K989 V990 G991 F992 F993 K994 R995 N996 R997 P998 P999 L1000 E1001 E1002 D1003 D1004 E1005 E1006 G1007 E1008

• Molecule 2: Integrin beta-3

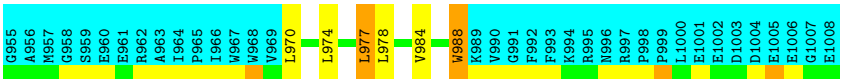
Chain B: 19% 6% • 73%



4.2.12 Score per residue for model 12

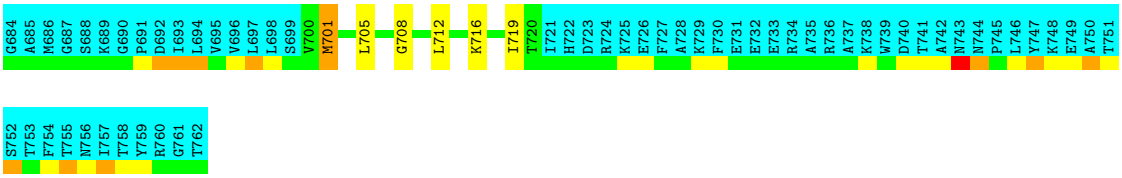
• Molecule 1: Integrin alpha-IIb

Chain A: 24% 7% • 65%



• Molecule 2: Integrin beta-3

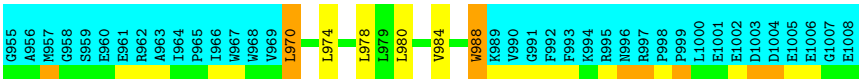
Chain B: 19% 6% • 73%



4.2.13 Score per residue for model 13

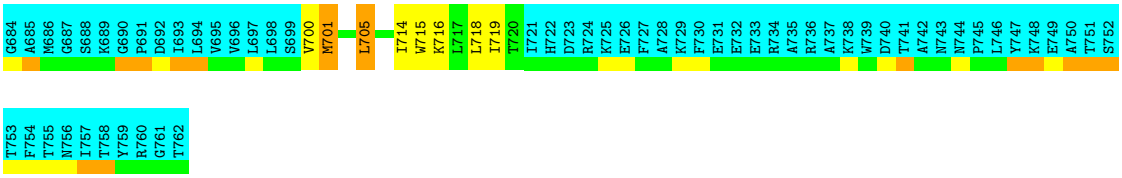
• Molecule 1: Integrin alpha-IIb

Chain A: 24% 7% • 65%



• Molecule 2: Integrin beta-3

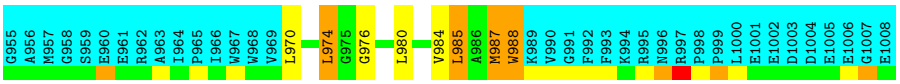
Chain B: 16% 8% • 73%



4.2.14 Score per residue for model 14

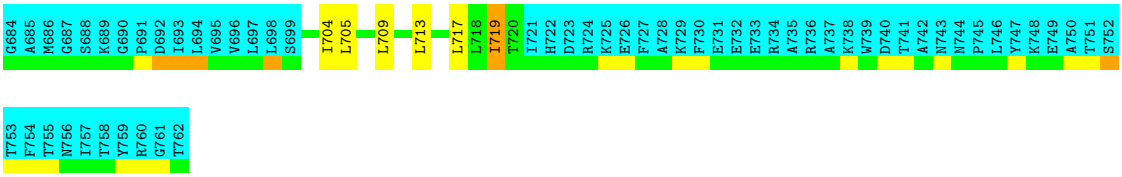
- Molecule 1: Integrin alpha-IIb

Chain A: 20% 7% 7% 65%



- Molecule 2: Integrin beta-3

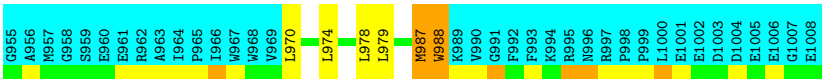
Chain B: 19% 6% • 73%



4.2.15 Score per residue for model 15

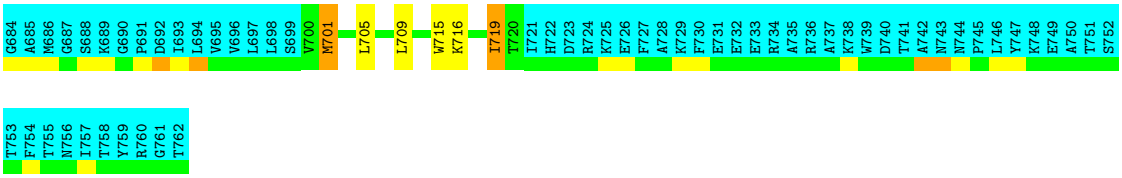
- Molecule 1: Integrin alpha-IIb

Chain A: 24% 7% • 65%



- Molecule 2: Integrin beta-3

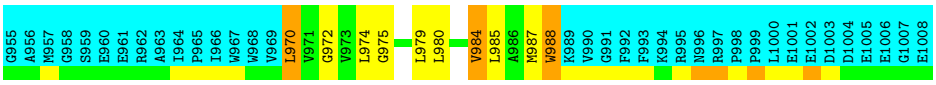
Chain B: 19% 5% • 73%



4.2.16 Score per residue for model 16

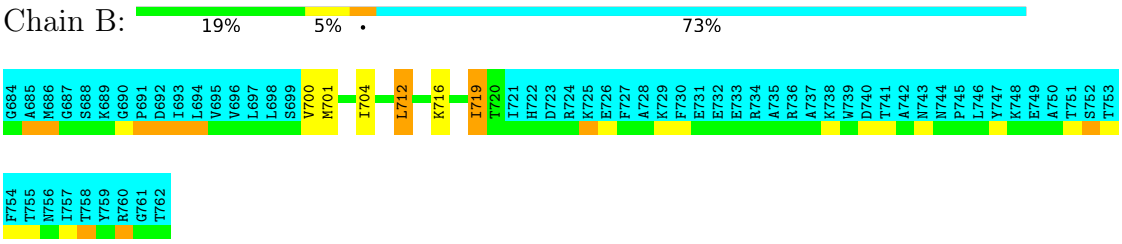
- Molecule 1: Integrin alpha-IIb

Chain A: 17% 13% 6% 65%



• Molecule 2: Integrin beta-3

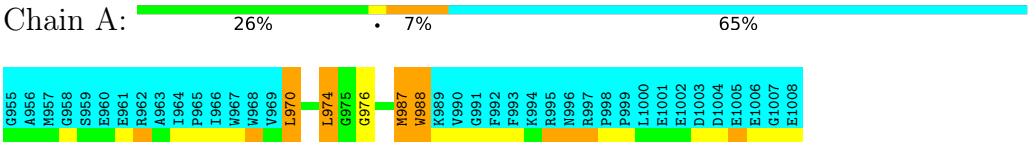
Chain B:



4.2.17 Score per residue for model 17

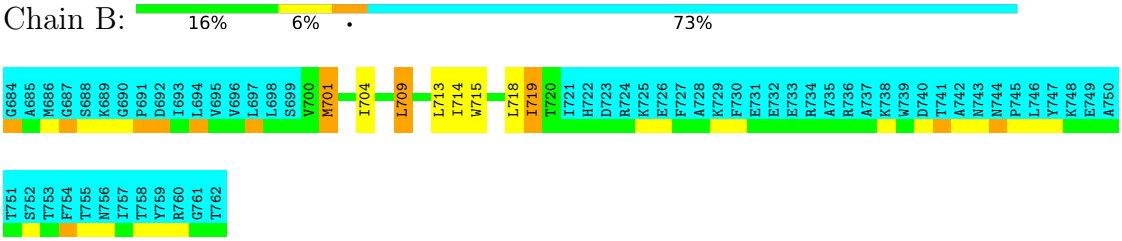
• Molecule 1: Integrin alpha-IIb

Chain A:



• Molecule 2: Integrin beta-3

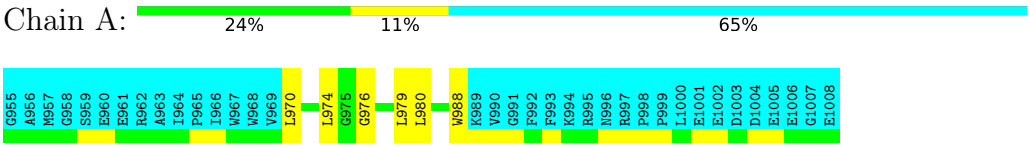
Chain B:



4.2.18 Score per residue for model 18

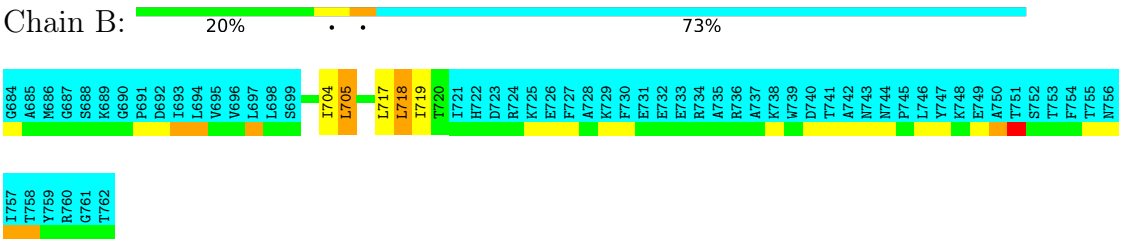
• Molecule 1: Integrin alpha-IIb

Chain A:



• Molecule 2: Integrin beta-3

Chain B:



4.2.19 Score per residue for model 19

- Molecule 1: Integrin alpha-IIb

Chain A: 22% 6% 7% 65%

G955 A956 M957 G958 S959 E960 E961 R962 A963 I964 P965 I966 W967 W968 V969 L970 V971 G972 V973 L974 L979 L985 A986 M987 W988 K989 V990 G991 F992 F993 K994 R995 N996 R997 P998 P999 L1000 E1001 E1002 D1003 D1004 E1005 E1006 G1007 E1008

- Molecule 2: Integrin beta-3

Chain B: 15% 8% • 73%

G684 A685 M686 G687 S688 K689 G690 P691 D692 I693 L694 V695 V696 L697 L698 S699 V700 M701 I704 L705 L713 I714 W715 K716 L717 L718 I719 T720 I721 H722 D723 R724 K725 E726 F727 A728 K729 F730 E731 E732 E733 R734 A735 R736 A737 K738 W739 D740 T741 A742 N743 N744 P745 L746 Y747 K748 E749 A750

T751 S752 T753 F754 T755 N756 I757 T758 Y759 R760 G761 T762

4.2.20 Score per residue for model 20

- Molecule 1: Integrin alpha-IIb

Chain A: 26% 6% • 65%

G955 A956 M957 G958 S959 E960 E961 R962 A963 I964 P965 I966 W967 W968 V969 L970 L974 L979 M987 W988 K989 V990 G991 F992 F993 K994 R995 N996 R997 P998 P999 L1000 E1001 E1002 D1003 D1004 E1005 E1006 G1007 E1008

- Molecule 2: Integrin beta-3

Chain B: 15% 6% 5% 73%

G684 A685 M686 G687 S688 K689 G690 P691 D692 I693 L694 V695 V696 L697 L698 S699 V700 M701 L705 G708 L712 L713 I714 W715 K716 L717 L718 I719 T720 I721 H722 D723 R724 K725 E726 F727 A728 K729 F730 E731 E732 E733 R734 A735 R736 A737 K738 W739 D740 T741 A742 N743 N744 P745 L746 Y747 K748

E749 A750 T751 S752 T753 F754 T755 N756 I757 T758 Y759 R760 G761 T762

5 Refinement protocol and experimental data overview (i)

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

Of the 98 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	refinement	2.15.0
X-PLOR NIH	structure solution	2.15.0

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	1528
Number of shifts mapped to atoms	1528
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

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	139	166	166	8±3
2	B	156	190	190	7±3
All	All	5900	7120	7120	216

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:987:MET:SD	2:B:719:ILE:HD11	0.81	2.15	3	1
1:A:988:TRP:NE1	2:B:719:ILE:HD11	0.76	1.95	12	8
1:A:972:GLY:C	2:B:704:ILE:HD11	0.69	2.07	8	3
1:A:988:TRP:CD1	2:B:719:ILE:HD11	0.66	2.25	15	5
1:A:972:GLY:O	2:B:704:ILE:HD11	0.65	1.91	8	4
1:A:984:VAL:HG13	2:B:715:TRP:CD1	0.64	2.26	13	2
1:A:987:MET:SD	1:A:988:TRP:N	0.64	2.70	16	2
1:A:984:VAL:HG13	2:B:715:TRP:CG	0.62	2.29	3	2
2:B:715:TRP:CZ3	2:B:718:LEU:HD13	0.62	2.29	3	1
1:A:978:LEU:C	1:A:978:LEU:HD13	0.62	2.15	12	2
1:A:980:LEU:O	1:A:980:LEU:HD23	0.60	1.96	8	1
1:A:988:TRP:CD1	2:B:715:TRP:NE1	0.60	2.69	3	5
2:B:701:MET:SD	2:B:701:MET:N	0.60	2.74	10	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:980:LEU:HD23	1:A:980:LEU:C	0.59	2.16	14	1
1:A:979:LEU:HD22	2:B:704:ILE:HG22	0.59	1.74	18	5
1:A:974:LEU:O	1:A:974:LEU:HD23	0.56	2.00	12	13
1:A:980:LEU:O	1:A:984:VAL:HG23	0.56	1.99	13	2
1:A:976:GLY:HA2	2:B:704:ILE:HG23	0.54	1.79	11	5
1:A:988:TRP:HE1	2:B:719:ILE:HD11	0.53	1.64	20	3
2:B:716:LYS:NZ	2:B:720:THR:OG1	0.53	2.41	20	1
1:A:980:LEU:HD11	1:A:984:VAL:HG23	0.51	1.83	16	1
1:A:970:LEU:O	1:A:974:LEU:N	0.51	2.42	14	19
1:A:978:LEU:HD13	1:A:978:LEU:O	0.50	2.07	1	4
1:A:974:LEU:O	1:A:974:LEU:HD13	0.50	2.07	1	2
2:B:712:LEU:C	2:B:712:LEU:HD23	0.49	2.28	11	1
1:A:988:TRP:HE1	2:B:719:ILE:CD1	0.48	2.21	8	11
1:A:980:LEU:O	1:A:984:VAL:CG2	0.48	2.61	13	2
1:A:988:TRP:CE2	2:B:719:ILE:HD11	0.48	2.44	12	3
1:A:987:MET:HG3	1:A:988:TRP:N	0.48	2.24	10	14
2:B:714:ILE:CD1	2:B:714:ILE:N	0.47	2.77	19	3
2:B:709:LEU:O	2:B:709:LEU:HD13	0.47	2.10	6	2
2:B:718:LEU:O	2:B:718:LEU:HD13	0.47	2.10	8	3
1:A:972:GLY:O	2:B:704:ILE:CD1	0.47	2.62	8	2
2:B:708:GLY:O	2:B:712:LEU:N	0.46	2.44	12	2
2:B:709:LEU:O	2:B:709:LEU:HD23	0.46	2.11	15	5
1:A:985:LEU:HD13	1:A:985:LEU:O	0.46	2.10	14	2
2:B:718:LEU:HD23	2:B:718:LEU:O	0.46	2.11	13	1
2:B:705:LEU:HD23	2:B:705:LEU:O	0.45	2.12	19	14
2:B:714:ILE:N	2:B:714:ILE:HD12	0.45	2.25	19	3
1:A:988:TRP:NE1	2:B:719:ILE:CD1	0.45	2.78	11	5
1:A:972:GLY:O	2:B:704:ILE:CG1	0.44	2.65	10	3
1:A:988:TRP:CD1	2:B:719:ILE:HG23	0.44	2.47	17	2
1:A:988:TRP:CD1	2:B:719:ILE:CG2	0.44	3.01	1	2
1:A:980:LEU:C	1:A:980:LEU:CD2	0.43	2.85	14	1
1:A:987:MET:CG	1:A:988:TRP:N	0.43	2.81	8	2
1:A:972:GLY:HA3	2:B:700:VAL:HG13	0.43	1.91	16	1
1:A:978:LEU:HD13	1:A:978:LEU:C	0.42	2.34	13	1
1:A:980:LEU:HD23	1:A:980:LEU:O	0.42	2.12	14	1
1:A:977:LEU:HD13	1:A:977:LEU:O	0.42	2.15	7	3
2:B:717:LEU:HD12	2:B:717:LEU:N	0.42	2.29	14	1
2:B:714:ILE:N	2:B:714:ILE:CD1	0.42	2.83	17	2
1:A:987:MET:SD	1:A:987:MET:C	0.42	2.98	8	2
2:B:713:LEU:O	2:B:713:LEU:HD23	0.42	2.15	17	2
1:A:984:VAL:O	1:A:987:MET:HG3	0.42	2.15	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:717:LEU:CD1	2:B:717:LEU:N	0.42	2.83	19	1
2:B:712:LEU:O	2:B:716:LYS:N	0.42	2.52	11	1
2:B:701:MET:N	2:B:701:MET:SD	0.42	2.93	5	1
1:A:974:LEU:HD23	1:A:974:LEU:C	0.41	2.35	20	3
1:A:976:GLY:O	1:A:980:LEU:N	0.41	2.43	8	2
1:A:978:LEU:C	1:A:978:LEU:CD1	0.41	2.87	12	2
2:B:712:LEU:O	2:B:712:LEU:HD13	0.41	2.16	16	1
2:B:713:LEU:HD23	2:B:713:LEU:O	0.41	2.16	4	2
1:A:988:TRP:CD1	2:B:719:ILE:CD1	0.41	3.02	15	1
2:B:717:LEU:N	2:B:717:LEU:CD2	0.41	2.83	18	1
2:B:717:LEU:N	2:B:717:LEU:CD1	0.40	2.84	10	1
1:A:987:MET:HE1	2:B:712:LEU:HD12	0.40	1.94	1	1
1:A:975:GLY:O	1:A:979:LEU:N	0.40	2.49	16	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	19/54 (35%)	19±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
2	B	21/79 (27%)	21±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	800/2660 (30%)	800 (100%)	0 (0%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	15/44 (34%)	12±1 (79±7%)	3±1 (21±7%)	3	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	16/64 (25%)	13±1 (80±7%)	3±1 (20±7%)	3 33
All	All	620/2160 (29%)	493 (80%)	127 (20%)	3 33

All 19 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	988	TRP	20
2	B	719	ILE	15
2	B	701	MET	13
1	A	987	MET	13
2	B	716	LYS	10
2	B	705	LEU	8
2	B	718	LEU	7
1	A	984	VAL	6
1	A	974	LEU	5
1	A	970	LEU	5
2	B	709	LEU	5
1	A	979	LEU	4
1	A	977	LEU	4
2	B	712	LEU	4
1	A	978	LEU	2
2	B	713	LEU	2
1	A	985	LEU	2
1	A	983	LEU	1
2	B	700	VAL	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 86% for the well-defined parts and 82% 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	1528
Number of shifts mapped to atoms	1528
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	132	0.10 ± 0.11	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	119	0.57 ± 0.04	Should be checked
$^{13}C'$	131	0.29 ± 0.05	None needed (< 0.5 ppm)
^{15}N	126	0.89 ± 0.09	Should be applied

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 86%, i.e. 511 atoms were assigned a chemical shift out of a possible 596. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	202/205 (99%)	82/85 (96%)	80/80 (100%)	40/40 (100%)
Sidechain	295/367 (80%)	207/254 (81%)	88/112 (79%)	0/1 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	14/24 (58%)	12/12 (100%)	0/10 (0%)	2/2 (100%)
Overall	511/596 (86%)	301/351 (86%)	168/202 (83%)	42/43 (98%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 1528 atoms were assigned a chemical shift out of a possible 1867. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	651/668 (97%)	262/274 (96%)	263/266 (99%)	126/128 (98%)
Sidechain	828/1064 (78%)	554/701 (79%)	265/330 (80%)	9/33 (27%)
Aromatic	49/135 (36%)	44/67 (66%)	0/62 (0%)	5/6 (83%)
Overall	1528/1867 (82%)	860/1042 (83%)	528/658 (80%)	140/167 (84%)

7.1.4 Statistically unusual chemical shifts (i)

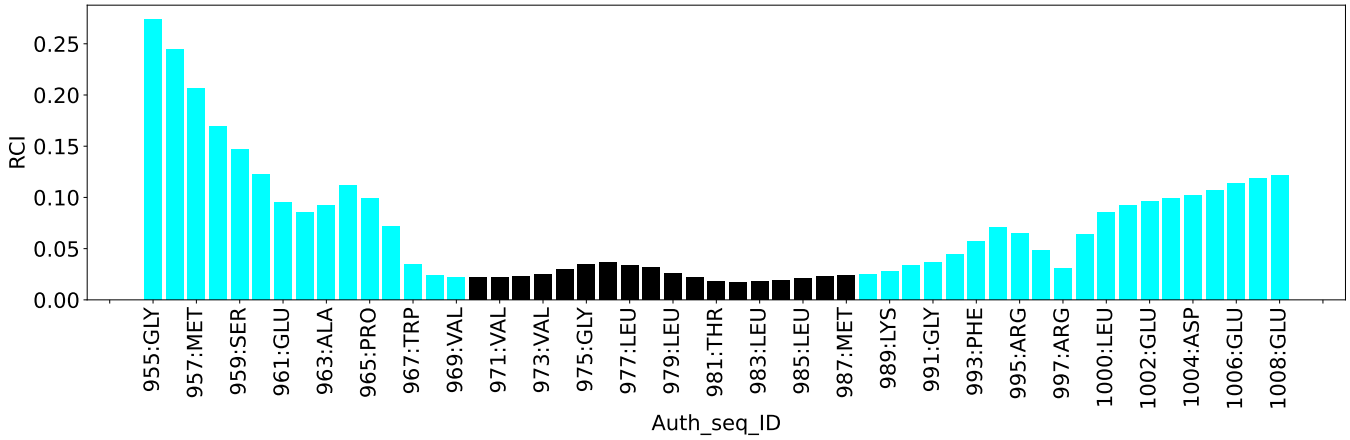
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	962	ARG	NE	110.62	76.53 – 92.65	16.1
1	A	995	ARG	NE	110.62	76.53 – 92.65	16.1
1	B	736	ARG	NE	110.44	76.53 – 92.65	16.0
1	B	734	ARG	NE	110.30	76.53 – 92.65	15.9
1	B	724	ARG	NE	110.26	76.53 – 92.65	15.9
1	A	997	ARG	CD	50.23	38.57 – 47.75	7.7

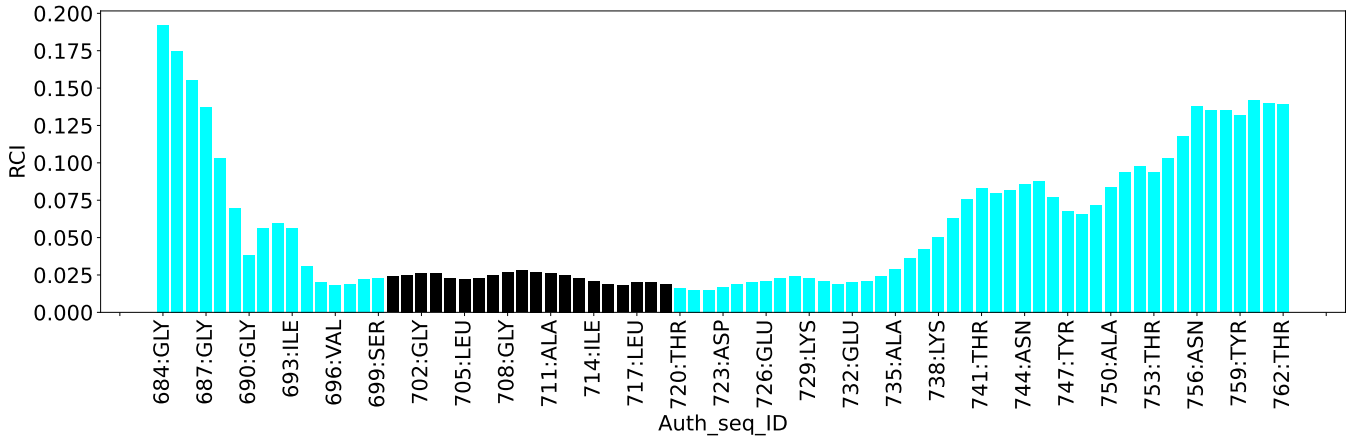
7.1.5 Random Coil Index (RCI) plots (i)

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 (i)

8.1 Conformationally restricting restraints (i)

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	4592
Intra-residue (|i-j|=0)	1320
Sequential (|i-j|=1)	1306
Medium range (|i-j|>1 and |i-j|<5)	1376
Long range (|i-j|≥5)	0
Inter-chain	164
Hydrogen bond restraints	426
Disulfide bond restraints	0
Total dihedral-angle restraints	148
Number of unmapped restraints	0
Number of restraints per residue	35.6
Number of long range restraints per residue[1]	0.0

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

8.2 Residual restraint violations (i)

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 (i)

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)	127.8	0.2
0.2-0.5 (Medium)	129.1	0.5
>0.5 (Large)	8.1	2.12

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	10.1	9.1
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

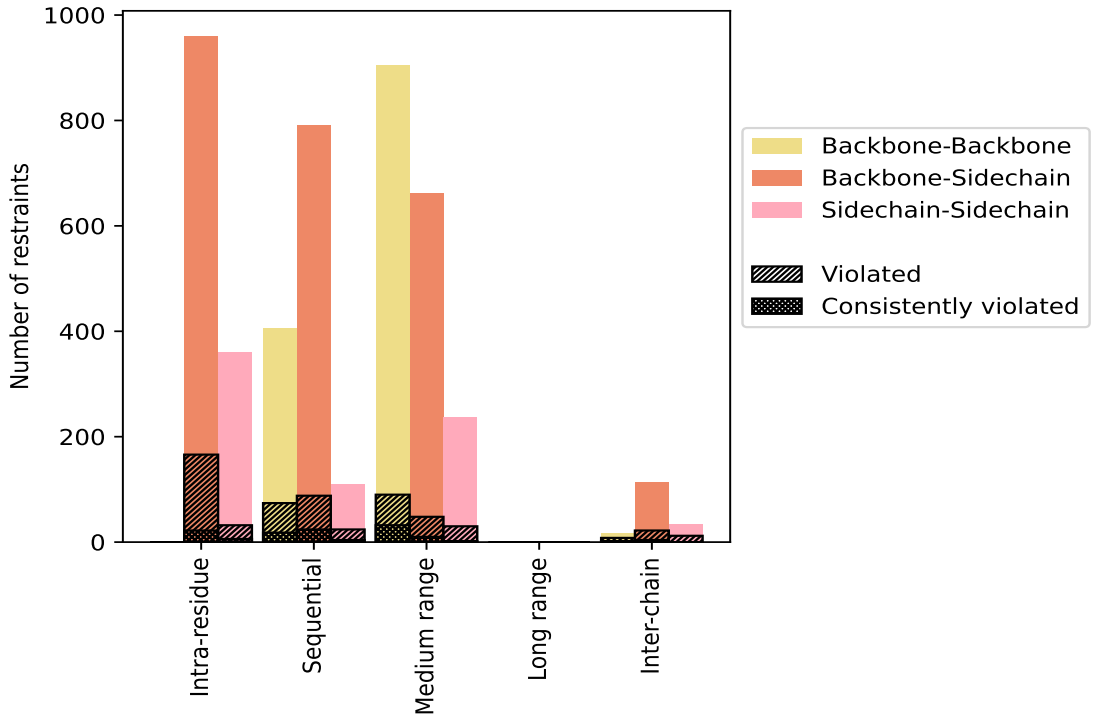
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	1320	28.7	198	15.0	4.3	28	2.1	0.6
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	960	20.9	166	17.3	3.6	22	2.3	0.5
Sidechain-Sidechain	360	7.8	32	8.9	0.7	6	1.7	0.1
Sequential (|i-j|=1)	1306	28.4	186	14.2	4.1	46	3.5	1.0
Backbone-Backbone	406	8.8	74	18.2	1.6	18	4.4	0.4
Backbone-Sidechain	790	17.2	88	11.1	1.9	24	3.0	0.5
Sidechain-Sidechain	110	2.4	24	21.8	0.5	4	3.6	0.1
Medium range (|i-j|>1 & |i-j|<5)	1376	30.0	154	11.2	3.4	44	3.2	1.0
Backbone-Backbone	478	10.4	76	15.9	1.7	32	6.7	0.7
Backbone-Sidechain	662	14.4	48	7.3	1.0	10	1.5	0.2
Sidechain-Sidechain	236	5.1	30	12.7	0.7	2	0.8	0.0
Long range (|i-j|≥5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	164	3.6	42	25.6	0.9	6	3.7	0.1
Backbone-Backbone	16	0.3	8	50.0	0.2	2	12.5	0.0
Backbone-Sidechain	114	2.5	22	19.3	0.5	4	3.5	0.1
Sidechain-Sidechain	34	0.7	12	35.3	0.3	0	0.0	0.0
Hydrogen bond	426	9.3	14	3.3	0.3	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	4592	100.0	594	12.9	12.9	124	2.7	2.7
Backbone-Backbone	1326	28.9	172	13.0	3.7	52	3.9	1.1
Backbone-Sidechain	2526	55.0	324	12.8	7.1	60	2.4	1.3
Sidechain-Sidechain	740	16.1	98	13.2	2.1	12	1.6	0.3

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

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



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

9.2 Distance violation statistics for each model (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	86	84	92	0	16	278	0.25	1.05	0.13	0.23
2	84	92	84	0	18	278	0.22	0.55	0.11	0.19
3	66	78	80	0	10	234	0.25	0.76	0.13	0.21
4	76	88	78	0	16	258	0.24	0.53	0.11	0.2
5	72	92	84	0	16	264	0.24	0.79	0.12	0.2
6	70	94	80	0	20	264	0.23	0.51	0.11	0.2
7	80	84	88	0	14	266	0.26	2.12	0.2	0.21
8	74	84	90	0	18	266	0.25	1.63	0.16	0.22
9	88	88	86	0	20	282	0.23	0.58	0.11	0.2
10	70	96	78	0	18	262	0.24	0.61	0.12	0.21
11	64	100	80	0	20	264	0.24	0.57	0.11	0.21

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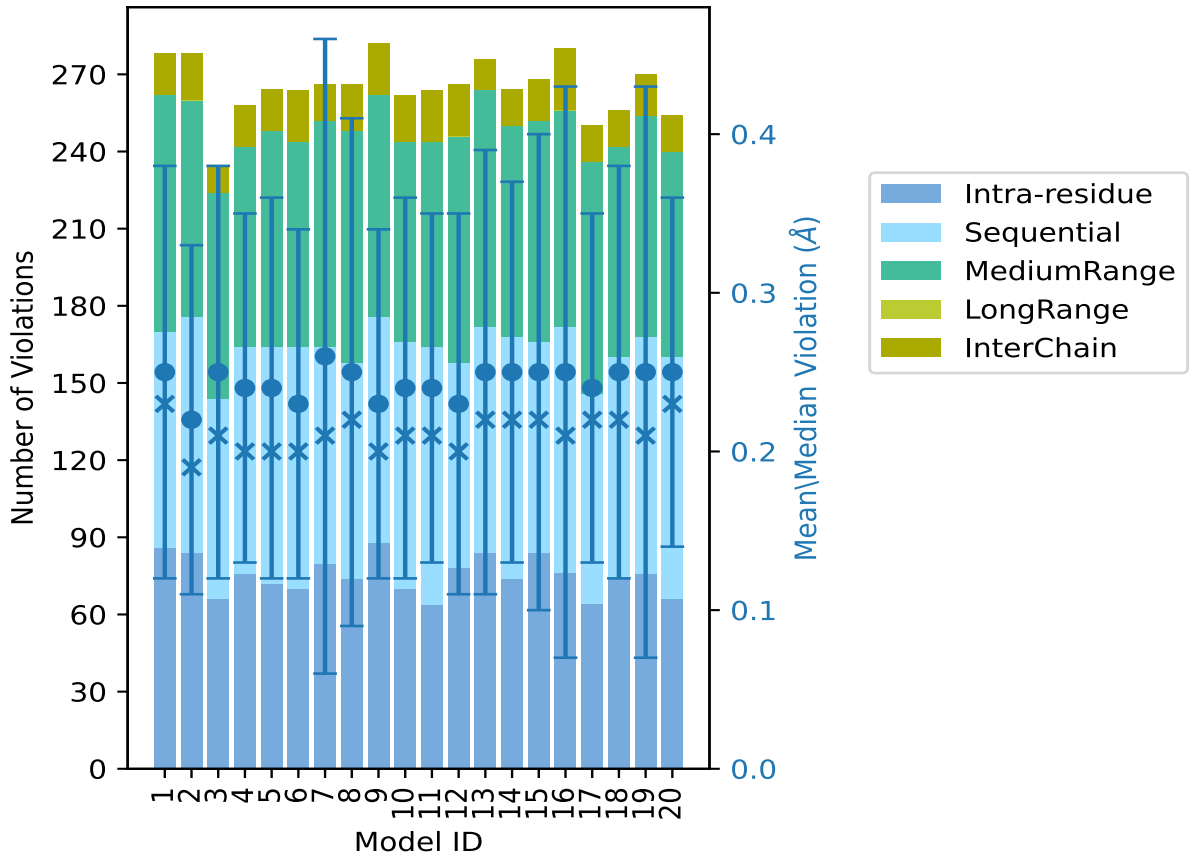
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	78	80	88	0	20	266	0.23	0.53	0.12	0.2
13	84	88	92	0	12	276	0.25	1.14	0.14	0.22
14	74	94	82	0	14	264	0.25	0.95	0.12	0.22
15	84	82	86	0	16	268	0.25	1.34	0.15	0.22
16	76	96	84	0	24	280	0.25	1.91	0.18	0.21
17	64	82	90	0	14	250	0.24	0.56	0.11	0.22
18	74	86	82	0	14	256	0.25	0.98	0.13	0.22
19	76	92	86	0	16	270	0.25	1.83	0.18	0.21
20	66	94	80	0	14	254	0.25	0.59	0.11	0.23

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

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



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

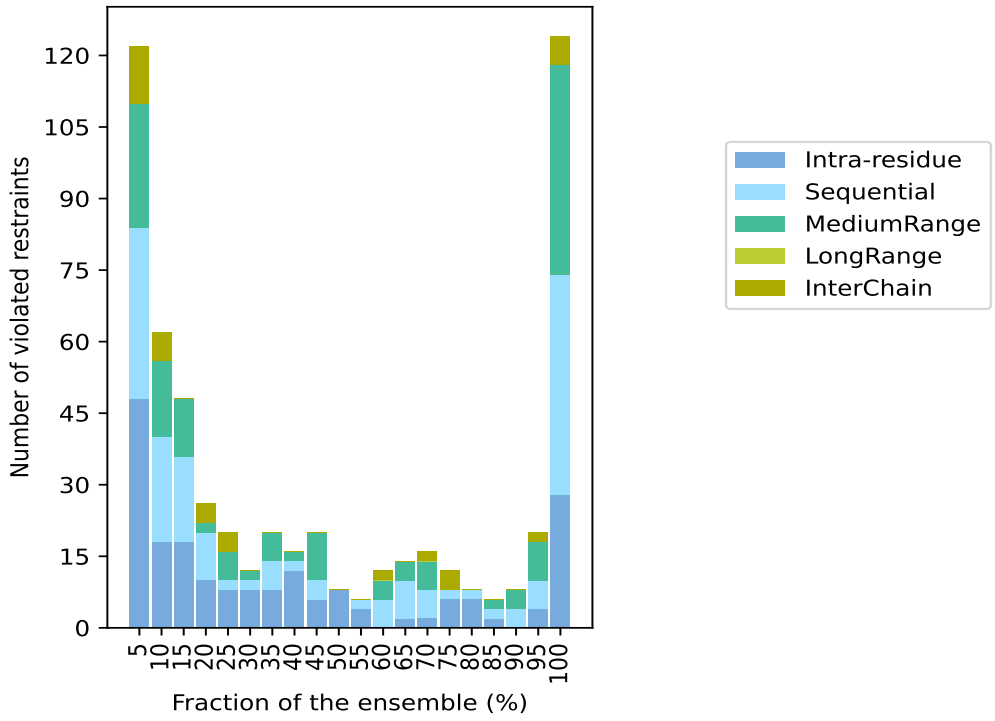
9.3 Distance violation statistics for the ensemble (i)

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, 3586(IR:1122, SQ:1120, MR:1222, LR:0, IC:122) 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]	%
48	36	26	0	12	122	1	5.0
18	22	16	0	6	62	2	10.0
18	18	12	0	0	48	3	15.0
10	10	2	0	4	26	4	20.0
8	2	6	0	4	20	5	25.0
8	2	2	0	0	12	6	30.0
8	6	6	0	0	20	7	35.0
12	2	2	0	0	16	8	40.0
6	4	10	0	0	20	9	45.0
8	0	0	0	0	8	10	50.0
4	2	0	0	0	6	11	55.0
0	6	4	0	2	12	12	60.0
2	8	4	0	0	14	13	65.0
2	6	6	0	2	16	14	70.0
6	2	0	0	4	12	15	75.0
6	2	0	0	0	8	16	80.0
2	2	2	0	0	6	17	85.0
0	4	4	0	0	8	18	90.0
4	6	8	0	2	20	19	95.0
28	46	44	0	6	124	20	100.0

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

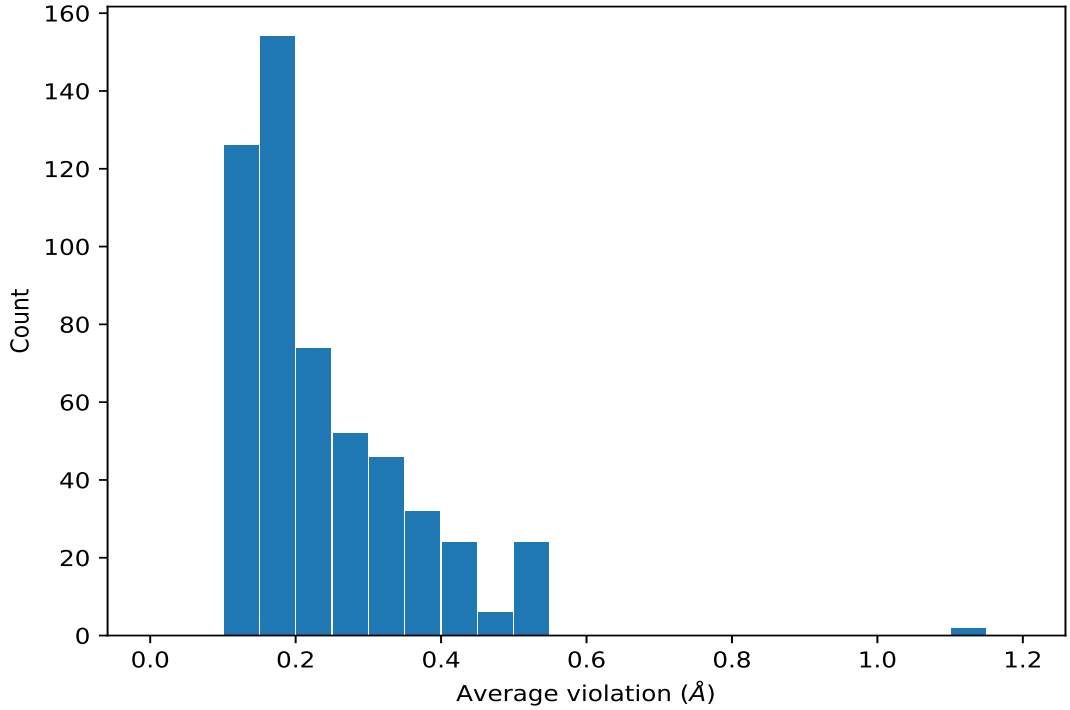
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(1,299)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	20	0.51	0.04	0.52
(1,2382)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	20	0.51	0.04	0.52
(1,1562)	2:B:725:LYS:H	2:B:725:LYS:HB3	20	0.5	0.01	0.5
(1,3645)	2:B:725:LYS:H	2:B:725:LYS:HB3	20	0.5	0.01	0.5
(1,283)	1:A:975:GLY:HA2	1:A:976:GLY:H	20	0.47	0.01	0.47
(1,2366)	1:A:975:GLY:HA2	1:A:976:GLY:H	20	0.47	0.01	0.47
(1,1632)	2:B:729:LYS:H	2:B:729:LYS:HG3	20	0.47	0.02	0.47
(1,3715)	2:B:729:LYS:H	2:B:729:LYS:HG3	20	0.47	0.02	0.47
(1,670)	1:A:992:PHE:HA	1:A:993:PHE:H	20	0.47	0.01	0.48
(1,2753)	1:A:992:PHE:HA	1:A:993:PHE:H	20	0.47	0.01	0.48
(1,1634)	2:B:729:LYS:HE3	2:B:729:LYS:HA	20	0.43	0.03	0.42
(1,3717)	2:B:729:LYS:HE3	2:B:729:LYS:HA	20	0.43	0.03	0.42
(1,689)	1:A:993:PHE:HA	1:A:994:LYS:H	20	0.42	0.04	0.42
(1,2772)	1:A:993:PHE:HA	1:A:994:LYS:H	20	0.42	0.04	0.42
(1,199)	1:A:970:LEU:HB2	1:A:971:VAL:H	20	0.42	0.06	0.4
(1,2282)	1:A:970:LEU:HB2	1:A:971:VAL:H	20	0.42	0.06	0.4

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,136)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	20	0.41	0.02	0.42
(1,2219)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	20	0.41	0.02	0.42
(1,2078)	1:A:988:TRP:H	2:B:719:ILE:HG12	20	0.4	0.06	0.41
(1,4161)	1:A:988:TRP:H	2:B:719:ILE:HG12	20	0.4	0.06	0.41
(1,755)	1:A:997:ARG:H	1:A:997:ARG:HG3	20	0.4	0.13	0.38
(1,2838)	1:A:997:ARG:H	1:A:997:ARG:HG3	20	0.4	0.13	0.38
(1,1630)	2:B:729:LYS:H	2:B:729:LYS:HB3	20	0.38	0.01	0.38
(1,3713)	2:B:729:LYS:H	2:B:729:LYS:HB3	20	0.38	0.01	0.38
(1,762)	1:A:997:ARG:HA	1:A:999:PRO:HD2	20	0.38	0.14	0.39
(1,2845)	1:A:997:ARG:HA	1:A:999:PRO:HD2	20	0.38	0.14	0.39
(1,478)	1:A:985:LEU:HB3	1:A:986:ALA:HA	20	0.36	0.02	0.36
(1,2561)	1:A:985:LEU:HB3	1:A:986:ALA:HA	20	0.36	0.02	0.36
(1,539)	1:A:987:MET:HB3	1:A:988:TRP:H	20	0.35	0.06	0.34
(1,2622)	1:A:987:MET:HB3	1:A:988:TRP:H	20	0.35	0.06	0.34
(1,706)	1:A:994:LYS:H	1:A:994:LYS:HB3	20	0.34	0.04	0.34
(1,2789)	1:A:994:LYS:H	1:A:994:LYS:HB3	20	0.34	0.04	0.34
(1,285)	1:A:975:GLY:HA3	1:A:977:LEU:H	20	0.33	0.04	0.34
(1,2368)	1:A:975:GLY:HA3	1:A:977:LEU:H	20	0.33	0.04	0.34
(1,141)	1:A:968:TRP:HB2	1:A:969:VAL:H	20	0.32	0.04	0.32
(1,2224)	1:A:968:TRP:HB2	1:A:969:VAL:H	20	0.32	0.04	0.32
(1,113)	1:A:967:TRP:H	1:A:968:TRP:HA	20	0.32	0.04	0.34
(1,2196)	1:A:967:TRP:H	1:A:968:TRP:HA	20	0.32	0.04	0.34
(1,416)	1:A:983:LEU:HB2	1:A:984:VAL:H	20	0.31	0.03	0.32
(1,602)	1:A:989:LYS:HA	1:A:991:GLY:H	20	0.31	0.02	0.31
(1,2499)	1:A:983:LEU:HB2	1:A:984:VAL:H	20	0.31	0.03	0.32
(1,2685)	1:A:989:LYS:HA	1:A:991:GLY:H	20	0.31	0.02	0.31
(1,577)	1:A:989:LYS:H	1:A:989:LYS:HB3	20	0.31	0.04	0.3
(1,2660)	1:A:989:LYS:H	1:A:989:LYS:HB3	20	0.31	0.04	0.3
(1,547)	1:A:987:MET:HG3	1:A:989:LYS:H	20	0.31	0.08	0.32
(1,2630)	1:A:987:MET:HG3	1:A:989:LYS:H	20	0.31	0.08	0.32
(1,516)	1:A:986:ALA:HA	1:A:988:TRP:H	20	0.3	0.05	0.3
(1,2599)	1:A:986:ALA:HA	1:A:988:TRP:H	20	0.3	0.05	0.3
(1,215)	1:A:971:VAL:HA	1:A:972:GLY:HA3	20	0.3	0.01	0.3
(1,2298)	1:A:971:VAL:HA	1:A:972:GLY:HA3	20	0.3	0.01	0.3
(1,1601)	2:B:726:GLU:HA	2:B:729:LYS:HB3	20	0.29	0.02	0.29
(1,3684)	2:B:726:GLU:HA	2:B:729:LYS:HB3	20	0.29	0.02	0.29
(1,5)	1:A:960:GLU:HA	1:A:961:GLU:H	20	0.29	0.06	0.28
(1,2088)	1:A:960:GLU:HA	1:A:961:GLU:H	20	0.29	0.06	0.28
(1,45)	1:A:964:ILE:HB	1:A:965:PRO:HD3	20	0.29	0.03	0.29
(1,2128)	1:A:964:ILE:HB	1:A:965:PRO:HD3	20	0.29	0.03	0.29
(1,519)	1:A:986:ALA:HA	1:A:989:LYS:H	20	0.28	0.02	0.28
(1,2602)	1:A:986:ALA:HA	1:A:989:LYS:H	20	0.28	0.02	0.28

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,480)	1:A:985:LEU:HA	1:A:986:ALA:H	20	0.28	0.0	0.28
(1,2563)	1:A:985:LEU:HA	1:A:986:ALA:H	20	0.28	0.0	0.28
(1,119)	1:A:967:TRP:HB2	1:A:968:TRP:H	20	0.27	0.04	0.28
(1,489)	1:A:985:LEU:HA	1:A:988:TRP:H	20	0.27	0.03	0.27
(1,2202)	1:A:967:TRP:HB2	1:A:968:TRP:H	20	0.27	0.04	0.28
(1,2572)	1:A:985:LEU:HA	1:A:988:TRP:H	20	0.27	0.03	0.27
(1,2047)	1:A:979:LEU:H	2:B:704:ILE:HB	20	0.27	0.05	0.26
(1,4130)	1:A:979:LEU:H	2:B:704:ILE:HB	20	0.27	0.05	0.26
(1,1799)	2:B:739:TRP:HB2	2:B:740:ASP:H	20	0.27	0.03	0.28
(1,3882)	2:B:739:TRP:HB2	2:B:740:ASP:H	20	0.27	0.03	0.28
(1,499)	1:A:985:LEU:HA	1:A:989:LYS:H	20	0.26	0.03	0.27
(1,2582)	1:A:985:LEU:HA	1:A:989:LYS:H	20	0.26	0.03	0.27
(1,1769)	2:B:738:LYS:H	2:B:738:LYS:HG3	20	0.26	0.04	0.27
(1,3852)	2:B:738:LYS:H	2:B:738:LYS:HG3	20	0.26	0.04	0.27
(1,1220)	2:B:708:GLY:H	2:B:710:ALA:H	20	0.26	0.05	0.25
(1,3303)	2:B:708:GLY:H	2:B:710:ALA:H	20	0.26	0.05	0.25
(1,590)	1:A:989:LYS:HB2	1:A:990:VAL:H	20	0.25	0.03	0.25
(1,2673)	1:A:989:LYS:HB2	1:A:990:VAL:H	20	0.25	0.03	0.25
(1,2060)	1:A:984:VAL:H	2:B:712:LEU:HA	20	0.25	0.08	0.23
(1,4143)	1:A:984:VAL:H	2:B:712:LEU:HA	20	0.25	0.08	0.23
(1,1862)	2:B:745:PRO:HA	2:B:746:LEU:H	20	0.25	0.06	0.24
(1,3945)	2:B:745:PRO:HA	2:B:746:LEU:H	20	0.25	0.06	0.24
(1,391)	1:A:982:ILE:H	1:A:983:LEU:HB3	20	0.24	0.03	0.23
(1,1890)	2:B:747:TYR:HB2	2:B:748:LYS:H	20	0.24	0.04	0.24
(1,2474)	1:A:982:ILE:H	1:A:983:LEU:HB3	20	0.24	0.03	0.23
(1,3973)	2:B:747:TYR:HB2	2:B:748:LYS:H	20	0.24	0.04	0.24
(1,393)	1:A:982:ILE:H	1:A:984:VAL:H	20	0.24	0.04	0.24
(1,2476)	1:A:982:ILE:H	1:A:984:VAL:H	20	0.24	0.04	0.24
(1,1787)	2:B:738:LYS:HA	2:B:740:ASP:H	20	0.23	0.02	0.24
(1,3870)	2:B:738:LYS:HA	2:B:740:ASP:H	20	0.23	0.02	0.24
(1,450)	1:A:984:VAL:HA	1:A:987:MET:H	20	0.22	0.04	0.22
(1,2533)	1:A:984:VAL:HA	1:A:987:MET:H	20	0.22	0.04	0.22
(1,118)	1:A:967:TRP:HA	1:A:968:TRP:HB3	20	0.22	0.05	0.22
(1,2201)	1:A:967:TRP:HA	1:A:968:TRP:HB3	20	0.22	0.05	0.22
(1,423)	1:A:983:LEU:H	1:A:985:LEU:H	20	0.2	0.03	0.2
(1,2506)	1:A:983:LEU:H	1:A:985:LEU:H	20	0.2	0.03	0.2
(1,1563)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	20	0.2	0.02	0.2
(1,3646)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	20	0.2	0.02	0.2
(1,125)	1:A:967:TRP:H	1:A:970:LEU:H	20	0.2	0.02	0.2
(1,2208)	1:A:967:TRP:H	1:A:970:LEU:H	20	0.2	0.02	0.2
(1,1128)	2:B:704:ILE:HB	2:B:705:LEU:HB2	20	0.2	0.03	0.2
(1,3211)	2:B:704:ILE:HB	2:B:705:LEU:HB2	20	0.2	0.03	0.2

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1635)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	20	0.19	0.02	0.2
(1,3718)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	20	0.19	0.02	0.2
(1,341)	1:A:979:LEU:HA	1:A:981:THR:H	20	0.18	0.04	0.17
(1,2424)	1:A:979:LEU:HA	1:A:981:THR:H	20	0.18	0.04	0.17
(1,426)	1:A:983:LEU:HA	1:A:985:LEU:H	20	0.18	0.04	0.18
(1,2509)	1:A:983:LEU:HA	1:A:985:LEU:H	20	0.18	0.04	0.18
(1,289)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	20	0.18	0.03	0.18
(1,684)	1:A:993:PHE:HB3	1:A:993:PHE:H	20	0.18	0.03	0.19
(1,2372)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	20	0.18	0.03	0.18
(1,2767)	1:A:993:PHE:HB3	1:A:993:PHE:H	20	0.18	0.03	0.19
(1,273)	1:A:974:LEU:H	1:A:975:GLY:HA2	20	0.18	0.03	0.18
(1,2356)	1:A:974:LEU:H	1:A:975:GLY:HA2	20	0.18	0.03	0.18
(1,485)	1:A:985:LEU:HA	1:A:987:MET:H	20	0.18	0.02	0.17
(1,2568)	1:A:985:LEU:HA	1:A:987:MET:H	20	0.18	0.02	0.17
(1,1236)	2:B:709:LEU:H	2:B:711:ALA:H	20	0.17	0.04	0.16
(1,3319)	2:B:709:LEU:H	2:B:711:ALA:H	20	0.17	0.04	0.16
(1,1496)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	20	0.17	0.04	0.16
(1,3579)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	20	0.17	0.04	0.16
(1,672)	1:A:992:PHE:HB3	1:A:993:PHE:H	20	0.17	0.03	0.17
(1,1561)	2:B:725:LYS:H	2:B:725:LYS:HG3	20	0.17	0.01	0.17
(1,2755)	1:A:992:PHE:HB3	1:A:993:PHE:H	20	0.17	0.03	0.17
(1,3644)	2:B:725:LYS:H	2:B:725:LYS:HG3	20	0.17	0.01	0.17
(1,1534)	2:B:724:ARG:H	2:B:724:ARG:HB3	20	0.13	0.01	0.13
(1,3617)	2:B:724:ARG:H	2:B:724:ARG:HB3	20	0.13	0.01	0.13
(1,1915)	2:B:749:GLU:H	2:B:749:GLU:HB3	19	0.29	0.09	0.26
(1,3998)	2:B:749:GLU:H	2:B:749:GLU:HB3	19	0.29	0.09	0.26
(1,460)	1:A:984:VAL:HA	1:A:988:TRP:HB3	19	0.28	0.05	0.29
(1,2543)	1:A:984:VAL:HA	1:A:988:TRP:HB3	19	0.28	0.05	0.29
(1,1917)	2:B:749:GLU:H	2:B:749:GLU:HG3	19	0.19	0.08	0.18
(1,4000)	2:B:749:GLU:H	2:B:749:GLU:HG3	19	0.19	0.08	0.18
(1,645)	1:A:990:VAL:HB	1:A:993:PHE:H	19	0.18	0.03	0.17
(1,2728)	1:A:990:VAL:HB	1:A:993:PHE:H	19	0.18	0.03	0.17
(1,2068)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	19	0.18	0.03	0.19
(1,4151)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	19	0.18	0.03	0.19
(1,1780)	2:B:738:LYS:HB3	2:B:739:TRP:H	19	0.17	0.04	0.16
(1,3863)	2:B:738:LYS:HB3	2:B:739:TRP:H	19	0.17	0.04	0.16
(1,850)	2:B:692:ASP:HA	2:B:693:ILE:H	19	0.17	0.03	0.16
(1,2933)	2:B:692:ASP:HA	2:B:693:ILE:H	19	0.17	0.03	0.16
(1,356)	1:A:980:LEU:HB3	1:A:981:THR:HA	19	0.16	0.04	0.15
(1,2439)	1:A:980:LEU:HB3	1:A:981:THR:HA	19	0.16	0.04	0.15
(1,548)	1:A:987:MET:HA	1:A:990:VAL:H	19	0.15	0.03	0.14
(1,2631)	1:A:987:MET:HA	1:A:990:VAL:H	19	0.15	0.03	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1555)	2:B:724:ARG:HA	2:B:728:ALA:H	19	0.14	0.02	0.13
(1,3638)	2:B:724:ARG:HA	2:B:728:ALA:H	19	0.14	0.02	0.13
(1,761)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	18	0.22	0.07	0.22
(1,2844)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	18	0.22	0.07	0.22
(1,1805)	2:B:740:ASP:HA	2:B:741:THR:H	18	0.2	0.09	0.17
(1,3888)	2:B:740:ASP:HA	2:B:741:THR:H	18	0.2	0.09	0.17
(1,225)	1:A:971:VAL:H	1:A:973:VAL:H	18	0.17	0.03	0.16
(1,2308)	1:A:971:VAL:H	1:A:973:VAL:H	18	0.17	0.03	0.16
(1,1798)	2:B:739:TRP:HB3	2:B:740:ASP:H	18	0.13	0.02	0.12
(1,3881)	2:B:739:TRP:HB3	2:B:740:ASP:H	18	0.13	0.02	0.12
(1,738)	1:A:995:ARG:HA	1:A:996:ASN:H	17	0.38	0.14	0.35
(1,2821)	1:A:995:ARG:HA	1:A:996:ASN:H	17	0.38	0.14	0.35
(1,1777)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	17	0.24	0.05	0.26
(1,3860)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	17	0.24	0.05	0.26
(1,1387)	2:B:717:LEU:H	2:B:719:ILE:H	17	0.16	0.07	0.13
(1,3470)	2:B:717:LEU:H	2:B:719:ILE:H	17	0.16	0.07	0.13
(1,1776)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	16	0.26	0.03	0.27
(1,3859)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	16	0.26	0.03	0.27
(1,870)	2:B:693:ILE:H	2:B:693:ILE:HB	16	0.2	0.08	0.18
(1,2953)	2:B:693:ILE:H	2:B:693:ILE:HB	16	0.2	0.08	0.18
(1,1885)	2:B:747:TYR:H	2:B:747:TYR:HB3	16	0.16	0.04	0.16
(1,3968)	2:B:747:TYR:H	2:B:747:TYR:HB3	16	0.16	0.04	0.16
(1,690)	1:A:993:PHE:HB2	1:A:994:LYS:H	16	0.15	0.03	0.14
(1,2773)	1:A:993:PHE:HB2	1:A:994:LYS:H	16	0.15	0.03	0.14
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD21	15	0.24	0.04	0.24
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD22	15	0.24	0.04	0.24
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD23	15	0.24	0.04	0.24
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD21	15	0.24	0.04	0.24
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD22	15	0.24	0.04	0.24
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD23	15	0.24	0.04	0.24
(1,175)	1:A:969:VAL:H	1:A:970:LEU:HB3	15	0.18	0.03	0.19
(1,2258)	1:A:969:VAL:H	1:A:970:LEU:HB3	15	0.18	0.03	0.19
(1,2074)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	15	0.15	0.04	0.13
(1,4157)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	15	0.15	0.04	0.13
(1,2018)	1:A:973:VAL:H	2:B:700:VAL:HA	15	0.15	0.04	0.13
(1,4101)	1:A:973:VAL:H	2:B:700:VAL:HA	15	0.15	0.04	0.13
(1,1767)	2:B:738:LYS:HA	2:B:738:LYS:HD3	15	0.15	0.05	0.14
(1,3850)	2:B:738:LYS:HA	2:B:738:LYS:HD3	15	0.15	0.05	0.14
(1,557)	1:A:988:TRP:H	1:A:988:TRP:HB3	15	0.14	0.02	0.13
(1,2640)	1:A:988:TRP:H	1:A:988:TRP:HB3	15	0.14	0.02	0.13
(1,639)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	14	0.43	0.02	0.43
(1,639)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	14	0.43	0.02	0.43

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,639)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	14	0.43	0.02	0.43
(1,2722)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	14	0.43	0.02	0.43
(1,2722)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	14	0.43	0.02	0.43
(1,2722)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	14	0.43	0.02	0.43
(1,1950)	2:B:754:PHE:HA	2:B:755:THR:H	14	0.26	0.04	0.27
(1,4033)	2:B:754:PHE:HA	2:B:755:THR:H	14	0.26	0.04	0.27
(1,841)	2:B:691:PRO:HD3	2:B:692:ASP:H	14	0.23	0.03	0.22
(1,2924)	2:B:691:PRO:HD3	2:B:692:ASP:H	14	0.23	0.03	0.22
(1,750)	1:A:996:ASN:HA	1:A:997:ARG:H	14	0.22	0.08	0.2
(1,2833)	1:A:996:ASN:HA	1:A:997:ARG:H	14	0.22	0.08	0.2
(1,576)	1:A:989:LYS:H	1:A:989:LYS:HD3	14	0.18	0.05	0.17
(1,2659)	1:A:989:LYS:H	1:A:989:LYS:HD3	14	0.18	0.05	0.17
(1,2079)	1:A:988:TRP:HE1	2:B:719:ILE:HB	14	0.18	0.03	0.18
(1,4162)	1:A:988:TRP:HE1	2:B:719:ILE:HB	14	0.18	0.03	0.18
(3,43)	1:A:981:THR:O	1:A:984:VAL:H	14	0.13	0.01	0.12
(3,202)	1:A:981:THR:O	1:A:984:VAL:H	14	0.13	0.01	0.12
(1,1623)	2:B:728:ALA:H	2:B:730:PHE:H	14	0.12	0.01	0.12
(1,3706)	2:B:728:ALA:H	2:B:730:PHE:H	14	0.12	0.01	0.12
(1,1102)	2:B:703:ALA:HA	2:B:706:LEU:HB3	14	0.12	0.01	0.11
(1,3185)	2:B:703:ALA:HA	2:B:706:LEU:HB3	14	0.12	0.01	0.11
(1,1661)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	13	1.14	0.59	1.05
(1,3744)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	13	1.14	0.59	1.05
(1,1819)	2:B:742:ALA:HA	2:B:743:ASN:H	13	0.26	0.09	0.23
(1,3902)	2:B:742:ALA:HA	2:B:743:ASN:H	13	0.26	0.09	0.23
(1,1412)	2:B:718:LEU:HB3	2:B:719:ILE:HG12	13	0.2	0.06	0.2
(1,3495)	2:B:718:LEU:HB3	2:B:719:ILE:HG12	13	0.2	0.06	0.2
(1,1814)	2:B:741:THR:HA	2:B:744:ASN:H	13	0.18	0.05	0.2
(1,3897)	2:B:741:THR:HA	2:B:744:ASN:H	13	0.18	0.05	0.2
(1,725)	1:A:994:LYS:HB3	1:A:995:ARG:HG3	13	0.16	0.06	0.14
(1,2808)	1:A:994:LYS:HB3	1:A:995:ARG:HG3	13	0.16	0.06	0.14
(1,1871)	2:B:746:LEU:H	2:B:746:LEU:HB2	13	0.14	0.02	0.13
(1,3954)	2:B:746:LEU:H	2:B:746:LEU:HB2	13	0.14	0.02	0.13
(1,7)	1:A:960:GLU:HB2	1:A:961:GLU:H	13	0.13	0.02	0.13
(1,2090)	1:A:960:GLU:HB2	1:A:961:GLU:H	13	0.13	0.02	0.13
(1,843)	2:B:691:PRO:HB3	2:B:692:ASP:H	12	0.26	0.06	0.22
(1,2926)	2:B:691:PRO:HB3	2:B:692:ASP:H	12	0.26	0.06	0.22
(1,1810)	2:B:741:THR:HA	2:B:742:ALA:H	12	0.25	0.11	0.19
(1,3893)	2:B:741:THR:HA	2:B:742:ALA:H	12	0.25	0.11	0.19
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG21	12	0.15	0.03	0.14
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG22	12	0.15	0.03	0.14
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG23	12	0.15	0.03	0.14
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG21	12	0.15	0.03	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG22	12	0.15	0.03	0.14
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG23	12	0.15	0.03	0.14
(1,395)	1:A:982:ILE:HA	1:A:985:LEU:HB3	12	0.15	0.03	0.14
(1,2478)	1:A:982:ILE:HA	1:A:985:LEU:HB3	12	0.15	0.03	0.14
(1,1949)	2:B:754:PHE:HB3	2:B:755:THR:H	12	0.14	0.02	0.13
(1,4032)	2:B:754:PHE:HB3	2:B:755:THR:H	12	0.14	0.02	0.13
(1,331)	1:A:978:LEU:HA	1:A:981:THR:H	12	0.13	0.01	0.13
(1,2414)	1:A:978:LEU:HA	1:A:981:THR:H	12	0.13	0.01	0.13
(1,81)	1:A:966:ILE:H	1:A:966:ILE:HG13	11	0.25	0.02	0.24
(1,2164)	1:A:966:ILE:H	1:A:966:ILE:HG13	11	0.25	0.02	0.24
(3,111)	2:B:710:ALA:O	2:B:714:ILE:H	11	0.14	0.03	0.14
(3,270)	2:B:710:ALA:O	2:B:714:ILE:H	11	0.14	0.03	0.14
(1,8)	1:A:961:GLU:H	1:A:961:GLU:HB3	11	0.14	0.03	0.12
(1,2091)	1:A:961:GLU:H	1:A:961:GLU:HB3	11	0.14	0.03	0.12
(1,1944)	2:B:753:THR:HA	2:B:754:PHE:H	11	0.13	0.02	0.12
(1,4027)	2:B:753:THR:HA	2:B:754:PHE:H	11	0.13	0.02	0.12
(1,195)	1:A:970:LEU:HD11	1:A:970:LEU:HA	10	0.37	0.13	0.42
(1,195)	1:A:970:LEU:HD12	1:A:970:LEU:HA	10	0.37	0.13	0.42
(1,195)	1:A:970:LEU:HD13	1:A:970:LEU:HA	10	0.37	0.13	0.42
(1,2278)	1:A:970:LEU:HD11	1:A:970:LEU:HA	10	0.37	0.13	0.42
(1,2278)	1:A:970:LEU:HD12	1:A:970:LEU:HA	10	0.37	0.13	0.42
(1,2278)	1:A:970:LEU:HD13	1:A:970:LEU:HA	10	0.37	0.13	0.42
(1,704)	1:A:994:LYS:H	1:A:994:LYS:HG3	10	0.17	0.08	0.14
(1,2787)	1:A:994:LYS:H	1:A:994:LYS:HG3	10	0.17	0.08	0.14
(1,950)	2:B:696:VAL:H	2:B:696:VAL:HB	10	0.11	0.0	0.11
(1,3033)	2:B:696:VAL:H	2:B:696:VAL:HB	10	0.11	0.0	0.11
(1,1572)	2:B:725:LYS:HD3	2:B:725:LYS:HB3	10	0.11	0.0	0.11
(1,3655)	2:B:725:LYS:HD3	2:B:725:LYS:HB3	10	0.11	0.0	0.11
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD11	9	0.36	0.02	0.36
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD12	9	0.36	0.02	0.36
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD13	9	0.36	0.02	0.36
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD11	9	0.36	0.02	0.36
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD12	9	0.36	0.02	0.36
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD13	9	0.36	0.02	0.36
(1,741)	1:A:995:ARG:HB3	1:A:997:ARG:H	9	0.35	0.11	0.3
(1,2824)	1:A:995:ARG:HB3	1:A:997:ARG:H	9	0.35	0.11	0.3
(1,737)	1:A:995:ARG:HB3	1:A:996:ASN:H	9	0.35	0.12	0.35
(1,2820)	1:A:995:ARG:HB3	1:A:996:ASN:H	9	0.35	0.12	0.35
(1,363)	1:A:981:THR:H	1:A:981:THR:HG21	9	0.3	0.02	0.3
(1,363)	1:A:981:THR:H	1:A:981:THR:HG22	9	0.3	0.02	0.3
(1,363)	1:A:981:THR:H	1:A:981:THR:HG23	9	0.3	0.02	0.3
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG21	9	0.3	0.02	0.3

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG22	9	0.3	0.02	0.3
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG23	9	0.3	0.02	0.3
(1,811)	1:A:1006:GLU:H	1:A:1006:GLU:HB3	9	0.22	0.14	0.14
(1,2894)	1:A:1006:GLU:H	1:A:1006:GLU:HB3	9	0.22	0.14	0.14
(1,208)	1:A:970:LEU:HB3	1:A:974:LEU:H	9	0.14	0.02	0.14
(1,2291)	1:A:970:LEU:HB3	1:A:974:LEU:H	9	0.14	0.02	0.14
(1,155)	1:A:968:TRP:HA	1:A:971:VAL:H	9	0.14	0.02	0.14
(1,2238)	1:A:968:TRP:HA	1:A:971:VAL:H	9	0.14	0.02	0.14
(1,120)	1:A:967:TRP:HB3	1:A:968:TRP:HB3	9	0.13	0.03	0.12
(1,2203)	1:A:967:TRP:HB3	1:A:968:TRP:HB3	9	0.13	0.03	0.12
(1,230)	1:A:971:VAL:HA	1:A:974:LEU:HB3	9	0.12	0.01	0.12
(1,2313)	1:A:971:VAL:HA	1:A:974:LEU:HB3	9	0.12	0.01	0.12
(1,1581)	2:B:725:LYS:HA	2:B:728:ALA:H	9	0.12	0.01	0.12
(1,3664)	2:B:725:LYS:HA	2:B:728:ALA:H	9	0.12	0.01	0.12
(1,743)	1:A:996:ASN:H	1:A:996:ASN:HB3	8	0.36	0.01	0.36
(1,2826)	1:A:996:ASN:H	1:A:996:ASN:HB3	8	0.36	0.01	0.36
(1,1828)	2:B:743:ASN:HB3	2:B:743:ASN:H	8	0.27	0.13	0.22
(1,3911)	2:B:743:ASN:HB3	2:B:743:ASN:H	8	0.27	0.13	0.22
(1,243)	1:A:972:GLY:H	1:A:976:GLY:H	8	0.2	0.03	0.2
(1,2326)	1:A:972:GLY:H	1:A:976:GLY:H	8	0.2	0.03	0.2
(1,807)	1:A:1005:GLU:H	1:A:1005:GLU:HB3	8	0.19	0.08	0.16
(1,2890)	1:A:1005:GLU:H	1:A:1005:GLU:HB3	8	0.19	0.08	0.16
(1,851)	2:B:692:ASP:H	2:B:693:ILE:H	8	0.16	0.05	0.14
(1,2934)	2:B:692:ASP:H	2:B:693:ILE:H	8	0.16	0.05	0.14
(1,437)	1:A:984:VAL:H	1:A:984:VAL:HG11	8	0.16	0.05	0.14
(1,437)	1:A:984:VAL:H	1:A:984:VAL:HG12	8	0.16	0.05	0.14
(1,437)	1:A:984:VAL:H	1:A:984:VAL:HG13	8	0.16	0.05	0.14
(1,742)	1:A:996:ASN:H	1:A:996:ASN:HB2	8	0.16	0.03	0.15
(1,2520)	1:A:984:VAL:H	1:A:984:VAL:HG11	8	0.16	0.05	0.14
(1,2520)	1:A:984:VAL:H	1:A:984:VAL:HG12	8	0.16	0.05	0.14
(1,2520)	1:A:984:VAL:H	1:A:984:VAL:HG13	8	0.16	0.05	0.14
(1,2825)	1:A:996:ASN:H	1:A:996:ASN:HB2	8	0.16	0.03	0.15
(1,729)	1:A:995:ARG:H	1:A:995:ARG:HB3	8	0.15	0.03	0.15
(1,2812)	1:A:995:ARG:H	1:A:995:ARG:HB3	8	0.15	0.03	0.15
(1,1662)	2:B:730:PHE:HE1	2:B:734:ARG:HD2	7	0.43	0.31	0.49
(1,3745)	2:B:730:PHE:HE1	2:B:734:ARG:HD2	7	0.43	0.31	0.49
(1,1718)	2:B:734:ARG:HD2	2:B:734:ARG:HB2	7	0.22	0.05	0.21
(1,3801)	2:B:734:ARG:HD2	2:B:734:ARG:HB2	7	0.22	0.05	0.21
(1,1659)	2:B:730:PHE:HB3	2:B:731:GLU:HG2	7	0.19	0.04	0.2
(1,3742)	2:B:730:PHE:HB3	2:B:731:GLU:HG2	7	0.19	0.04	0.2
(1,1838)	2:B:744:ASN:H	2:B:744:ASN:HB2	7	0.19	0.17	0.12
(1,3921)	2:B:744:ASN:H	2:B:744:ASN:HB2	7	0.19	0.17	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1537)	2:B:724:ARG:HD3	2:B:724:ARG:HB3	7	0.15	0.03	0.15
(1,3620)	2:B:724:ARG:HD3	2:B:724:ARG:HB3	7	0.15	0.03	0.15
(1,724)	1:A:994:LYS:HB2	1:A:995:ARG:HG3	7	0.15	0.02	0.14
(1,2807)	1:A:994:LYS:HB2	1:A:995:ARG:HG3	7	0.15	0.02	0.14
(1,275)	1:A:974:LEU:HB2	1:A:975:GLY:H	7	0.14	0.04	0.12
(1,2358)	1:A:974:LEU:HB2	1:A:975:GLY:H	7	0.14	0.04	0.12
(1,104)	1:A:966:ILE:HA	1:A:970:LEU:H	7	0.13	0.01	0.14
(1,2187)	1:A:966:ILE:HA	1:A:970:LEU:H	7	0.13	0.01	0.14
(1,321)	1:A:977:LEU:HB2	1:A:981:THR:H	7	0.13	0.01	0.12
(1,2404)	1:A:977:LEU:HB2	1:A:981:THR:H	7	0.13	0.01	0.12
(1,791)	1:A:1002:GLU:H	1:A:1002:GLU:HB3	7	0.12	0.01	0.11
(1,2874)	1:A:1002:GLU:H	1:A:1002:GLU:HB3	7	0.12	0.01	0.11
(1,624)	1:A:990:VAL:HB	1:A:991:GLY:H	6	0.31	0.03	0.31
(1,2707)	1:A:990:VAL:HB	1:A:991:GLY:H	6	0.31	0.03	0.31
(1,1826)	2:B:743:ASN:HB2	2:B:743:ASN:H	6	0.2	0.03	0.2
(1,3909)	2:B:743:ASN:HB2	2:B:743:ASN:H	6	0.2	0.03	0.2
(1,14)	1:A:962:ARG:H	1:A:962:ARG:HB2	6	0.2	0.04	0.2
(1,2097)	1:A:962:ARG:H	1:A:962:ARG:HB2	6	0.2	0.04	0.2
(1,132)	1:A:968:TRP:H	1:A:968:TRP:HB3	6	0.14	0.02	0.14
(1,2215)	1:A:968:TRP:H	1:A:968:TRP:HB3	6	0.14	0.02	0.14
(1,106)	1:A:967:TRP:H	1:A:967:TRP:HB3	6	0.14	0.02	0.13
(1,2189)	1:A:967:TRP:H	1:A:967:TRP:HB3	6	0.14	0.02	0.13
(3,24)	1:A:974:LEU:O	1:A:978:LEU:H	6	0.12	0.01	0.12
(3,183)	1:A:974:LEU:O	1:A:978:LEU:H	6	0.12	0.01	0.12
(1,432)	1:A:983:LEU:HB2	1:A:987:MET:H	6	0.11	0.01	0.11
(1,2515)	1:A:983:LEU:HB2	1:A:987:MET:H	6	0.11	0.01	0.11
(1,186)	1:A:970:LEU:HA	1:A:970:LEU:HD21	5	0.51	0.01	0.5
(1,186)	1:A:970:LEU:HA	1:A:970:LEU:HD22	5	0.51	0.01	0.5
(1,186)	1:A:970:LEU:HA	1:A:970:LEU:HD23	5	0.51	0.01	0.5
(1,2269)	1:A:970:LEU:HA	1:A:970:LEU:HD21	5	0.51	0.01	0.5
(1,2269)	1:A:970:LEU:HA	1:A:970:LEU:HD22	5	0.51	0.01	0.5
(1,2269)	1:A:970:LEU:HA	1:A:970:LEU:HD23	5	0.51	0.01	0.5
(1,790)	1:A:1001:GLU:H	1:A:1001:GLU:HB2	5	0.31	0.22	0.16
(1,2873)	1:A:1001:GLU:H	1:A:1001:GLU:HB2	5	0.31	0.22	0.16
(1,1951)	2:B:755:THR:H	2:B:755:THR:HB	5	0.23	0.1	0.18
(1,4034)	2:B:755:THR:H	2:B:755:THR:HB	5	0.23	0.1	0.18
(1,1835)	2:B:743:ASN:HA	2:B:744:ASN:H	5	0.19	0.04	0.16
(1,3918)	2:B:743:ASN:HA	2:B:744:ASN:H	5	0.19	0.04	0.16
(1,1968)	2:B:757:ILE:H	2:B:757:ILE:HG12	5	0.15	0.01	0.15
(1,4051)	2:B:757:ILE:H	2:B:757:ILE:HG12	5	0.15	0.01	0.15
(1,2028)	1:A:974:LEU:H	2:B:704:ILE:HG13	5	0.14	0.01	0.14
(1,4111)	1:A:974:LEU:H	2:B:704:ILE:HG13	5	0.14	0.01	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,183)	1:A:969:VAL:H	1:A:972:GLY:HA3	5	0.13	0.02	0.12
(1,2266)	1:A:969:VAL:H	1:A:972:GLY:HA3	5	0.13	0.02	0.12
(1,1786)	2:B:738:LYS:H	2:B:740:ASP:H	5	0.12	0.01	0.12
(1,3869)	2:B:738:LYS:H	2:B:740:ASP:H	5	0.12	0.01	0.12
(1,1470)	2:B:720:THR:HG21	2:B:724:ARG:HD3	5	0.12	0.01	0.11
(1,1470)	2:B:720:THR:HG22	2:B:724:ARG:HD3	5	0.12	0.01	0.11
(1,1470)	2:B:720:THR:HG23	2:B:724:ARG:HD3	5	0.12	0.01	0.11
(1,3553)	2:B:720:THR:HG21	2:B:724:ARG:HD3	5	0.12	0.01	0.11
(1,3553)	2:B:720:THR:HG22	2:B:724:ARG:HD3	5	0.12	0.01	0.11
(1,3553)	2:B:720:THR:HG23	2:B:724:ARG:HD3	5	0.12	0.01	0.11
(1,2073)	1:A:988:TRP:HE1	2:B:715:TRP:HD1	5	0.12	0.01	0.12
(1,4156)	1:A:988:TRP:HE1	2:B:715:TRP:HD1	5	0.12	0.01	0.12
(1,1873)	2:B:746:LEU:H	2:B:746:LEU:HB3	4	0.52	0.02	0.52
(1,3956)	2:B:746:LEU:H	2:B:746:LEU:HB3	4	0.52	0.02	0.52
(1,1820)	2:B:742:ALA:HB1	2:B:743:ASN:H	4	0.24	0.07	0.28
(1,1820)	2:B:742:ALA:HB2	2:B:743:ASN:H	4	0.24	0.07	0.28
(1,1820)	2:B:742:ALA:HB3	2:B:743:ASN:H	4	0.24	0.07	0.28
(1,3903)	2:B:742:ALA:HB1	2:B:743:ASN:H	4	0.24	0.07	0.28
(1,3903)	2:B:742:ALA:HB2	2:B:743:ASN:H	4	0.24	0.07	0.28
(1,3903)	2:B:742:ALA:HB3	2:B:743:ASN:H	4	0.24	0.07	0.28
(1,1957)	2:B:756:ASN:H	2:B:756:ASN:HB2	4	0.23	0.18	0.14
(1,4040)	2:B:756:ASN:H	2:B:756:ASN:HB2	4	0.23	0.18	0.14
(1,803)	1:A:1004:ASP:HA	1:A:1005:GLU:H	4	0.18	0.08	0.14
(1,2886)	1:A:1004:ASP:HA	1:A:1005:GLU:H	4	0.18	0.08	0.14
(1,2080)	1:A:988:TRP:HE1	2:B:719:ILE:HG21	4	0.16	0.04	0.16
(1,2080)	1:A:988:TRP:HE1	2:B:719:ILE:HG22	4	0.16	0.04	0.16
(1,2080)	1:A:988:TRP:HE1	2:B:719:ILE:HG23	4	0.16	0.04	0.16
(1,4163)	1:A:988:TRP:HE1	2:B:719:ILE:HG21	4	0.16	0.04	0.16
(1,4163)	1:A:988:TRP:HE1	2:B:719:ILE:HG22	4	0.16	0.04	0.16
(1,4163)	1:A:988:TRP:HE1	2:B:719:ILE:HG23	4	0.16	0.04	0.16
(1,1811)	2:B:741:THR:HB	2:B:742:ALA:H	4	0.16	0.07	0.12
(1,3894)	2:B:741:THR:HB	2:B:742:ALA:H	4	0.16	0.07	0.12
(1,718)	1:A:994:LYS:HB2	1:A:995:ARG:H	4	0.15	0.03	0.15
(1,2801)	1:A:994:LYS:HB2	1:A:995:ARG:H	4	0.15	0.03	0.15
(1,848)	2:B:692:ASP:H	2:B:692:ASP:HB3	4	0.15	0.05	0.13
(1,2931)	2:B:692:ASP:H	2:B:692:ASP:HB3	4	0.15	0.05	0.13
(1,693)	1:A:993:PHE:H	1:A:994:LYS:HD3	4	0.14	0.03	0.14
(1,2776)	1:A:993:PHE:H	1:A:994:LYS:HD3	4	0.14	0.03	0.14
(1,802)	1:A:1004:ASP:H	1:A:1004:ASP:HB2	4	0.14	0.04	0.12
(1,2885)	1:A:1004:ASP:H	1:A:1004:ASP:HB2	4	0.14	0.04	0.12
(1,99)	1:A:966:ILE:HA	1:A:969:VAL:H	4	0.12	0.01	0.12
(1,2182)	1:A:966:ILE:HA	1:A:969:VAL:H	4	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,408)	1:A:983:LEU:H	1:A:983:LEU:HB3	4	0.12	0.01	0.12
(1,2010)	1:A:969:VAL:HA	2:B:700:VAL:H	4	0.12	0.01	0.12
(1,2491)	1:A:983:LEU:H	1:A:983:LEU:HB3	4	0.12	0.01	0.12
(1,4093)	1:A:969:VAL:HA	2:B:700:VAL:H	4	0.12	0.01	0.12
(1,268)	1:A:974:LEU:HD21	1:A:974:LEU:HA	3	0.54	0.0	0.54
(1,268)	1:A:974:LEU:HD22	1:A:974:LEU:HA	3	0.54	0.0	0.54
(1,268)	1:A:974:LEU:HD23	1:A:974:LEU:HA	3	0.54	0.0	0.54
(1,2351)	1:A:974:LEU:HD21	1:A:974:LEU:HA	3	0.54	0.0	0.54
(1,2351)	1:A:974:LEU:HD22	1:A:974:LEU:HA	3	0.54	0.0	0.54
(1,2351)	1:A:974:LEU:HD23	1:A:974:LEU:HA	3	0.54	0.0	0.54
(1,1987)	2:B:759:TYR:H	2:B:759:TYR:HB2	3	0.41	0.21	0.55
(1,4070)	2:B:759:TYR:H	2:B:759:TYR:HB2	3	0.41	0.21	0.55
(1,1946)	2:B:754:PHE:H	2:B:754:PHE:HB3	3	0.41	0.12	0.39
(1,4029)	2:B:754:PHE:H	2:B:754:PHE:HB3	3	0.41	0.12	0.39
(1,1931)	2:B:751:THR:HA	2:B:752:SER:H	3	0.39	0.19	0.52
(1,4014)	2:B:751:THR:HA	2:B:752:SER:H	3	0.39	0.19	0.52
(1,778)	1:A:1000:LEU:H	1:A:1000:LEU:HB3	3	0.36	0.19	0.37
(1,2861)	1:A:1000:LEU:H	1:A:1000:LEU:HB3	3	0.36	0.19	0.37
(1,312)	1:A:977:LEU:HD11	1:A:977:LEU:HA	3	0.3	0.15	0.23
(1,312)	1:A:977:LEU:HD12	1:A:977:LEU:HA	3	0.3	0.15	0.23
(1,312)	1:A:977:LEU:HD13	1:A:977:LEU:HA	3	0.3	0.15	0.23
(1,2395)	1:A:977:LEU:HD11	1:A:977:LEU:HA	3	0.3	0.15	0.23
(1,2395)	1:A:977:LEU:HD12	1:A:977:LEU:HA	3	0.3	0.15	0.23
(1,2395)	1:A:977:LEU:HD13	1:A:977:LEU:HA	3	0.3	0.15	0.23
(1,1984)	2:B:758:THR:HA	2:B:759:TYR:H	3	0.28	0.0	0.28
(1,4067)	2:B:758:THR:HA	2:B:759:TYR:H	3	0.28	0.0	0.28
(1,849)	2:B:692:ASP:HB3	2:B:693:ILE:H	3	0.23	0.12	0.2
(1,2932)	2:B:692:ASP:HB3	2:B:693:ILE:H	3	0.23	0.12	0.2
(1,533)	1:A:987:MET:H	1:A:987:MET:HG2	3	0.2	0.03	0.21
(1,2616)	1:A:987:MET:H	1:A:987:MET:HG2	3	0.2	0.03	0.21
(1,487)	1:A:985:LEU:H	1:A:987:MET:HG2	3	0.19	0.06	0.17
(1,2570)	1:A:985:LEU:H	1:A:987:MET:HG2	3	0.19	0.06	0.17
(1,760)	1:A:997:ARG:HA	1:A:999:PRO:HD3	3	0.19	0.07	0.16
(1,2843)	1:A:997:ARG:HA	1:A:999:PRO:HD3	3	0.19	0.07	0.16
(1,740)	1:A:995:ARG:H	1:A:996:ASN:H	3	0.18	0.04	0.2
(1,801)	1:A:1004:ASP:H	1:A:1004:ASP:HB3	3	0.18	0.09	0.13
(1,2823)	1:A:995:ARG:H	1:A:996:ASN:H	3	0.18	0.04	0.2
(1,2884)	1:A:1004:ASP:H	1:A:1004:ASP:HB3	3	0.18	0.09	0.13
(1,1924)	2:B:750:ALA:H	2:B:751:THR:H	3	0.18	0.02	0.18
(1,4007)	2:B:750:ALA:H	2:B:751:THR:H	3	0.18	0.02	0.18
(1,342)	1:A:979:LEU:HA	1:A:982:ILE:HB	3	0.17	0.04	0.16
(1,2425)	1:A:979:LEU:HA	1:A:982:ILE:HB	3	0.17	0.04	0.16

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1880)	2:B:746:LEU:HB2	2:B:747:TYR:H	3	0.17	0.03	0.17
(1,3963)	2:B:746:LEU:HB2	2:B:747:TYR:H	3	0.17	0.03	0.17
(1,1425)	2:B:718:LEU:HD21	2:B:721:ILE:HB	3	0.15	0.03	0.16
(1,1425)	2:B:718:LEU:HD22	2:B:721:ILE:HB	3	0.15	0.03	0.16
(1,1425)	2:B:718:LEU:HD23	2:B:721:ILE:HB	3	0.15	0.03	0.16
(1,3508)	2:B:718:LEU:HD21	2:B:721:ILE:HB	3	0.15	0.03	0.16
(1,3508)	2:B:718:LEU:HD22	2:B:721:ILE:HB	3	0.15	0.03	0.16
(1,3508)	2:B:718:LEU:HD23	2:B:721:ILE:HB	3	0.15	0.03	0.16
(1,1821)	2:B:742:ALA:HB1	2:B:743:ASN:HD22	3	0.15	0.02	0.15
(1,1821)	2:B:742:ALA:HB2	2:B:743:ASN:HD22	3	0.15	0.02	0.15
(1,1821)	2:B:742:ALA:HB3	2:B:743:ASN:HD22	3	0.15	0.02	0.15
(1,3904)	2:B:742:ALA:HB1	2:B:743:ASN:HD22	3	0.15	0.02	0.15
(1,3904)	2:B:742:ALA:HB2	2:B:743:ASN:HD22	3	0.15	0.02	0.15
(1,3904)	2:B:742:ALA:HB3	2:B:743:ASN:HD22	3	0.15	0.02	0.15
(1,611)	1:A:989:LYS:HE3	1:A:993:PHE:HE1	3	0.13	0.02	0.12
(1,1774)	2:B:738:LYS:HE3	2:B:738:LYS:HB3	3	0.13	0.03	0.11
(1,2694)	1:A:989:LYS:HE3	1:A:993:PHE:HE1	3	0.13	0.02	0.12
(1,3857)	2:B:738:LYS:HE3	2:B:738:LYS:HB3	3	0.13	0.03	0.11
(3,52)	1:A:984:VAL:O	1:A:987:MET:H	3	0.13	0.02	0.13
(3,211)	1:A:984:VAL:O	1:A:987:MET:H	3	0.13	0.02	0.13
(1,1273)	2:B:712:LEU:HB3	2:B:713:LEU:HB2	3	0.12	0.01	0.13
(1,3356)	2:B:712:LEU:HB3	2:B:713:LEU:HB2	3	0.12	0.01	0.13
(1,638)	1:A:990:VAL:H	1:A:992:PHE:H	3	0.12	0.01	0.12
(1,2721)	1:A:990:VAL:H	1:A:992:PHE:H	3	0.12	0.01	0.12
(1,1565)	2:B:725:LYS:HE3	2:B:725:LYS:HG3	3	0.11	0.0	0.11
(1,3648)	2:B:725:LYS:HE3	2:B:725:LYS:HG3	3	0.11	0.0	0.11
(1,647)	1:A:991:GLY:H	1:A:992:PHE:H	3	0.11	0.0	0.11
(1,2730)	1:A:991:GLY:H	1:A:992:PHE:H	3	0.11	0.0	0.11
(1,1380)	2:B:717:LEU:HD11	2:B:717:LEU:HA	2	0.5	0.01	0.5
(1,1380)	2:B:717:LEU:HD12	2:B:717:LEU:HA	2	0.5	0.01	0.5
(1,1380)	2:B:717:LEU:HD13	2:B:717:LEU:HA	2	0.5	0.01	0.5
(1,3463)	2:B:717:LEU:HD11	2:B:717:LEU:HA	2	0.5	0.01	0.5
(1,3463)	2:B:717:LEU:HD12	2:B:717:LEU:HA	2	0.5	0.01	0.5
(1,3463)	2:B:717:LEU:HD13	2:B:717:LEU:HA	2	0.5	0.01	0.5
(1,776)	1:A:999:PRO:HA	1:A:1000:LEU:H	2	0.34	0.09	0.34
(1,2859)	1:A:999:PRO:HA	1:A:1000:LEU:H	2	0.34	0.09	0.34
(1,83)	1:A:966:ILE:H	1:A:966:ILE:HG12	2	0.33	0.01	0.33
(1,2166)	1:A:966:ILE:H	1:A:966:ILE:HG12	2	0.33	0.01	0.33
(1,1990)	2:B:759:TYR:HA	2:B:760:ARG:H	2	0.32	0.2	0.32
(1,4073)	2:B:759:TYR:HA	2:B:760:ARG:H	2	0.32	0.2	0.32
(1,787)	1:A:1000:LEU:HA	1:A:1001:GLU:H	2	0.32	0.1	0.32
(1,2870)	1:A:1000:LEU:HA	1:A:1001:GLU:H	2	0.32	0.1	0.32

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,809)	1:A:1005:GLU:HB2	1:A:1006:GLU:H	2	0.3	0.01	0.3
(1,2892)	1:A:1005:GLU:HB2	1:A:1006:GLU:H	2	0.3	0.01	0.3
(1,1963)	2:B:756:ASN:HA	2:B:757:ILE:H	2	0.26	0.01	0.26
(1,4046)	2:B:756:ASN:HA	2:B:757:ILE:H	2	0.26	0.01	0.26
(1,1715)	2:B:734:ARG:HD3	2:B:734:ARG:HB2	2	0.24	0.03	0.24
(1,3798)	2:B:734:ARG:HD3	2:B:734:ARG:HB2	2	0.24	0.03	0.24
(1,1927)	2:B:751:THR:H	2:B:751:THR:HG21	2	0.22	0.09	0.22
(1,1927)	2:B:751:THR:H	2:B:751:THR:HG22	2	0.22	0.09	0.22
(1,1927)	2:B:751:THR:H	2:B:751:THR:HG23	2	0.22	0.09	0.22
(1,4010)	2:B:751:THR:H	2:B:751:THR:HG21	2	0.22	0.09	0.22
(1,4010)	2:B:751:THR:H	2:B:751:THR:HG22	2	0.22	0.09	0.22
(1,4010)	2:B:751:THR:H	2:B:751:THR:HG23	2	0.22	0.09	0.22
(1,869)	2:B:693:ILE:H	2:B:693:ILE:HG12	2	0.2	0.01	0.2
(1,2952)	2:B:693:ILE:H	2:B:693:ILE:HG12	2	0.2	0.01	0.2
(1,44)	1:A:964:ILE:H	1:A:965:PRO:HB2	2	0.19	0.03	0.19
(1,2127)	1:A:964:ILE:H	1:A:965:PRO:HB2	2	0.19	0.03	0.19
(1,1830)	2:B:743:ASN:H	2:B:743:ASN:HD22	2	0.18	0.01	0.18
(1,3913)	2:B:743:ASN:H	2:B:743:ASN:HD22	2	0.18	0.01	0.18
(1,488)	1:A:985:LEU:H	1:A:987:MET:HG3	2	0.18	0.06	0.18
(1,2571)	1:A:985:LEU:H	1:A:987:MET:HG3	2	0.18	0.06	0.18
(1,751)	1:A:996:ASN:H	1:A:997:ARG:H	2	0.17	0.05	0.17
(1,798)	1:A:1003:ASP:H	1:A:1003:ASP:HB2	2	0.17	0.02	0.17
(1,813)	1:A:1006:GLU:H	1:A:1006:GLU:HB2	2	0.17	0.02	0.17
(1,2834)	1:A:996:ASN:H	1:A:997:ARG:H	2	0.17	0.05	0.17
(1,2881)	1:A:1003:ASP:H	1:A:1003:ASP:HB2	2	0.17	0.02	0.17
(1,2896)	1:A:1006:GLU:H	1:A:1006:GLU:HB2	2	0.17	0.02	0.17
(1,2038)	1:A:976:GLY:H	2:B:707:ILE:HB	2	0.16	0.03	0.16
(1,2048)	1:A:979:LEU:H	2:B:707:ILE:HB	2	0.16	0.03	0.16
(1,4121)	1:A:976:GLY:H	2:B:707:ILE:HB	2	0.16	0.03	0.16
(1,4131)	1:A:979:LEU:H	2:B:707:ILE:HB	2	0.16	0.03	0.16
(1,1658)	2:B:730:PHE:HB3	2:B:731:GLU:HG3	2	0.15	0.03	0.15
(1,3741)	2:B:730:PHE:HB3	2:B:731:GLU:HG3	2	0.15	0.03	0.15
(1,46)	1:A:964:ILE:HB	1:A:965:PRO:HD2	2	0.14	0.0	0.14
(1,1235)	2:B:709:LEU:HB3	2:B:710:ALA:HA	2	0.14	0.02	0.14
(1,2129)	1:A:964:ILE:HB	1:A:965:PRO:HD2	2	0.14	0.0	0.14
(1,3318)	2:B:709:LEU:HB3	2:B:710:ALA:HA	2	0.14	0.02	0.14
(1,976)	2:B:697:LEU:HB3	2:B:699:SER:H	2	0.13	0.02	0.13
(1,3059)	2:B:697:LEU:HB3	2:B:699:SER:H	2	0.13	0.02	0.13
(3,81)	2:B:700:VAL:O	2:B:704:ILE:H	2	0.13	0.01	0.13
(3,240)	2:B:700:VAL:O	2:B:704:ILE:H	2	0.13	0.01	0.13
(1,864)	2:B:692:ASP:H	2:B:696:VAL:H	2	0.12	0.01	0.12
(1,2002)	1:A:968:TRP:HE1	2:B:693:ILE:HB	2	0.12	0.02	0.12

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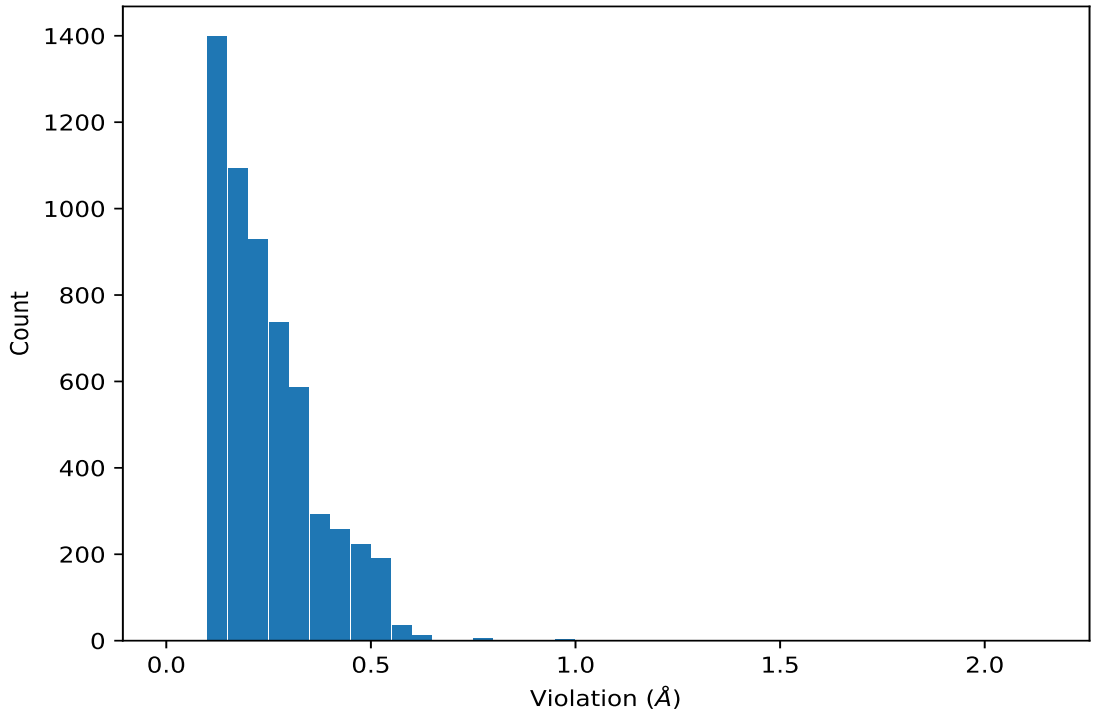
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2947)	2:B:692:ASP:H	2:B:696:VAL:H	2	0.12	0.01	0.12
(1,4085)	1:A:968:TRP:HE1	2:B:693:ILE:HB	2	0.12	0.02	0.12
(1,63)	1:A:965:PRO:HG3	1:A:967:TRP:HB2	2	0.12	0.0	0.12
(1,701)	1:A:993:PHE:HA	1:A:996:ASN:H	2	0.12	0.01	0.12
(1,1065)	2:B:701:MET:HG3	2:B:704:ILE:HG13	2	0.12	0.01	0.12
(1,2146)	1:A:965:PRO:HG3	1:A:967:TRP:HB2	2	0.12	0.0	0.12
(1,2784)	1:A:993:PHE:HA	1:A:996:ASN:H	2	0.12	0.01	0.12
(1,3148)	2:B:701:MET:HG3	2:B:704:ILE:HG13	2	0.12	0.01	0.12
(1,451)	1:A:984:VAL:H	1:A:987:MET:H	2	0.12	0.0	0.12
(1,697)	1:A:993:PHE:H	1:A:995:ARG:H	2	0.12	0.0	0.12
(1,1739)	2:B:736:ARG:H	2:B:736:ARG:HB3	2	0.12	0.0	0.12
(1,2534)	1:A:984:VAL:H	1:A:987:MET:H	2	0.12	0.0	0.12
(1,2780)	1:A:993:PHE:H	1:A:995:ARG:H	2	0.12	0.0	0.12
(1,3822)	2:B:736:ARG:H	2:B:736:ARG:HB3	2	0.12	0.0	0.12
(1,1966)	2:B:756:ASN:H	2:B:757:ILE:HD11	2	0.11	0.0	0.11
(1,1966)	2:B:756:ASN:H	2:B:757:ILE:HD12	2	0.11	0.0	0.11
(1,1966)	2:B:756:ASN:H	2:B:757:ILE:HD13	2	0.11	0.0	0.11
(1,4049)	2:B:756:ASN:H	2:B:757:ILE:HD11	2	0.11	0.0	0.11
(1,4049)	2:B:756:ASN:H	2:B:757:ILE:HD12	2	0.11	0.0	0.11
(1,4049)	2:B:756:ASN:H	2:B:757:ILE:HD13	2	0.11	0.0	0.11

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3744)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	7	2.12
(1,1661)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	7	2.12
(1,3744)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	16	1.91
(1,1661)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	16	1.91
(1,3744)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	19	1.83
(1,1661)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	19	1.83
(1,3744)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	8	1.63
(1,1661)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	8	1.63
(1,3744)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	15	1.34
(1,1661)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	15	1.34
(1,3744)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	13	1.14
(1,1661)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	13	1.14
(1,3744)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	1	1.05
(1,1661)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	1	1.05
(1,3744)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	18	0.98
(1,1661)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	18	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3744)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	14	0.95
(1,1661)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	14	0.95
(1,3745)	2:B:730:PHE:HE1	2:B:734:ARG:HD2	7	0.93
(1,1662)	2:B:730:PHE:HE1	2:B:734:ARG:HD2	7	0.93
(1,3744)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	5	0.79
(1,1661)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	5	0.79
(1,3745)	2:B:730:PHE:HE1	2:B:734:ARG:HD2	16	0.77
(1,1662)	2:B:730:PHE:HE1	2:B:734:ARG:HD2	16	0.77
(1,3744)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	3	0.76
(1,1661)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	3	0.76
(1,762)	1:A:997:ARG:HA	1:A:999:PRO:HD2	19	0.64
(1,2845)	1:A:997:ARG:HA	1:A:999:PRO:HD2	19	0.64
(1,3820)	2:B:736:ARG:H	2:B:736:ARG:HB2	15	0.62
(1,1737)	2:B:736:ARG:H	2:B:736:ARG:HB2	15	0.62
(1,806)	1:A:1005:GLU:H	1:A:1005:GLU:HB2	14	0.61
(1,755)	1:A:997:ARG:H	1:A:997:ARG:HG3	18	0.61
(1,737)	1:A:995:ARG:HB3	1:A:996:ASN:H	10	0.61
(1,2889)	1:A:1005:GLU:H	1:A:1005:GLU:HB2	14	0.61
(1,2838)	1:A:997:ARG:H	1:A:997:ARG:HG3	18	0.61
(1,2820)	1:A:995:ARG:HB3	1:A:996:ASN:H	10	0.61
(1,3921)	2:B:744:ASN:H	2:B:744:ASN:HB2	13	0.6
(1,1838)	2:B:744:ASN:H	2:B:744:ASN:HB2	13	0.6
(1,790)	1:A:1001:GLU:H	1:A:1001:GLU:HB2	7	0.59
(1,738)	1:A:995:ARG:HA	1:A:996:ASN:H	20	0.59
(1,2873)	1:A:1001:GLU:H	1:A:1001:GLU:HB2	7	0.59
(1,2821)	1:A:995:ARG:HA	1:A:996:ASN:H	20	0.59
(1,778)	1:A:1000:LEU:H	1:A:1000:LEU:HB3	9	0.58
(1,738)	1:A:995:ARG:HA	1:A:996:ASN:H	13	0.58
(1,4070)	2:B:759:TYR:H	2:B:759:TYR:HB2	10	0.58
(1,4061)	2:B:757:ILE:HA	2:B:758:THR:H	18	0.58
(1,2861)	1:A:1000:LEU:H	1:A:1000:LEU:HB3	9	0.58
(1,2821)	1:A:995:ARG:HA	1:A:996:ASN:H	13	0.58
(1,1987)	2:B:759:TYR:H	2:B:759:TYR:HB2	10	0.58
(1,1978)	2:B:757:ILE:HA	2:B:758:THR:H	18	0.58
(1,790)	1:A:1001:GLU:H	1:A:1001:GLU:HB2	1	0.57
(1,4029)	2:B:754:PHE:H	2:B:754:PHE:HB3	11	0.57
(1,299)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	14	0.57
(1,2873)	1:A:1001:GLU:H	1:A:1001:GLU:HB2	1	0.57
(1,2382)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	14	0.57
(1,1946)	2:B:754:PHE:H	2:B:754:PHE:HB3	11	0.57
(1,762)	1:A:997:ARG:HA	1:A:999:PRO:HD2	10	0.56
(1,755)	1:A:997:ARG:H	1:A:997:ARG:HG3	3	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,755)	1:A:997:ARG:H	1:A:997:ARG:HG3	20	0.56
(1,3956)	2:B:746:LEU:H	2:B:746:LEU:HB3	20	0.56
(1,299)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	16	0.56
(1,299)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	17	0.56
(1,2845)	1:A:997:ARG:HA	1:A:999:PRO:HD2	10	0.56
(1,2838)	1:A:997:ARG:H	1:A:997:ARG:HG3	3	0.56
(1,2838)	1:A:997:ARG:H	1:A:997:ARG:HG3	20	0.56
(1,2382)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	16	0.56
(1,2382)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	17	0.56
(1,1873)	2:B:746:LEU:H	2:B:746:LEU:HB3	20	0.56
(1,5)	1:A:960:GLU:HA	1:A:961:GLU:H	3	0.55
(1,4070)	2:B:759:TYR:H	2:B:759:TYR:HB2	9	0.55
(1,4040)	2:B:756:ASN:H	2:B:756:ASN:HB2	2	0.55
(1,2088)	1:A:960:GLU:HA	1:A:961:GLU:H	3	0.55
(1,1987)	2:B:759:TYR:H	2:B:759:TYR:HB2	9	0.55
(1,1957)	2:B:756:ASN:H	2:B:756:ASN:HB2	2	0.55
(1,777)	1:A:1000:LEU:H	1:A:1000:LEU:HB2	15	0.54
(1,755)	1:A:997:ARG:H	1:A:997:ARG:HG3	11	0.54
(1,738)	1:A:995:ARG:HA	1:A:996:ASN:H	17	0.54
(1,547)	1:A:987:MET:HG3	1:A:989:LYS:H	1	0.54
(1,299)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	11	0.54
(1,2860)	1:A:1000:LEU:H	1:A:1000:LEU:HB2	15	0.54
(1,2838)	1:A:997:ARG:H	1:A:997:ARG:HG3	11	0.54
(1,2821)	1:A:995:ARG:HA	1:A:996:ASN:H	17	0.54
(1,268)	1:A:974:LEU:HD21	1:A:974:LEU:HA	10	0.54
(1,268)	1:A:974:LEU:HD22	1:A:974:LEU:HA	10	0.54
(1,268)	1:A:974:LEU:HD23	1:A:974:LEU:HA	10	0.54
(1,268)	1:A:974:LEU:HD21	1:A:974:LEU:HA	13	0.54
(1,268)	1:A:974:LEU:HD22	1:A:974:LEU:HA	13	0.54
(1,268)	1:A:974:LEU:HD23	1:A:974:LEU:HA	13	0.54
(1,2630)	1:A:987:MET:HG3	1:A:989:LYS:H	1	0.54
(1,2382)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	11	0.54
(1,2351)	1:A:974:LEU:HD21	1:A:974:LEU:HA	10	0.54
(1,2351)	1:A:974:LEU:HD22	1:A:974:LEU:HA	10	0.54
(1,2351)	1:A:974:LEU:HD23	1:A:974:LEU:HA	10	0.54
(1,2351)	1:A:974:LEU:HD21	1:A:974:LEU:HA	13	0.54
(1,2351)	1:A:974:LEU:HD22	1:A:974:LEU:HA	13	0.54
(1,2351)	1:A:974:LEU:HD23	1:A:974:LEU:HA	13	0.54
(1,762)	1:A:997:ARG:HA	1:A:999:PRO:HD2	12	0.53
(1,762)	1:A:997:ARG:HA	1:A:999:PRO:HD2	15	0.53
(1,755)	1:A:997:ARG:H	1:A:997:ARG:HG3	12	0.53
(1,755)	1:A:997:ARG:H	1:A:997:ARG:HG3	17	0.53

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,741)	1:A:995:ARG:HB3	1:A:997:ARG:H	20	0.53
(1,4073)	2:B:759:TYR:HA	2:B:760:ARG:H	19	0.53
(1,4014)	2:B:751:THR:HA	2:B:752:SER:H	8	0.53
(1,3998)	2:B:749:GLU:H	2:B:749:GLU:HB3	8	0.53
(1,3956)	2:B:746:LEU:H	2:B:746:LEU:HB3	13	0.53
(1,299)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	3	0.53
(1,299)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	4	0.53
(1,299)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	12	0.53
(1,299)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	13	0.53
(1,2845)	1:A:997:ARG:HA	1:A:999:PRO:HD2	12	0.53
(1,2845)	1:A:997:ARG:HA	1:A:999:PRO:HD2	15	0.53
(1,2838)	1:A:997:ARG:H	1:A:997:ARG:HG3	12	0.53
(1,2838)	1:A:997:ARG:H	1:A:997:ARG:HG3	17	0.53
(1,2824)	1:A:995:ARG:HB3	1:A:997:ARG:H	20	0.53
(1,268)	1:A:974:LEU:HD21	1:A:974:LEU:HA	16	0.53
(1,268)	1:A:974:LEU:HD22	1:A:974:LEU:HA	16	0.53
(1,268)	1:A:974:LEU:HD23	1:A:974:LEU:HA	16	0.53
(1,2382)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	3	0.53
(1,2382)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	4	0.53
(1,2382)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	12	0.53
(1,2382)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	13	0.53
(1,2351)	1:A:974:LEU:HD21	1:A:974:LEU:HA	16	0.53
(1,2351)	1:A:974:LEU:HD22	1:A:974:LEU:HA	16	0.53
(1,2351)	1:A:974:LEU:HD23	1:A:974:LEU:HA	16	0.53
(1,2269)	1:A:970:LEU:HA	1:A:970:LEU:HD21	11	0.53
(1,2269)	1:A:970:LEU:HA	1:A:970:LEU:HD22	11	0.53
(1,2269)	1:A:970:LEU:HA	1:A:970:LEU:HD23	11	0.53
(1,1990)	2:B:759:TYR:HA	2:B:760:ARG:H	19	0.53
(1,1931)	2:B:751:THR:HA	2:B:752:SER:H	8	0.53
(1,1915)	2:B:749:GLU:H	2:B:749:GLU:HB3	8	0.53
(1,1873)	2:B:746:LEU:H	2:B:746:LEU:HB3	13	0.53
(1,186)	1:A:970:LEU:HA	1:A:970:LEU:HD21	11	0.53
(1,186)	1:A:970:LEU:HA	1:A:970:LEU:HD22	11	0.53
(1,186)	1:A:970:LEU:HA	1:A:970:LEU:HD23	11	0.53
(1,738)	1:A:995:ARG:HA	1:A:996:ASN:H	4	0.52
(1,689)	1:A:993:PHE:HA	1:A:994:LYS:H	3	0.52
(1,4014)	2:B:751:THR:HA	2:B:752:SER:H	19	0.52
(1,3998)	2:B:749:GLU:H	2:B:749:GLU:HB3	11	0.52
(1,3745)	2:B:730:PHE:HE1	2:B:734:ARG:HD2	8	0.52
(1,299)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	15	0.52
(1,299)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	18	0.52
(1,2821)	1:A:995:ARG:HA	1:A:996:ASN:H	4	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2772)	1:A:993:PHE:HA	1:A:994:LYS:H	3	0.52
(1,2382)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	15	0.52
(1,2382)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	18	0.52
(1,2282)	1:A:970:LEU:HB2	1:A:971:VAL:H	12	0.52
(1,199)	1:A:970:LEU:HB2	1:A:971:VAL:H	12	0.52
(1,1931)	2:B:751:THR:HA	2:B:752:SER:H	19	0.52
(1,1915)	2:B:749:GLU:H	2:B:749:GLU:HB3	11	0.52
(1,1662)	2:B:730:PHE:HE1	2:B:734:ARG:HD2	8	0.52
(1,762)	1:A:997:ARG:HA	1:A:999:PRO:HD2	2	0.51
(1,539)	1:A:987:MET:HB3	1:A:988:TRP:H	12	0.51
(1,4161)	1:A:988:TRP:H	2:B:719:ILE:HG12	18	0.51
(1,3956)	2:B:746:LEU:H	2:B:746:LEU:HB3	3	0.51
(1,3645)	2:B:725:LYS:H	2:B:725:LYS:HB3	6	0.51
(1,3645)	2:B:725:LYS:H	2:B:725:LYS:HB3	7	0.51
(1,3463)	2:B:717:LEU:HD11	2:B:717:LEU:HA	5	0.51
(1,3463)	2:B:717:LEU:HD12	2:B:717:LEU:HA	5	0.51
(1,3463)	2:B:717:LEU:HD13	2:B:717:LEU:HA	5	0.51
(1,312)	1:A:977:LEU:HD11	1:A:977:LEU:HA	4	0.51
(1,312)	1:A:977:LEU:HD12	1:A:977:LEU:HA	4	0.51
(1,312)	1:A:977:LEU:HD13	1:A:977:LEU:HA	4	0.51
(1,299)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	2	0.51
(1,299)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	7	0.51
(1,299)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	9	0.51
(1,299)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	20	0.51
(1,2845)	1:A:997:ARG:HA	1:A:999:PRO:HD2	2	0.51
(1,2622)	1:A:987:MET:HB3	1:A:988:TRP:H	12	0.51
(1,2395)	1:A:977:LEU:HD11	1:A:977:LEU:HA	4	0.51
(1,2395)	1:A:977:LEU:HD12	1:A:977:LEU:HA	4	0.51
(1,2395)	1:A:977:LEU:HD13	1:A:977:LEU:HA	4	0.51
(1,2382)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	2	0.51
(1,2382)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	7	0.51
(1,2382)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	9	0.51
(1,2382)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	20	0.51
(1,2282)	1:A:970:LEU:HB2	1:A:971:VAL:H	10	0.51
(1,2269)	1:A:970:LEU:HA	1:A:970:LEU:HD21	18	0.51
(1,2269)	1:A:970:LEU:HA	1:A:970:LEU:HD22	18	0.51
(1,2269)	1:A:970:LEU:HA	1:A:970:LEU:HD23	18	0.51
(1,2078)	1:A:988:TRP:H	2:B:719:ILE:HG12	18	0.51
(1,199)	1:A:970:LEU:HB2	1:A:971:VAL:H	10	0.51
(1,1873)	2:B:746:LEU:H	2:B:746:LEU:HB3	3	0.51
(1,186)	1:A:970:LEU:HA	1:A:970:LEU:HD21	18	0.51
(1,186)	1:A:970:LEU:HA	1:A:970:LEU:HD22	18	0.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,186)	1:A:970:LEU:HA	1:A:970:LEU:HD23	18	0.51
(1,1562)	2:B:725:LYS:H	2:B:725:LYS:HB3	6	0.51
(1,1562)	2:B:725:LYS:H	2:B:725:LYS:HB3	7	0.51
(1,1380)	2:B:717:LEU:HD11	2:B:717:LEU:HA	5	0.51
(1,1380)	2:B:717:LEU:HD12	2:B:717:LEU:HA	5	0.51
(1,1380)	2:B:717:LEU:HD13	2:B:717:LEU:HA	5	0.51
(1,996)	2:B:698:LEU:HD21	2:B:698:LEU:HA	9	0.5
(1,996)	2:B:698:LEU:HD22	2:B:698:LEU:HA	9	0.5
(1,996)	2:B:698:LEU:HD23	2:B:698:LEU:HA	9	0.5
(1,741)	1:A:995:ARG:HB3	1:A:997:ARG:H	17	0.5
(1,3956)	2:B:746:LEU:H	2:B:746:LEU:HB3	5	0.5
(1,3902)	2:B:742:ALA:HA	2:B:743:ASN:H	19	0.5
(1,3888)	2:B:740:ASP:HA	2:B:741:THR:H	12	0.5
(1,3717)	2:B:729:LYS:HE3	2:B:729:LYS:HA	7	0.5
(1,3715)	2:B:729:LYS:H	2:B:729:LYS:HG3	8	0.5
(1,3715)	2:B:729:LYS:H	2:B:729:LYS:HG3	9	0.5
(1,3715)	2:B:729:LYS:H	2:B:729:LYS:HG3	10	0.5
(1,3715)	2:B:729:LYS:H	2:B:729:LYS:HG3	17	0.5
(1,3645)	2:B:725:LYS:H	2:B:725:LYS:HB3	1	0.5
(1,3645)	2:B:725:LYS:H	2:B:725:LYS:HB3	2	0.5
(1,3645)	2:B:725:LYS:H	2:B:725:LYS:HB3	3	0.5
(1,3645)	2:B:725:LYS:H	2:B:725:LYS:HB3	5	0.5
(1,3645)	2:B:725:LYS:H	2:B:725:LYS:HB3	8	0.5
(1,3645)	2:B:725:LYS:H	2:B:725:LYS:HB3	10	0.5
(1,3645)	2:B:725:LYS:H	2:B:725:LYS:HB3	12	0.5
(1,3645)	2:B:725:LYS:H	2:B:725:LYS:HB3	14	0.5
(1,3645)	2:B:725:LYS:H	2:B:725:LYS:HB3	15	0.5
(1,3645)	2:B:725:LYS:H	2:B:725:LYS:HB3	18	0.5
(1,3463)	2:B:717:LEU:HD11	2:B:717:LEU:HA	17	0.5
(1,3463)	2:B:717:LEU:HD12	2:B:717:LEU:HA	17	0.5
(1,3463)	2:B:717:LEU:HD13	2:B:717:LEU:HA	17	0.5
(1,3079)	2:B:698:LEU:HD21	2:B:698:LEU:HA	9	0.5
(1,3079)	2:B:698:LEU:HD22	2:B:698:LEU:HA	9	0.5
(1,3079)	2:B:698:LEU:HD23	2:B:698:LEU:HA	9	0.5
(1,283)	1:A:975:GLY:HA2	1:A:976:GLY:H	12	0.5
(1,2824)	1:A:995:ARG:HB3	1:A:997:ARG:H	17	0.5
(1,2366)	1:A:975:GLY:HA2	1:A:976:GLY:H	12	0.5
(1,2282)	1:A:970:LEU:HB2	1:A:971:VAL:H	8	0.5
(1,2282)	1:A:970:LEU:HB2	1:A:971:VAL:H	14	0.5
(1,2269)	1:A:970:LEU:HA	1:A:970:LEU:HD21	1	0.5
(1,2269)	1:A:970:LEU:HA	1:A:970:LEU:HD22	1	0.5
(1,2269)	1:A:970:LEU:HA	1:A:970:LEU:HD23	1	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2269)	1:A:970:LEU:HA	1:A:970:LEU:HD21	4	0.5
(1,2269)	1:A:970:LEU:HA	1:A:970:LEU:HD22	4	0.5
(1,2269)	1:A:970:LEU:HA	1:A:970:LEU:HD23	4	0.5
(1,2269)	1:A:970:LEU:HA	1:A:970:LEU:HD21	20	0.5
(1,2269)	1:A:970:LEU:HA	1:A:970:LEU:HD22	20	0.5
(1,2269)	1:A:970:LEU:HA	1:A:970:LEU:HD23	20	0.5
(1,199)	1:A:970:LEU:HB2	1:A:971:VAL:H	8	0.5
(1,199)	1:A:970:LEU:HB2	1:A:971:VAL:H	14	0.5
(1,1873)	2:B:746:LEU:H	2:B:746:LEU:HB3	5	0.5
(1,186)	1:A:970:LEU:HA	1:A:970:LEU:HD21	1	0.5
(1,186)	1:A:970:LEU:HA	1:A:970:LEU:HD22	1	0.5
(1,186)	1:A:970:LEU:HA	1:A:970:LEU:HD23	1	0.5
(1,186)	1:A:970:LEU:HA	1:A:970:LEU:HD21	4	0.5
(1,186)	1:A:970:LEU:HA	1:A:970:LEU:HD22	4	0.5
(1,186)	1:A:970:LEU:HA	1:A:970:LEU:HD23	4	0.5
(1,186)	1:A:970:LEU:HA	1:A:970:LEU:HD21	20	0.5
(1,186)	1:A:970:LEU:HA	1:A:970:LEU:HD22	20	0.5
(1,186)	1:A:970:LEU:HA	1:A:970:LEU:HD23	20	0.5
(1,1819)	2:B:742:ALA:HA	2:B:743:ASN:H	19	0.5
(1,1805)	2:B:740:ASP:HA	2:B:741:THR:H	12	0.5
(1,1634)	2:B:729:LYS:HE3	2:B:729:LYS:HA	7	0.5
(1,1632)	2:B:729:LYS:H	2:B:729:LYS:HG3	8	0.5
(1,1632)	2:B:729:LYS:H	2:B:729:LYS:HG3	9	0.5
(1,1632)	2:B:729:LYS:H	2:B:729:LYS:HG3	10	0.5
(1,1632)	2:B:729:LYS:H	2:B:729:LYS:HG3	17	0.5
(1,1562)	2:B:725:LYS:H	2:B:725:LYS:HB3	1	0.5
(1,1562)	2:B:725:LYS:H	2:B:725:LYS:HB3	2	0.5
(1,1562)	2:B:725:LYS:H	2:B:725:LYS:HB3	3	0.5
(1,1562)	2:B:725:LYS:H	2:B:725:LYS:HB3	5	0.5
(1,1562)	2:B:725:LYS:H	2:B:725:LYS:HB3	8	0.5
(1,1562)	2:B:725:LYS:H	2:B:725:LYS:HB3	10	0.5
(1,1562)	2:B:725:LYS:H	2:B:725:LYS:HB3	12	0.5
(1,1562)	2:B:725:LYS:H	2:B:725:LYS:HB3	14	0.5
(1,1562)	2:B:725:LYS:H	2:B:725:LYS:HB3	15	0.5
(1,1562)	2:B:725:LYS:H	2:B:725:LYS:HB3	18	0.5
(1,1380)	2:B:717:LEU:HD11	2:B:717:LEU:HA	17	0.5
(1,1380)	2:B:717:LEU:HD12	2:B:717:LEU:HA	17	0.5
(1,1380)	2:B:717:LEU:HD13	2:B:717:LEU:HA	17	0.5
(1,670)	1:A:992:PHE:HA	1:A:993:PHE:H	6	0.49
(1,3745)	2:B:730:PHE:HE1	2:B:734:ARG:HD2	6	0.49
(1,3717)	2:B:729:LYS:HE3	2:B:729:LYS:HA	16	0.49
(1,3715)	2:B:729:LYS:H	2:B:729:LYS:HG3	4	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3715)	2:B:729:LYS:H	2:B:729:LYS:HG3	13	0.49
(1,3715)	2:B:729:LYS:H	2:B:729:LYS:HG3	19	0.49
(1,3645)	2:B:725:LYS:H	2:B:725:LYS:HB3	4	0.49
(1,3645)	2:B:725:LYS:H	2:B:725:LYS:HB3	9	0.49
(1,3645)	2:B:725:LYS:H	2:B:725:LYS:HB3	11	0.49
(1,3645)	2:B:725:LYS:H	2:B:725:LYS:HB3	13	0.49
(1,3645)	2:B:725:LYS:H	2:B:725:LYS:HB3	16	0.49
(1,3645)	2:B:725:LYS:H	2:B:725:LYS:HB3	17	0.49
(1,3645)	2:B:725:LYS:H	2:B:725:LYS:HB3	19	0.49
(1,3645)	2:B:725:LYS:H	2:B:725:LYS:HB3	20	0.49
(1,299)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	1	0.49
(1,299)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	5	0.49
(1,299)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	10	0.49
(1,283)	1:A:975:GLY:HA2	1:A:976:GLY:H	14	0.49
(1,2753)	1:A:992:PHE:HA	1:A:993:PHE:H	6	0.49
(1,2382)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	1	0.49
(1,2382)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	5	0.49
(1,2382)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	10	0.49
(1,2366)	1:A:975:GLY:HA2	1:A:976:GLY:H	14	0.49
(1,2278)	1:A:970:LEU:HD11	1:A:970:LEU:HA	3	0.49
(1,2278)	1:A:970:LEU:HD12	1:A:970:LEU:HA	3	0.49
(1,2278)	1:A:970:LEU:HD13	1:A:970:LEU:HA	3	0.49
(1,2278)	1:A:970:LEU:HD11	1:A:970:LEU:HA	5	0.49
(1,2278)	1:A:970:LEU:HD12	1:A:970:LEU:HA	5	0.49
(1,2278)	1:A:970:LEU:HD13	1:A:970:LEU:HA	5	0.49
(1,2278)	1:A:970:LEU:HD11	1:A:970:LEU:HA	6	0.49
(1,2278)	1:A:970:LEU:HD12	1:A:970:LEU:HA	6	0.49
(1,2278)	1:A:970:LEU:HD13	1:A:970:LEU:HA	6	0.49
(1,2278)	1:A:970:LEU:HD11	1:A:970:LEU:HA	9	0.49
(1,2278)	1:A:970:LEU:HD12	1:A:970:LEU:HA	9	0.49
(1,2278)	1:A:970:LEU:HD13	1:A:970:LEU:HA	9	0.49
(1,2278)	1:A:970:LEU:HD11	1:A:970:LEU:HA	15	0.49
(1,2278)	1:A:970:LEU:HD12	1:A:970:LEU:HA	15	0.49
(1,2278)	1:A:970:LEU:HD13	1:A:970:LEU:HA	15	0.49
(1,195)	1:A:970:LEU:HD11	1:A:970:LEU:HA	3	0.49
(1,195)	1:A:970:LEU:HD12	1:A:970:LEU:HA	3	0.49
(1,195)	1:A:970:LEU:HD13	1:A:970:LEU:HA	3	0.49
(1,195)	1:A:970:LEU:HD11	1:A:970:LEU:HA	5	0.49
(1,195)	1:A:970:LEU:HD12	1:A:970:LEU:HA	5	0.49
(1,195)	1:A:970:LEU:HD13	1:A:970:LEU:HA	5	0.49
(1,195)	1:A:970:LEU:HD11	1:A:970:LEU:HA	6	0.49
(1,195)	1:A:970:LEU:HD12	1:A:970:LEU:HA	6	0.49

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,195)	1:A:970:LEU:HD13	1:A:970:LEU:HA	6	0.49
(1,195)	1:A:970:LEU:HD11	1:A:970:LEU:HA	9	0.49
(1,195)	1:A:970:LEU:HD12	1:A:970:LEU:HA	9	0.49
(1,195)	1:A:970:LEU:HD13	1:A:970:LEU:HA	9	0.49
(1,195)	1:A:970:LEU:HD11	1:A:970:LEU:HA	15	0.49
(1,195)	1:A:970:LEU:HD12	1:A:970:LEU:HA	15	0.49
(1,195)	1:A:970:LEU:HD13	1:A:970:LEU:HA	15	0.49
(1,1662)	2:B:730:PHE:HE1	2:B:734:ARG:HD2	6	0.49
(1,1634)	2:B:729:LYS:HE3	2:B:729:LYS:HA	16	0.49
(1,1632)	2:B:729:LYS:H	2:B:729:LYS:HG3	4	0.49
(1,1632)	2:B:729:LYS:H	2:B:729:LYS:HG3	13	0.49
(1,1632)	2:B:729:LYS:H	2:B:729:LYS:HG3	19	0.49
(1,1562)	2:B:725:LYS:H	2:B:725:LYS:HB3	4	0.49
(1,1562)	2:B:725:LYS:H	2:B:725:LYS:HB3	9	0.49
(1,1562)	2:B:725:LYS:H	2:B:725:LYS:HB3	11	0.49
(1,1562)	2:B:725:LYS:H	2:B:725:LYS:HB3	13	0.49
(1,1562)	2:B:725:LYS:H	2:B:725:LYS:HB3	16	0.49
(1,1562)	2:B:725:LYS:H	2:B:725:LYS:HB3	17	0.49
(1,1562)	2:B:725:LYS:H	2:B:725:LYS:HB3	19	0.49
(1,1562)	2:B:725:LYS:H	2:B:725:LYS:HB3	20	0.49
(1,762)	1:A:997:ARG:HA	1:A:999:PRO:HD2	8	0.48
(1,741)	1:A:995:ARG:HB3	1:A:997:ARG:H	13	0.48
(1,738)	1:A:995:ARG:HA	1:A:996:ASN:H	1	0.48
(1,670)	1:A:992:PHE:HA	1:A:993:PHE:H	7	0.48
(1,670)	1:A:992:PHE:HA	1:A:993:PHE:H	8	0.48
(1,670)	1:A:992:PHE:HA	1:A:993:PHE:H	11	0.48
(1,670)	1:A:992:PHE:HA	1:A:993:PHE:H	13	0.48
(1,670)	1:A:992:PHE:HA	1:A:993:PHE:H	14	0.48
(1,670)	1:A:992:PHE:HA	1:A:993:PHE:H	15	0.48
(1,670)	1:A:992:PHE:HA	1:A:993:PHE:H	16	0.48
(1,670)	1:A:992:PHE:HA	1:A:993:PHE:H	17	0.48
(1,670)	1:A:992:PHE:HA	1:A:993:PHE:H	18	0.48
(1,639)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	9	0.48
(1,639)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	9	0.48
(1,639)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	9	0.48
(1,3893)	2:B:741:THR:HA	2:B:742:ALA:H	1	0.48
(1,3715)	2:B:729:LYS:H	2:B:729:LYS:HG3	14	0.48
(1,3715)	2:B:729:LYS:H	2:B:729:LYS:HG3	18	0.48
(1,2845)	1:A:997:ARG:HA	1:A:999:PRO:HD2	8	0.48
(1,283)	1:A:975:GLY:HA2	1:A:976:GLY:H	2	0.48
(1,283)	1:A:975:GLY:HA2	1:A:976:GLY:H	4	0.48
(1,283)	1:A:975:GLY:HA2	1:A:976:GLY:H	5	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,283)	1:A:975:GLY:HA2	1:A:976:GLY:H	6	0.48
(1,283)	1:A:975:GLY:HA2	1:A:976:GLY:H	7	0.48
(1,283)	1:A:975:GLY:HA2	1:A:976:GLY:H	13	0.48
(1,283)	1:A:975:GLY:HA2	1:A:976:GLY:H	16	0.48
(1,2824)	1:A:995:ARG:HB3	1:A:997:ARG:H	13	0.48
(1,2821)	1:A:995:ARG:HA	1:A:996:ASN:H	1	0.48
(1,2753)	1:A:992:PHE:HA	1:A:993:PHE:H	7	0.48
(1,2753)	1:A:992:PHE:HA	1:A:993:PHE:H	8	0.48
(1,2753)	1:A:992:PHE:HA	1:A:993:PHE:H	11	0.48
(1,2753)	1:A:992:PHE:HA	1:A:993:PHE:H	13	0.48
(1,2753)	1:A:992:PHE:HA	1:A:993:PHE:H	14	0.48
(1,2753)	1:A:992:PHE:HA	1:A:993:PHE:H	15	0.48
(1,2753)	1:A:992:PHE:HA	1:A:993:PHE:H	16	0.48
(1,2753)	1:A:992:PHE:HA	1:A:993:PHE:H	17	0.48
(1,2753)	1:A:992:PHE:HA	1:A:993:PHE:H	18	0.48
(1,2722)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	9	0.48
(1,2722)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	9	0.48
(1,2722)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	9	0.48
(1,2366)	1:A:975:GLY:HA2	1:A:976:GLY:H	2	0.48
(1,2366)	1:A:975:GLY:HA2	1:A:976:GLY:H	4	0.48
(1,2366)	1:A:975:GLY:HA2	1:A:976:GLY:H	5	0.48
(1,2366)	1:A:975:GLY:HA2	1:A:976:GLY:H	6	0.48
(1,2366)	1:A:975:GLY:HA2	1:A:976:GLY:H	7	0.48
(1,2366)	1:A:975:GLY:HA2	1:A:976:GLY:H	13	0.48
(1,2366)	1:A:975:GLY:HA2	1:A:976:GLY:H	16	0.48
(1,1810)	2:B:741:THR:HA	2:B:742:ALA:H	1	0.48
(1,1632)	2:B:729:LYS:H	2:B:729:LYS:HG3	14	0.48
(1,1632)	2:B:729:LYS:H	2:B:729:LYS:HG3	18	0.48
(1,811)	1:A:1006:GLU:H	1:A:1006:GLU:HB3	2	0.47
(1,762)	1:A:997:ARG:HA	1:A:999:PRO:HD2	3	0.47
(1,689)	1:A:993:PHE:HA	1:A:994:LYS:H	9	0.47
(1,689)	1:A:993:PHE:HA	1:A:994:LYS:H	15	0.47
(1,689)	1:A:993:PHE:HA	1:A:994:LYS:H	20	0.47
(1,670)	1:A:992:PHE:HA	1:A:993:PHE:H	3	0.47
(1,670)	1:A:992:PHE:HA	1:A:993:PHE:H	4	0.47
(1,670)	1:A:992:PHE:HA	1:A:993:PHE:H	9	0.47
(1,670)	1:A:992:PHE:HA	1:A:993:PHE:H	10	0.47
(1,670)	1:A:992:PHE:HA	1:A:993:PHE:H	20	0.47
(1,4161)	1:A:988:TRP:H	2:B:719:ILE:HG12	11	0.47
(1,4161)	1:A:988:TRP:H	2:B:719:ILE:HG12	13	0.47
(1,4000)	2:B:749:GLU:H	2:B:749:GLU:HG3	10	0.47
(1,3715)	2:B:729:LYS:H	2:B:729:LYS:HG3	3	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3715)	2:B:729:LYS:H	2:B:729:LYS:HG3	12	0.47
(1,3715)	2:B:729:LYS:H	2:B:729:LYS:HG3	20	0.47
(1,2894)	1:A:1006:GLU:H	1:A:1006:GLU:HB3	2	0.47
(1,2845)	1:A:997:ARG:HA	1:A:999:PRO:HD2	3	0.47
(1,283)	1:A:975:GLY:HA2	1:A:976:GLY:H	1	0.47
(1,283)	1:A:975:GLY:HA2	1:A:976:GLY:H	9	0.47
(1,283)	1:A:975:GLY:HA2	1:A:976:GLY:H	11	0.47
(1,283)	1:A:975:GLY:HA2	1:A:976:GLY:H	15	0.47
(1,283)	1:A:975:GLY:HA2	1:A:976:GLY:H	17	0.47
(1,283)	1:A:975:GLY:HA2	1:A:976:GLY:H	18	0.47
(1,283)	1:A:975:GLY:HA2	1:A:976:GLY:H	19	0.47
(1,283)	1:A:975:GLY:HA2	1:A:976:GLY:H	20	0.47
(1,2772)	1:A:993:PHE:HA	1:A:994:LYS:H	9	0.47
(1,2772)	1:A:993:PHE:HA	1:A:994:LYS:H	15	0.47
(1,2772)	1:A:993:PHE:HA	1:A:994:LYS:H	20	0.47
(1,2753)	1:A:992:PHE:HA	1:A:993:PHE:H	3	0.47
(1,2753)	1:A:992:PHE:HA	1:A:993:PHE:H	4	0.47
(1,2753)	1:A:992:PHE:HA	1:A:993:PHE:H	9	0.47
(1,2753)	1:A:992:PHE:HA	1:A:993:PHE:H	10	0.47
(1,2753)	1:A:992:PHE:HA	1:A:993:PHE:H	20	0.47
(1,2366)	1:A:975:GLY:HA2	1:A:976:GLY:H	1	0.47
(1,2366)	1:A:975:GLY:HA2	1:A:976:GLY:H	9	0.47
(1,2366)	1:A:975:GLY:HA2	1:A:976:GLY:H	11	0.47
(1,2366)	1:A:975:GLY:HA2	1:A:976:GLY:H	15	0.47
(1,2366)	1:A:975:GLY:HA2	1:A:976:GLY:H	17	0.47
(1,2366)	1:A:975:GLY:HA2	1:A:976:GLY:H	18	0.47
(1,2366)	1:A:975:GLY:HA2	1:A:976:GLY:H	19	0.47
(1,2366)	1:A:975:GLY:HA2	1:A:976:GLY:H	20	0.47
(1,2078)	1:A:988:TRP:H	2:B:719:ILE:HG12	11	0.47
(1,2078)	1:A:988:TRP:H	2:B:719:ILE:HG12	13	0.47
(1,1917)	2:B:749:GLU:H	2:B:749:GLU:HG3	10	0.47
(1,1632)	2:B:729:LYS:H	2:B:729:LYS:HG3	3	0.47
(1,1632)	2:B:729:LYS:H	2:B:729:LYS:HG3	12	0.47
(1,1632)	2:B:729:LYS:H	2:B:729:LYS:HG3	20	0.47
(1,755)	1:A:997:ARG:H	1:A:997:ARG:HG3	4	0.46
(1,670)	1:A:992:PHE:HA	1:A:993:PHE:H	2	0.46
(1,670)	1:A:992:PHE:HA	1:A:993:PHE:H	5	0.46
(1,539)	1:A:987:MET:HB3	1:A:988:TRP:H	13	0.46
(1,3893)	2:B:741:THR:HA	2:B:742:ALA:H	6	0.46
(1,3717)	2:B:729:LYS:HE3	2:B:729:LYS:HA	4	0.46
(1,3715)	2:B:729:LYS:H	2:B:729:LYS:HG3	1	0.46
(1,3715)	2:B:729:LYS:H	2:B:729:LYS:HG3	2	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3715)	2:B:729:LYS:H	2:B:729:LYS:HG3	5	0.46
(1,3715)	2:B:729:LYS:H	2:B:729:LYS:HG3	6	0.46
(1,3715)	2:B:729:LYS:H	2:B:729:LYS:HG3	7	0.46
(1,2838)	1:A:997:ARG:H	1:A:997:ARG:HG3	4	0.46
(1,283)	1:A:975:GLY:HA2	1:A:976:GLY:H	3	0.46
(1,283)	1:A:975:GLY:HA2	1:A:976:GLY:H	8	0.46
(1,283)	1:A:975:GLY:HA2	1:A:976:GLY:H	10	0.46
(1,2753)	1:A:992:PHE:HA	1:A:993:PHE:H	2	0.46
(1,2753)	1:A:992:PHE:HA	1:A:993:PHE:H	5	0.46
(1,2622)	1:A:987:MET:HB3	1:A:988:TRP:H	13	0.46
(1,2366)	1:A:975:GLY:HA2	1:A:976:GLY:H	3	0.46
(1,2366)	1:A:975:GLY:HA2	1:A:976:GLY:H	8	0.46
(1,2366)	1:A:975:GLY:HA2	1:A:976:GLY:H	10	0.46
(1,1810)	2:B:741:THR:HA	2:B:742:ALA:H	6	0.46
(1,1634)	2:B:729:LYS:HE3	2:B:729:LYS:HA	4	0.46
(1,1632)	2:B:729:LYS:H	2:B:729:LYS:HG3	1	0.46
(1,1632)	2:B:729:LYS:H	2:B:729:LYS:HG3	2	0.46
(1,1632)	2:B:729:LYS:H	2:B:729:LYS:HG3	5	0.46
(1,1632)	2:B:729:LYS:H	2:B:729:LYS:HG3	6	0.46
(1,1632)	2:B:729:LYS:H	2:B:729:LYS:HG3	7	0.46
(1,800)	1:A:1003:ASP:HA	1:A:1004:ASP:H	1	0.45
(1,755)	1:A:997:ARG:H	1:A:997:ARG:HG3	5	0.45
(1,738)	1:A:995:ARG:HA	1:A:996:ASN:H	5	0.45
(1,738)	1:A:995:ARG:HA	1:A:996:ASN:H	16	0.45
(1,670)	1:A:992:PHE:HA	1:A:993:PHE:H	12	0.45
(1,670)	1:A:992:PHE:HA	1:A:993:PHE:H	19	0.45
(1,639)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	13	0.45
(1,639)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	13	0.45
(1,639)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	13	0.45
(1,3911)	2:B:743:ASN:HB3	2:B:743:ASN:H	7	0.45
(1,3911)	2:B:743:ASN:HB3	2:B:743:ASN:H	18	0.45
(1,3715)	2:B:729:LYS:H	2:B:729:LYS:HG3	11	0.45
(1,3715)	2:B:729:LYS:H	2:B:729:LYS:HG3	15	0.45
(1,299)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	6	0.45
(1,299)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	19	0.45
(1,2883)	1:A:1003:ASP:HA	1:A:1004:ASP:H	1	0.45
(1,2838)	1:A:997:ARG:H	1:A:997:ARG:HG3	5	0.45
(1,2821)	1:A:995:ARG:HA	1:A:996:ASN:H	5	0.45
(1,2821)	1:A:995:ARG:HA	1:A:996:ASN:H	16	0.45
(1,2753)	1:A:992:PHE:HA	1:A:993:PHE:H	12	0.45
(1,2753)	1:A:992:PHE:HA	1:A:993:PHE:H	19	0.45
(1,2722)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	13	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2722)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	13	0.45
(1,2722)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	13	0.45
(1,2382)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	6	0.45
(1,2382)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	19	0.45
(1,2282)	1:A:970:LEU:HB2	1:A:971:VAL:H	19	0.45
(1,199)	1:A:970:LEU:HB2	1:A:971:VAL:H	19	0.45
(1,1828)	2:B:743:ASN:HB3	2:B:743:ASN:H	7	0.45
(1,1828)	2:B:743:ASN:HB3	2:B:743:ASN:H	18	0.45
(1,1632)	2:B:729:LYS:H	2:B:729:LYS:HG3	11	0.45
(1,1632)	2:B:729:LYS:H	2:B:729:LYS:HG3	15	0.45
(1,811)	1:A:1006:GLU:H	1:A:1006:GLU:HB3	13	0.44
(1,762)	1:A:997:ARG:HA	1:A:999:PRO:HD2	11	0.44
(1,738)	1:A:995:ARG:HA	1:A:996:ASN:H	14	0.44
(1,706)	1:A:994:LYS:H	1:A:994:LYS:HB3	3	0.44
(1,689)	1:A:993:PHE:HA	1:A:994:LYS:H	19	0.44
(1,670)	1:A:992:PHE:HA	1:A:993:PHE:H	1	0.44
(1,639)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	1	0.44
(1,639)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	1	0.44
(1,639)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	1	0.44
(1,639)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	2	0.44
(1,639)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	2	0.44
(1,639)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	2	0.44
(1,639)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	6	0.44
(1,639)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	6	0.44
(1,639)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	6	0.44
(1,639)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	12	0.44
(1,639)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	12	0.44
(1,639)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	12	0.44
(1,539)	1:A:987:MET:HB3	1:A:988:TRP:H	11	0.44
(1,4161)	1:A:988:TRP:H	2:B:719:ILE:HG12	5	0.44
(1,3717)	2:B:729:LYS:HE3	2:B:729:LYS:HA	9	0.44
(1,299)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	8	0.44
(1,2894)	1:A:1006:GLU:H	1:A:1006:GLU:HB3	13	0.44
(1,2845)	1:A:997:ARG:HA	1:A:999:PRO:HD2	11	0.44
(1,2821)	1:A:995:ARG:HA	1:A:996:ASN:H	14	0.44
(1,2789)	1:A:994:LYS:H	1:A:994:LYS:HB3	3	0.44
(1,2772)	1:A:993:PHE:HA	1:A:994:LYS:H	19	0.44
(1,2753)	1:A:992:PHE:HA	1:A:993:PHE:H	1	0.44
(1,2722)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	1	0.44
(1,2722)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	1	0.44
(1,2722)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	1	0.44
(1,2722)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	2	0.44

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2722)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	2	0.44
(1,2722)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	2	0.44
(1,2722)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	6	0.44
(1,2722)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	6	0.44
(1,2722)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	6	0.44
(1,2722)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	12	0.44
(1,2722)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	12	0.44
(1,2722)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	12	0.44
(1,2622)	1:A:987:MET:HB3	1:A:988:TRP:H	11	0.44
(1,2382)	1:A:976:GLY:HA3	1:A:979:LEU:HB3	8	0.44
(1,2078)	1:A:988:TRP:H	2:B:719:ILE:HG12	5	0.44
(1,1634)	2:B:729:LYS:HE3	2:B:729:LYS:HA	9	0.44
(1,776)	1:A:999:PRO:HA	1:A:1000:LEU:H	11	0.43
(1,689)	1:A:993:PHE:HA	1:A:994:LYS:H	6	0.43
(1,689)	1:A:993:PHE:HA	1:A:994:LYS:H	8	0.43
(1,639)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	4	0.43
(1,639)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	4	0.43
(1,639)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	4	0.43
(1,639)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	19	0.43
(1,639)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	19	0.43
(1,639)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	19	0.43
(1,639)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	20	0.43
(1,639)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	20	0.43
(1,639)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	20	0.43
(1,4161)	1:A:988:TRP:H	2:B:719:ILE:HG12	6	0.43
(1,4161)	1:A:988:TRP:H	2:B:719:ILE:HG12	19	0.43
(1,4143)	1:A:984:VAL:H	2:B:712:LEU:HA	1	0.43
(1,3717)	2:B:729:LYS:HE3	2:B:729:LYS:HA	5	0.43
(1,3717)	2:B:729:LYS:HE3	2:B:729:LYS:HA	6	0.43
(1,3717)	2:B:729:LYS:HE3	2:B:729:LYS:HA	19	0.43
(1,3435)	2:B:716:LYS:HE3	2:B:716:LYS:HG2	7	0.43
(1,2859)	1:A:999:PRO:HA	1:A:1000:LEU:H	11	0.43
(1,2772)	1:A:993:PHE:HA	1:A:994:LYS:H	6	0.43
(1,2772)	1:A:993:PHE:HA	1:A:994:LYS:H	8	0.43
(1,2722)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	4	0.43
(1,2722)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	4	0.43
(1,2722)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	4	0.43
(1,2722)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	19	0.43
(1,2722)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	19	0.43
(1,2722)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	19	0.43
(1,2722)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	20	0.43
(1,2722)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	20	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2722)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	20	0.43
(1,2282)	1:A:970:LEU:HB2	1:A:971:VAL:H	13	0.43
(1,2282)	1:A:970:LEU:HB2	1:A:971:VAL:H	17	0.43
(1,2219)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	17	0.43
(1,2078)	1:A:988:TRP:H	2:B:719:ILE:HG12	6	0.43
(1,2078)	1:A:988:TRP:H	2:B:719:ILE:HG12	19	0.43
(1,2060)	1:A:984:VAL:H	2:B:712:LEU:HA	1	0.43
(1,199)	1:A:970:LEU:HB2	1:A:971:VAL:H	13	0.43
(1,199)	1:A:970:LEU:HB2	1:A:971:VAL:H	17	0.43
(1,1634)	2:B:729:LYS:HE3	2:B:729:LYS:HA	5	0.43
(1,1634)	2:B:729:LYS:HE3	2:B:729:LYS:HA	6	0.43
(1,1634)	2:B:729:LYS:HE3	2:B:729:LYS:HA	19	0.43
(1,136)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	17	0.43
(1,1352)	2:B:716:LYS:HE3	2:B:716:LYS:HG2	7	0.43
(1,787)	1:A:1000:LEU:HA	1:A:1001:GLU:H	9	0.42
(1,737)	1:A:995:ARG:HB3	1:A:996:ASN:H	14	0.42
(1,689)	1:A:993:PHE:HA	1:A:994:LYS:H	2	0.42
(1,689)	1:A:993:PHE:HA	1:A:994:LYS:H	10	0.42
(1,689)	1:A:993:PHE:HA	1:A:994:LYS:H	18	0.42
(1,639)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	3	0.42
(1,639)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	3	0.42
(1,639)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	3	0.42
(1,639)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	7	0.42
(1,639)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	7	0.42
(1,639)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	7	0.42
(1,4161)	1:A:988:TRP:H	2:B:719:ILE:HG12	2	0.42
(1,4161)	1:A:988:TRP:H	2:B:719:ILE:HG12	3	0.42
(1,4161)	1:A:988:TRP:H	2:B:719:ILE:HG12	10	0.42
(1,3902)	2:B:742:ALA:HA	2:B:743:ASN:H	12	0.42
(1,3717)	2:B:729:LYS:HE3	2:B:729:LYS:HA	1	0.42
(1,3717)	2:B:729:LYS:HE3	2:B:729:LYS:HA	3	0.42
(1,3717)	2:B:729:LYS:HE3	2:B:729:LYS:HA	8	0.42
(1,3717)	2:B:729:LYS:HE3	2:B:729:LYS:HA	10	0.42
(1,3717)	2:B:729:LYS:HE3	2:B:729:LYS:HA	11	0.42
(1,3717)	2:B:729:LYS:HE3	2:B:729:LYS:HA	14	0.42
(1,3717)	2:B:729:LYS:HE3	2:B:729:LYS:HA	17	0.42
(1,2870)	1:A:1000:LEU:HA	1:A:1001:GLU:H	9	0.42
(1,2820)	1:A:995:ARG:HB3	1:A:996:ASN:H	14	0.42
(1,2772)	1:A:993:PHE:HA	1:A:994:LYS:H	2	0.42
(1,2772)	1:A:993:PHE:HA	1:A:994:LYS:H	10	0.42
(1,2772)	1:A:993:PHE:HA	1:A:994:LYS:H	18	0.42
(1,2722)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	3	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2722)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	3	0.42
(1,2722)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	3	0.42
(1,2722)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	7	0.42
(1,2722)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	7	0.42
(1,2722)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	7	0.42
(1,2282)	1:A:970:LEU:HB2	1:A:971:VAL:H	2	0.42
(1,2219)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	1	0.42
(1,2219)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	2	0.42
(1,2219)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	5	0.42
(1,2219)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	7	0.42
(1,2219)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	8	0.42
(1,2219)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	9	0.42
(1,2219)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	10	0.42
(1,2219)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	12	0.42
(1,2219)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	13	0.42
(1,2219)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	14	0.42
(1,2219)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	15	0.42
(1,2219)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	16	0.42
(1,2219)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	19	0.42
(1,2219)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	20	0.42
(1,2078)	1:A:988:TRP:H	2:B:719:ILE:HG12	2	0.42
(1,2078)	1:A:988:TRP:H	2:B:719:ILE:HG12	3	0.42
(1,2078)	1:A:988:TRP:H	2:B:719:ILE:HG12	10	0.42
(1,199)	1:A:970:LEU:HB2	1:A:971:VAL:H	2	0.42
(1,1819)	2:B:742:ALA:HA	2:B:743:ASN:H	12	0.42
(1,1634)	2:B:729:LYS:HE3	2:B:729:LYS:HA	1	0.42
(1,1634)	2:B:729:LYS:HE3	2:B:729:LYS:HA	3	0.42
(1,1634)	2:B:729:LYS:HE3	2:B:729:LYS:HA	8	0.42
(1,1634)	2:B:729:LYS:HE3	2:B:729:LYS:HA	10	0.42
(1,1634)	2:B:729:LYS:HE3	2:B:729:LYS:HA	11	0.42
(1,1634)	2:B:729:LYS:HE3	2:B:729:LYS:HA	14	0.42
(1,1634)	2:B:729:LYS:HE3	2:B:729:LYS:HA	17	0.42
(1,136)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	1	0.42
(1,136)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	2	0.42
(1,136)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	5	0.42
(1,136)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	7	0.42
(1,136)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	8	0.42
(1,136)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	9	0.42
(1,136)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	10	0.42
(1,136)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	12	0.42
(1,136)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	13	0.42
(1,136)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	14	0.42

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,136)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	15	0.42
(1,136)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	16	0.42
(1,136)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	19	0.42
(1,136)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	20	0.42
(1,762)	1:A:997:ARG:HA	1:A:999:PRO:HD2	9	0.41
(1,762)	1:A:997:ARG:HA	1:A:999:PRO:HD2	14	0.41
(1,704)	1:A:994:LYS:H	1:A:994:LYS:HG3	3	0.41
(1,689)	1:A:993:PHE:HA	1:A:994:LYS:H	4	0.41
(1,689)	1:A:993:PHE:HA	1:A:994:LYS:H	7	0.41
(1,689)	1:A:993:PHE:HA	1:A:994:LYS:H	11	0.41
(1,689)	1:A:993:PHE:HA	1:A:994:LYS:H	12	0.41
(1,689)	1:A:993:PHE:HA	1:A:994:LYS:H	16	0.41
(1,639)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	5	0.41
(1,639)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	5	0.41
(1,639)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	5	0.41
(1,478)	1:A:985:LEU:HB3	1:A:986:ALA:HA	1	0.41
(1,4161)	1:A:988:TRP:H	2:B:719:ILE:HG12	7	0.41
(1,4161)	1:A:988:TRP:H	2:B:719:ILE:HG12	8	0.41
(1,4161)	1:A:988:TRP:H	2:B:719:ILE:HG12	9	0.41
(1,4161)	1:A:988:TRP:H	2:B:719:ILE:HG12	15	0.41
(1,4161)	1:A:988:TRP:H	2:B:719:ILE:HG12	17	0.41
(1,4143)	1:A:984:VAL:H	2:B:712:LEU:HA	17	0.41
(1,3911)	2:B:743:ASN:HB3	2:B:743:ASN:H	15	0.41
(1,3717)	2:B:729:LYS:HE3	2:B:729:LYS:HA	12	0.41
(1,3717)	2:B:729:LYS:HE3	2:B:729:LYS:HA	13	0.41
(1,3717)	2:B:729:LYS:HE3	2:B:729:LYS:HA	18	0.41
(1,3717)	2:B:729:LYS:HE3	2:B:729:LYS:HA	20	0.41
(1,3715)	2:B:729:LYS:H	2:B:729:LYS:HG3	16	0.41
(1,2845)	1:A:997:ARG:HA	1:A:999:PRO:HD2	9	0.41
(1,2845)	1:A:997:ARG:HA	1:A:999:PRO:HD2	14	0.41
(1,2787)	1:A:994:LYS:H	1:A:994:LYS:HG3	3	0.41
(1,2772)	1:A:993:PHE:HA	1:A:994:LYS:H	4	0.41
(1,2772)	1:A:993:PHE:HA	1:A:994:LYS:H	7	0.41
(1,2772)	1:A:993:PHE:HA	1:A:994:LYS:H	11	0.41
(1,2772)	1:A:993:PHE:HA	1:A:994:LYS:H	12	0.41
(1,2772)	1:A:993:PHE:HA	1:A:994:LYS:H	16	0.41
(1,2722)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	5	0.41
(1,2722)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	5	0.41
(1,2722)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	5	0.41
(1,2561)	1:A:985:LEU:HB3	1:A:986:ALA:HA	1	0.41
(1,2282)	1:A:970:LEU:HB2	1:A:971:VAL:H	7	0.41
(1,2219)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	3	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2219)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	6	0.41
(1,2219)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	18	0.41
(1,2078)	1:A:988:TRP:H	2:B:719:ILE:HG12	7	0.41
(1,2078)	1:A:988:TRP:H	2:B:719:ILE:HG12	8	0.41
(1,2078)	1:A:988:TRP:H	2:B:719:ILE:HG12	9	0.41
(1,2078)	1:A:988:TRP:H	2:B:719:ILE:HG12	15	0.41
(1,2078)	1:A:988:TRP:H	2:B:719:ILE:HG12	17	0.41
(1,2060)	1:A:984:VAL:H	2:B:712:LEU:HA	17	0.41
(1,199)	1:A:970:LEU:HB2	1:A:971:VAL:H	7	0.41
(1,1828)	2:B:743:ASN:HB3	2:B:743:ASN:H	15	0.41
(1,1634)	2:B:729:LYS:HE3	2:B:729:LYS:HA	12	0.41
(1,1634)	2:B:729:LYS:HE3	2:B:729:LYS:HA	13	0.41
(1,1634)	2:B:729:LYS:HE3	2:B:729:LYS:HA	18	0.41
(1,1634)	2:B:729:LYS:HE3	2:B:729:LYS:HA	20	0.41
(1,1632)	2:B:729:LYS:H	2:B:729:LYS:HG3	16	0.41
(1,136)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	3	0.41
(1,136)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	6	0.41
(1,136)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	18	0.41
(1,755)	1:A:997:ARG:H	1:A:997:ARG:HG3	13	0.4
(1,706)	1:A:994:LYS:H	1:A:994:LYS:HB3	20	0.4
(1,639)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	15	0.4
(1,639)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	15	0.4
(1,639)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	15	0.4
(1,639)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	17	0.4
(1,639)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	17	0.4
(1,639)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	17	0.4
(1,516)	1:A:986:ALA:HA	1:A:988:TRP:H	1	0.4
(1,516)	1:A:986:ALA:HA	1:A:988:TRP:H	16	0.4
(1,4154)	1:A:988:TRP:H	2:B:712:LEU:HD11	1	0.4
(1,4154)	1:A:988:TRP:H	2:B:712:LEU:HD12	1	0.4
(1,4154)	1:A:988:TRP:H	2:B:712:LEU:HD13	1	0.4
(1,3717)	2:B:729:LYS:HE3	2:B:729:LYS:HA	15	0.4
(1,285)	1:A:975:GLY:HA3	1:A:977:LEU:H	11	0.4
(1,2838)	1:A:997:ARG:H	1:A:997:ARG:HG3	13	0.4
(1,2789)	1:A:994:LYS:H	1:A:994:LYS:HB3	20	0.4
(1,2722)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	15	0.4
(1,2722)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	15	0.4
(1,2722)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	15	0.4
(1,2722)	1:A:990:VAL:HG11	1:A:992:PHE:HB3	17	0.4
(1,2722)	1:A:990:VAL:HG12	1:A:992:PHE:HB3	17	0.4
(1,2722)	1:A:990:VAL:HG13	1:A:992:PHE:HB3	17	0.4
(1,2599)	1:A:986:ALA:HA	1:A:988:TRP:H	1	0.4

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2599)	1:A:986:ALA:HA	1:A:988:TRP:H	16	0.4
(1,2368)	1:A:975:GLY:HA3	1:A:977:LEU:H	11	0.4
(1,2282)	1:A:970:LEU:HB2	1:A:971:VAL:H	5	0.4
(1,2282)	1:A:970:LEU:HB2	1:A:971:VAL:H	9	0.4
(1,2282)	1:A:970:LEU:HB2	1:A:971:VAL:H	15	0.4
(1,2282)	1:A:970:LEU:HB2	1:A:971:VAL:H	16	0.4
(1,2224)	1:A:968:TRP:HB2	1:A:969:VAL:H	11	0.4
(1,2071)	1:A:988:TRP:H	2:B:712:LEU:HD11	1	0.4
(1,2071)	1:A:988:TRP:H	2:B:712:LEU:HD12	1	0.4
(1,2071)	1:A:988:TRP:H	2:B:712:LEU:HD13	1	0.4
(1,199)	1:A:970:LEU:HB2	1:A:971:VAL:H	5	0.4
(1,199)	1:A:970:LEU:HB2	1:A:971:VAL:H	9	0.4
(1,199)	1:A:970:LEU:HB2	1:A:971:VAL:H	15	0.4
(1,199)	1:A:970:LEU:HB2	1:A:971:VAL:H	16	0.4
(1,1634)	2:B:729:LYS:HE3	2:B:729:LYS:HA	15	0.4
(1,141)	1:A:968:TRP:HB2	1:A:969:VAL:H	11	0.4
(1,849)	2:B:692:ASP:HB3	2:B:693:ILE:H	14	0.39
(1,755)	1:A:997:ARG:H	1:A:997:ARG:HG3	16	0.39
(1,750)	1:A:996:ASN:HA	1:A:997:ARG:H	10	0.39
(1,737)	1:A:995:ARG:HB3	1:A:996:ASN:H	16	0.39
(1,689)	1:A:993:PHE:HA	1:A:994:LYS:H	5	0.39
(1,689)	1:A:993:PHE:HA	1:A:994:LYS:H	14	0.39
(1,539)	1:A:987:MET:HB3	1:A:988:TRP:H	3	0.39
(1,478)	1:A:985:LEU:HB3	1:A:986:ALA:HA	7	0.39
(1,4029)	2:B:754:PHE:H	2:B:754:PHE:HB3	17	0.39
(1,3998)	2:B:749:GLU:H	2:B:749:GLU:HB3	6	0.39
(1,3713)	2:B:729:LYS:H	2:B:729:LYS:HB3	1	0.39
(1,3713)	2:B:729:LYS:H	2:B:729:LYS:HB3	2	0.39
(1,3713)	2:B:729:LYS:H	2:B:729:LYS:HB3	5	0.39
(1,3713)	2:B:729:LYS:H	2:B:729:LYS:HB3	6	0.39
(1,3713)	2:B:729:LYS:H	2:B:729:LYS:HB3	11	0.39
(1,3713)	2:B:729:LYS:H	2:B:729:LYS:HB3	15	0.39
(1,3713)	2:B:729:LYS:H	2:B:729:LYS:HB3	16	0.39
(1,3303)	2:B:708:GLY:H	2:B:710:ALA:H	12	0.39
(1,2932)	2:B:692:ASP:HB3	2:B:693:ILE:H	14	0.39
(1,285)	1:A:975:GLY:HA3	1:A:977:LEU:H	1	0.39
(1,285)	1:A:975:GLY:HA3	1:A:977:LEU:H	18	0.39
(1,2838)	1:A:997:ARG:H	1:A:997:ARG:HG3	16	0.39
(1,2833)	1:A:996:ASN:HA	1:A:997:ARG:H	10	0.39
(1,2820)	1:A:995:ARG:HB3	1:A:996:ASN:H	16	0.39
(1,2772)	1:A:993:PHE:HA	1:A:994:LYS:H	5	0.39
(1,2772)	1:A:993:PHE:HA	1:A:994:LYS:H	14	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2622)	1:A:987:MET:HB3	1:A:988:TRP:H	3	0.39
(1,2561)	1:A:985:LEU:HB3	1:A:986:ALA:HA	7	0.39
(1,2368)	1:A:975:GLY:HA3	1:A:977:LEU:H	1	0.39
(1,2368)	1:A:975:GLY:HA3	1:A:977:LEU:H	18	0.39
(1,2282)	1:A:970:LEU:HB2	1:A:971:VAL:H	3	0.39
(1,199)	1:A:970:LEU:HB2	1:A:971:VAL:H	3	0.39
(1,1946)	2:B:754:PHE:H	2:B:754:PHE:HB3	17	0.39
(1,1915)	2:B:749:GLU:H	2:B:749:GLU:HB3	6	0.39
(1,1630)	2:B:729:LYS:H	2:B:729:LYS:HB3	1	0.39
(1,1630)	2:B:729:LYS:H	2:B:729:LYS:HB3	2	0.39
(1,1630)	2:B:729:LYS:H	2:B:729:LYS:HB3	5	0.39
(1,1630)	2:B:729:LYS:H	2:B:729:LYS:HB3	6	0.39
(1,1630)	2:B:729:LYS:H	2:B:729:LYS:HB3	11	0.39
(1,1630)	2:B:729:LYS:H	2:B:729:LYS:HB3	15	0.39
(1,1630)	2:B:729:LYS:H	2:B:729:LYS:HB3	16	0.39
(1,1220)	2:B:708:GLY:H	2:B:710:ALA:H	12	0.39
(1,870)	2:B:693:ILE:H	2:B:693:ILE:HB	9	0.38
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD11	13	0.38
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD12	13	0.38
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD13	13	0.38
(1,755)	1:A:997:ARG:H	1:A:997:ARG:HG3	14	0.38
(1,737)	1:A:995:ARG:HB3	1:A:996:ASN:H	5	0.38
(1,706)	1:A:994:LYS:H	1:A:994:LYS:HB3	5	0.38
(1,689)	1:A:993:PHE:HA	1:A:994:LYS:H	13	0.38
(1,689)	1:A:993:PHE:HA	1:A:994:LYS:H	17	0.38
(1,478)	1:A:985:LEU:HB3	1:A:986:ALA:HA	4	0.38
(1,478)	1:A:985:LEU:HB3	1:A:986:ALA:HA	12	0.38
(1,4161)	1:A:988:TRP:H	2:B:719:ILE:HG12	12	0.38
(1,3717)	2:B:729:LYS:HE3	2:B:729:LYS:HA	2	0.38
(1,3713)	2:B:729:LYS:H	2:B:729:LYS:HB3	3	0.38
(1,3713)	2:B:729:LYS:H	2:B:729:LYS:HB3	7	0.38
(1,3713)	2:B:729:LYS:H	2:B:729:LYS:HB3	10	0.38
(1,3713)	2:B:729:LYS:H	2:B:729:LYS:HB3	12	0.38
(1,3713)	2:B:729:LYS:H	2:B:729:LYS:HB3	13	0.38
(1,3713)	2:B:729:LYS:H	2:B:729:LYS:HB3	14	0.38
(1,3713)	2:B:729:LYS:H	2:B:729:LYS:HB3	18	0.38
(1,3713)	2:B:729:LYS:H	2:B:729:LYS:HB3	20	0.38
(1,2953)	2:B:693:ILE:H	2:B:693:ILE:HB	9	0.38
(1,285)	1:A:975:GLY:HA3	1:A:977:LEU:H	15	0.38
(1,2838)	1:A:997:ARG:H	1:A:997:ARG:HG3	14	0.38
(1,2820)	1:A:995:ARG:HB3	1:A:996:ASN:H	5	0.38
(1,2789)	1:A:994:LYS:H	1:A:994:LYS:HB3	5	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2772)	1:A:993:PHE:HA	1:A:994:LYS:H	13	0.38
(1,2772)	1:A:993:PHE:HA	1:A:994:LYS:H	17	0.38
(1,2561)	1:A:985:LEU:HB3	1:A:986:ALA:HA	4	0.38
(1,2561)	1:A:985:LEU:HB3	1:A:986:ALA:HA	12	0.38
(1,2368)	1:A:975:GLY:HA3	1:A:977:LEU:H	15	0.38
(1,2282)	1:A:970:LEU:HB2	1:A:971:VAL:H	4	0.38
(1,2282)	1:A:970:LEU:HB2	1:A:971:VAL:H	11	0.38
(1,2224)	1:A:968:TRP:HB2	1:A:969:VAL:H	9	0.38
(1,2219)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	11	0.38
(1,2196)	1:A:967:TRP:H	1:A:968:TRP:HA	18	0.38
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD11	13	0.38
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD12	13	0.38
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD13	13	0.38
(1,2078)	1:A:988:TRP:H	2:B:719:ILE:HG12	12	0.38
(1,199)	1:A:970:LEU:HB2	1:A:971:VAL:H	4	0.38
(1,199)	1:A:970:LEU:HB2	1:A:971:VAL:H	11	0.38
(1,1634)	2:B:729:LYS:HE3	2:B:729:LYS:HA	2	0.38
(1,1630)	2:B:729:LYS:H	2:B:729:LYS:HB3	3	0.38
(1,1630)	2:B:729:LYS:H	2:B:729:LYS:HB3	7	0.38
(1,1630)	2:B:729:LYS:H	2:B:729:LYS:HB3	10	0.38
(1,1630)	2:B:729:LYS:H	2:B:729:LYS:HB3	12	0.38
(1,1630)	2:B:729:LYS:H	2:B:729:LYS:HB3	13	0.38
(1,1630)	2:B:729:LYS:H	2:B:729:LYS:HB3	14	0.38
(1,1630)	2:B:729:LYS:H	2:B:729:LYS:HB3	18	0.38
(1,1630)	2:B:729:LYS:H	2:B:729:LYS:HB3	20	0.38
(1,141)	1:A:968:TRP:HB2	1:A:969:VAL:H	9	0.38
(1,136)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	11	0.38
(1,113)	1:A:967:TRP:H	1:A:968:TRP:HA	18	0.38
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD11	19	0.37
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD12	19	0.37
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD13	19	0.37
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD11	20	0.37
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD12	20	0.37
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD13	20	0.37
(1,778)	1:A:1000:LEU:H	1:A:1000:LEU:HB3	1	0.37
(1,762)	1:A:997:ARG:HA	1:A:999:PRO:HD2	7	0.37
(1,761)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	18	0.37
(1,743)	1:A:996:ASN:H	1:A:996:ASN:HB3	3	0.37
(1,743)	1:A:996:ASN:H	1:A:996:ASN:HB3	12	0.37
(1,706)	1:A:994:LYS:H	1:A:994:LYS:HB3	18	0.37
(1,602)	1:A:989:LYS:HA	1:A:991:GLY:H	9	0.37
(1,547)	1:A:987:MET:HG3	1:A:989:LYS:H	4	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,516)	1:A:986:ALA:HA	1:A:988:TRP:H	8	0.37
(1,478)	1:A:985:LEU:HB3	1:A:986:ALA:HA	2	0.37
(1,478)	1:A:985:LEU:HB3	1:A:986:ALA:HA	6	0.37
(1,478)	1:A:985:LEU:HB3	1:A:986:ALA:HA	20	0.37
(1,460)	1:A:984:VAL:HA	1:A:988:TRP:HB3	19	0.37
(1,3945)	2:B:745:PRO:HA	2:B:746:LEU:H	20	0.37
(1,3713)	2:B:729:LYS:H	2:B:729:LYS:HB3	8	0.37
(1,3713)	2:B:729:LYS:H	2:B:729:LYS:HB3	9	0.37
(1,3713)	2:B:729:LYS:H	2:B:729:LYS:HB3	17	0.37
(1,3713)	2:B:729:LYS:H	2:B:729:LYS:HB3	19	0.37
(1,2861)	1:A:1000:LEU:H	1:A:1000:LEU:HB3	1	0.37
(1,285)	1:A:975:GLY:HA3	1:A:977:LEU:H	3	0.37
(1,285)	1:A:975:GLY:HA3	1:A:977:LEU:H	20	0.37
(1,2845)	1:A:997:ARG:HA	1:A:999:PRO:HD2	7	0.37
(1,2844)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	18	0.37
(1,2826)	1:A:996:ASN:H	1:A:996:ASN:HB3	3	0.37
(1,2826)	1:A:996:ASN:H	1:A:996:ASN:HB3	12	0.37
(1,2789)	1:A:994:LYS:H	1:A:994:LYS:HB3	18	0.37
(1,2685)	1:A:989:LYS:HA	1:A:991:GLY:H	9	0.37
(1,2630)	1:A:987:MET:HG3	1:A:989:LYS:H	4	0.37
(1,2599)	1:A:986:ALA:HA	1:A:988:TRP:H	8	0.37
(1,2561)	1:A:985:LEU:HB3	1:A:986:ALA:HA	2	0.37
(1,2561)	1:A:985:LEU:HB3	1:A:986:ALA:HA	6	0.37
(1,2561)	1:A:985:LEU:HB3	1:A:986:ALA:HA	20	0.37
(1,2543)	1:A:984:VAL:HA	1:A:988:TRP:HB3	19	0.37
(1,2368)	1:A:975:GLY:HA3	1:A:977:LEU:H	3	0.37
(1,2368)	1:A:975:GLY:HA3	1:A:977:LEU:H	20	0.37
(1,2282)	1:A:970:LEU:HB2	1:A:971:VAL:H	6	0.37
(1,2282)	1:A:970:LEU:HB2	1:A:971:VAL:H	18	0.37
(1,2224)	1:A:968:TRP:HB2	1:A:969:VAL:H	4	0.37
(1,2224)	1:A:968:TRP:HB2	1:A:969:VAL:H	16	0.37
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD11	19	0.37
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD12	19	0.37
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD13	19	0.37
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD11	20	0.37
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD12	20	0.37
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD13	20	0.37
(1,199)	1:A:970:LEU:HB2	1:A:971:VAL:H	6	0.37
(1,199)	1:A:970:LEU:HB2	1:A:971:VAL:H	18	0.37
(1,1862)	2:B:745:PRO:HA	2:B:746:LEU:H	20	0.37
(1,1630)	2:B:729:LYS:H	2:B:729:LYS:HB3	8	0.37
(1,1630)	2:B:729:LYS:H	2:B:729:LYS:HB3	9	0.37

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1630)	2:B:729:LYS:H	2:B:729:LYS:HB3	17	0.37
(1,1630)	2:B:729:LYS:H	2:B:729:LYS:HB3	19	0.37
(1,141)	1:A:968:TRP:HB2	1:A:969:VAL:H	4	0.37
(1,141)	1:A:968:TRP:HB2	1:A:969:VAL:H	16	0.37
(1,870)	2:B:693:ILE:H	2:B:693:ILE:HB	17	0.36
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD11	5	0.36
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD12	5	0.36
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD13	5	0.36
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD11	12	0.36
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD12	12	0.36
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD13	12	0.36
(1,762)	1:A:997:ARG:HA	1:A:999:PRO:HD2	1	0.36
(1,755)	1:A:997:ARG:H	1:A:997:ARG:HG3	6	0.36
(1,743)	1:A:996:ASN:H	1:A:996:ASN:HB3	2	0.36
(1,743)	1:A:996:ASN:H	1:A:996:ASN:HB3	9	0.36
(1,743)	1:A:996:ASN:H	1:A:996:ASN:HB3	19	0.36
(1,741)	1:A:995:ARG:HB3	1:A:997:ARG:H	4	0.36
(1,706)	1:A:994:LYS:H	1:A:994:LYS:HB3	6	0.36
(1,706)	1:A:994:LYS:H	1:A:994:LYS:HB3	13	0.36
(1,689)	1:A:993:PHE:HA	1:A:994:LYS:H	1	0.36
(1,577)	1:A:989:LYS:H	1:A:989:LYS:HB3	6	0.36
(1,577)	1:A:989:LYS:H	1:A:989:LYS:HB3	11	0.36
(1,577)	1:A:989:LYS:H	1:A:989:LYS:HB3	15	0.36
(1,547)	1:A:987:MET:HG3	1:A:989:LYS:H	19	0.36
(1,539)	1:A:987:MET:HB3	1:A:988:TRP:H	1	0.36
(1,478)	1:A:985:LEU:HB3	1:A:986:ALA:HA	5	0.36
(1,478)	1:A:985:LEU:HB3	1:A:986:ALA:HA	9	0.36
(1,478)	1:A:985:LEU:HB3	1:A:986:ALA:HA	10	0.36
(1,478)	1:A:985:LEU:HB3	1:A:986:ALA:HA	14	0.36
(1,478)	1:A:985:LEU:HB3	1:A:986:ALA:HA	16	0.36
(1,460)	1:A:984:VAL:HA	1:A:988:TRP:HB3	10	0.36
(1,416)	1:A:983:LEU:HB2	1:A:984:VAL:H	11	0.36
(1,4130)	1:A:979:LEU:H	2:B:704:ILE:HB	5	0.36
(1,4034)	2:B:755:THR:H	2:B:755:THR:HB	17	0.36
(1,3945)	2:B:745:PRO:HA	2:B:746:LEU:H	7	0.36
(1,3713)	2:B:729:LYS:H	2:B:729:LYS:HB3	4	0.36
(1,3470)	2:B:717:LEU:H	2:B:719:ILE:H	18	0.36
(1,2953)	2:B:693:ILE:H	2:B:693:ILE:HB	17	0.36
(1,285)	1:A:975:GLY:HA3	1:A:977:LEU:H	4	0.36
(1,2845)	1:A:997:ARG:HA	1:A:999:PRO:HD2	1	0.36
(1,2838)	1:A:997:ARG:H	1:A:997:ARG:HG3	6	0.36
(1,2826)	1:A:996:ASN:H	1:A:996:ASN:HB3	2	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2826)	1:A:996:ASN:H	1:A:996:ASN:HB3	9	0.36
(1,2826)	1:A:996:ASN:H	1:A:996:ASN:HB3	19	0.36
(1,2824)	1:A:995:ARG:HB3	1:A:997:ARG:H	4	0.36
(1,2789)	1:A:994:LYS:H	1:A:994:LYS:HB3	6	0.36
(1,2789)	1:A:994:LYS:H	1:A:994:LYS:HB3	13	0.36
(1,2772)	1:A:993:PHE:HA	1:A:994:LYS:H	1	0.36
(1,2660)	1:A:989:LYS:H	1:A:989:LYS:HB3	6	0.36
(1,2660)	1:A:989:LYS:H	1:A:989:LYS:HB3	11	0.36
(1,2660)	1:A:989:LYS:H	1:A:989:LYS:HB3	15	0.36
(1,2630)	1:A:987:MET:HG3	1:A:989:LYS:H	19	0.36
(1,2622)	1:A:987:MET:HB3	1:A:988:TRP:H	1	0.36
(1,2561)	1:A:985:LEU:HB3	1:A:986:ALA:HA	5	0.36
(1,2561)	1:A:985:LEU:HB3	1:A:986:ALA:HA	9	0.36
(1,2561)	1:A:985:LEU:HB3	1:A:986:ALA:HA	10	0.36
(1,2561)	1:A:985:LEU:HB3	1:A:986:ALA:HA	14	0.36
(1,2561)	1:A:985:LEU:HB3	1:A:986:ALA:HA	16	0.36
(1,2543)	1:A:984:VAL:HA	1:A:988:TRP:HB3	10	0.36
(1,2499)	1:A:983:LEU:HB2	1:A:984:VAL:H	11	0.36
(1,2368)	1:A:975:GLY:HA3	1:A:977:LEU:H	4	0.36
(1,2224)	1:A:968:TRP:HB2	1:A:969:VAL:H	3	0.36
(1,2196)	1:A:967:TRP:H	1:A:968:TRP:HA	1	0.36
(1,2196)	1:A:967:TRP:H	1:A:968:TRP:HA	3	0.36
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD11	5	0.36
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD12	5	0.36
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD13	5	0.36
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD11	12	0.36
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD12	12	0.36
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD13	12	0.36
(1,2047)	1:A:979:LEU:H	2:B:704:ILE:HB	5	0.36
(1,1951)	2:B:755:THR:H	2:B:755:THR:HB	17	0.36
(1,1862)	2:B:745:PRO:HA	2:B:746:LEU:H	7	0.36
(1,1630)	2:B:729:LYS:H	2:B:729:LYS:HB3	4	0.36
(1,141)	1:A:968:TRP:HB2	1:A:969:VAL:H	3	0.36
(1,1387)	2:B:717:LEU:H	2:B:719:ILE:H	18	0.36
(1,113)	1:A:967:TRP:H	1:A:968:TRP:HA	1	0.36
(1,113)	1:A:967:TRP:H	1:A:968:TRP:HA	3	0.36
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD11	7	0.35
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD12	7	0.35
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD13	7	0.35
(1,743)	1:A:996:ASN:H	1:A:996:ASN:HB3	7	0.35
(1,743)	1:A:996:ASN:H	1:A:996:ASN:HB3	8	0.35
(1,743)	1:A:996:ASN:H	1:A:996:ASN:HB3	15	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,738)	1:A:995:ARG:HA	1:A:996:ASN:H	15	0.35
(1,737)	1:A:995:ARG:HB3	1:A:996:ASN:H	1	0.35
(1,725)	1:A:994:LYS:HB3	1:A:995:ARG:HG3	17	0.35
(1,706)	1:A:994:LYS:H	1:A:994:LYS:HB3	11	0.35
(1,706)	1:A:994:LYS:H	1:A:994:LYS:HB3	14	0.35
(1,624)	1:A:990:VAL:HB	1:A:991:GLY:H	10	0.35
(1,577)	1:A:989:LYS:H	1:A:989:LYS:HB3	5	0.35
(1,539)	1:A:987:MET:HB3	1:A:988:TRP:H	17	0.35
(1,478)	1:A:985:LEU:HB3	1:A:986:ALA:HA	17	0.35
(1,478)	1:A:985:LEU:HB3	1:A:986:ALA:HA	19	0.35
(1,4130)	1:A:979:LEU:H	2:B:704:ILE:HB	12	0.35
(1,4034)	2:B:755:THR:H	2:B:755:THR:HB	11	0.35
(1,3684)	2:B:726:GLU:HA	2:B:729:LYS:HB3	16	0.35
(1,285)	1:A:975:GLY:HA3	1:A:977:LEU:H	10	0.35
(1,285)	1:A:975:GLY:HA3	1:A:977:LEU:H	16	0.35
(1,285)	1:A:975:GLY:HA3	1:A:977:LEU:H	17	0.35
(1,2826)	1:A:996:ASN:H	1:A:996:ASN:HB3	7	0.35
(1,2826)	1:A:996:ASN:H	1:A:996:ASN:HB3	8	0.35
(1,2826)	1:A:996:ASN:H	1:A:996:ASN:HB3	15	0.35
(1,2821)	1:A:995:ARG:HA	1:A:996:ASN:H	15	0.35
(1,2820)	1:A:995:ARG:HB3	1:A:996:ASN:H	1	0.35
(1,2808)	1:A:994:LYS:HB3	1:A:995:ARG:HG3	17	0.35
(1,2789)	1:A:994:LYS:H	1:A:994:LYS:HB3	11	0.35
(1,2789)	1:A:994:LYS:H	1:A:994:LYS:HB3	14	0.35
(1,2707)	1:A:990:VAL:HB	1:A:991:GLY:H	10	0.35
(1,2660)	1:A:989:LYS:H	1:A:989:LYS:HB3	5	0.35
(1,2622)	1:A:987:MET:HB3	1:A:988:TRP:H	17	0.35
(1,2561)	1:A:985:LEU:HB3	1:A:986:ALA:HA	17	0.35
(1,2561)	1:A:985:LEU:HB3	1:A:986:ALA:HA	19	0.35
(1,2368)	1:A:975:GLY:HA3	1:A:977:LEU:H	10	0.35
(1,2368)	1:A:975:GLY:HA3	1:A:977:LEU:H	16	0.35
(1,2368)	1:A:975:GLY:HA3	1:A:977:LEU:H	17	0.35
(1,2278)	1:A:970:LEU:HD11	1:A:970:LEU:HA	19	0.35
(1,2278)	1:A:970:LEU:HD12	1:A:970:LEU:HA	19	0.35
(1,2278)	1:A:970:LEU:HD13	1:A:970:LEU:HA	19	0.35
(1,2224)	1:A:968:TRP:HB2	1:A:969:VAL:H	8	0.35
(1,2224)	1:A:968:TRP:HB2	1:A:969:VAL:H	18	0.35
(1,2219)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	4	0.35
(1,2196)	1:A:967:TRP:H	1:A:968:TRP:HA	12	0.35
(1,2196)	1:A:967:TRP:H	1:A:968:TRP:HA	15	0.35
(1,2196)	1:A:967:TRP:H	1:A:968:TRP:HA	16	0.35
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD11	7	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD12	7	0.35
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD13	7	0.35
(1,2047)	1:A:979:LEU:H	2:B:704:ILE:HB	12	0.35
(1,1951)	2:B:755:THR:H	2:B:755:THR:HB	11	0.35
(1,195)	1:A:970:LEU:HD11	1:A:970:LEU:HA	19	0.35
(1,195)	1:A:970:LEU:HD12	1:A:970:LEU:HA	19	0.35
(1,195)	1:A:970:LEU:HD13	1:A:970:LEU:HA	19	0.35
(1,1601)	2:B:726:GLU:HA	2:B:729:LYS:HB3	16	0.35
(1,141)	1:A:968:TRP:HB2	1:A:969:VAL:H	8	0.35
(1,141)	1:A:968:TRP:HB2	1:A:969:VAL:H	18	0.35
(1,136)	1:A:968:TRP:HB3	1:A:968:TRP:HZ3	4	0.35
(1,113)	1:A:967:TRP:H	1:A:968:TRP:HA	12	0.35
(1,113)	1:A:967:TRP:H	1:A:968:TRP:HA	15	0.35
(1,113)	1:A:967:TRP:H	1:A:968:TRP:HA	16	0.35
(1,843)	2:B:691:PRO:HB3	2:B:692:ASP:H	6	0.34
(1,843)	2:B:691:PRO:HB3	2:B:692:ASP:H	7	0.34
(1,843)	2:B:691:PRO:HB3	2:B:692:ASP:H	10	0.34
(1,843)	2:B:691:PRO:HB3	2:B:692:ASP:H	12	0.34
(1,83)	1:A:966:ILE:H	1:A:966:ILE:HG12	15	0.34
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD11	1	0.34
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD12	1	0.34
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD13	1	0.34
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD11	8	0.34
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD12	8	0.34
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD13	8	0.34
(1,738)	1:A:995:ARG:HA	1:A:996:ASN:H	7	0.34
(1,706)	1:A:994:LYS:H	1:A:994:LYS:HB3	8	0.34
(1,706)	1:A:994:LYS:H	1:A:994:LYS:HB3	16	0.34
(1,602)	1:A:989:LYS:HA	1:A:991:GLY:H	14	0.34
(1,577)	1:A:989:LYS:H	1:A:989:LYS:HB3	8	0.34
(1,577)	1:A:989:LYS:H	1:A:989:LYS:HB3	16	0.34
(1,547)	1:A:987:MET:HG3	1:A:989:LYS:H	2	0.34
(1,547)	1:A:987:MET:HG3	1:A:989:LYS:H	6	0.34
(1,547)	1:A:987:MET:HG3	1:A:989:LYS:H	7	0.34
(1,539)	1:A:987:MET:HB3	1:A:988:TRP:H	5	0.34
(1,539)	1:A:987:MET:HB3	1:A:988:TRP:H	14	0.34
(1,539)	1:A:987:MET:HB3	1:A:988:TRP:H	15	0.34
(1,539)	1:A:987:MET:HB3	1:A:988:TRP:H	19	0.34
(1,539)	1:A:987:MET:HB3	1:A:988:TRP:H	20	0.34
(1,489)	1:A:985:LEU:HA	1:A:988:TRP:H	16	0.34
(1,478)	1:A:985:LEU:HB3	1:A:986:ALA:HA	3	0.34
(1,478)	1:A:985:LEU:HB3	1:A:986:ALA:HA	8	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,478)	1:A:985:LEU:HB3	1:A:986:ALA:HA	13	0.34
(1,478)	1:A:985:LEU:HB3	1:A:986:ALA:HA	15	0.34
(1,478)	1:A:985:LEU:HB3	1:A:986:ALA:HA	18	0.34
(1,460)	1:A:984:VAL:HA	1:A:988:TRP:HB3	9	0.34
(1,4161)	1:A:988:TRP:H	2:B:719:ILE:HG12	16	0.34
(1,416)	1:A:983:LEU:HB2	1:A:984:VAL:H	2	0.34
(1,416)	1:A:983:LEU:HB2	1:A:984:VAL:H	10	0.34
(1,416)	1:A:983:LEU:HB2	1:A:984:VAL:H	13	0.34
(1,4143)	1:A:984:VAL:H	2:B:712:LEU:HA	18	0.34
(1,4130)	1:A:979:LEU:H	2:B:704:ILE:HB	4	0.34
(1,3973)	2:B:747:TYR:HB2	2:B:748:LYS:H	19	0.34
(1,2926)	2:B:691:PRO:HB3	2:B:692:ASP:H	6	0.34
(1,2926)	2:B:691:PRO:HB3	2:B:692:ASP:H	7	0.34
(1,2926)	2:B:691:PRO:HB3	2:B:692:ASP:H	10	0.34
(1,2926)	2:B:691:PRO:HB3	2:B:692:ASP:H	12	0.34
(1,2821)	1:A:995:ARG:HA	1:A:996:ASN:H	7	0.34
(1,2789)	1:A:994:LYS:H	1:A:994:LYS:HB3	8	0.34
(1,2789)	1:A:994:LYS:H	1:A:994:LYS:HB3	16	0.34
(1,2685)	1:A:989:LYS:HA	1:A:991:GLY:H	14	0.34
(1,2660)	1:A:989:LYS:H	1:A:989:LYS:HB3	8	0.34
(1,2660)	1:A:989:LYS:H	1:A:989:LYS:HB3	16	0.34
(1,2630)	1:A:987:MET:HG3	1:A:989:LYS:H	2	0.34
(1,2630)	1:A:987:MET:HG3	1:A:989:LYS:H	6	0.34
(1,2630)	1:A:987:MET:HG3	1:A:989:LYS:H	7	0.34
(1,2622)	1:A:987:MET:HB3	1:A:988:TRP:H	5	0.34
(1,2622)	1:A:987:MET:HB3	1:A:988:TRP:H	14	0.34
(1,2622)	1:A:987:MET:HB3	1:A:988:TRP:H	15	0.34
(1,2622)	1:A:987:MET:HB3	1:A:988:TRP:H	19	0.34
(1,2622)	1:A:987:MET:HB3	1:A:988:TRP:H	20	0.34
(1,2572)	1:A:985:LEU:HA	1:A:988:TRP:H	16	0.34
(1,2561)	1:A:985:LEU:HB3	1:A:986:ALA:HA	3	0.34
(1,2561)	1:A:985:LEU:HB3	1:A:986:ALA:HA	8	0.34
(1,2561)	1:A:985:LEU:HB3	1:A:986:ALA:HA	13	0.34
(1,2561)	1:A:985:LEU:HB3	1:A:986:ALA:HA	15	0.34
(1,2561)	1:A:985:LEU:HB3	1:A:986:ALA:HA	18	0.34
(1,2543)	1:A:984:VAL:HA	1:A:988:TRP:HB3	9	0.34
(1,2499)	1:A:983:LEU:HB2	1:A:984:VAL:H	2	0.34
(1,2499)	1:A:983:LEU:HB2	1:A:984:VAL:H	10	0.34
(1,2499)	1:A:983:LEU:HB2	1:A:984:VAL:H	13	0.34
(1,2224)	1:A:968:TRP:HB2	1:A:969:VAL:H	13	0.34
(1,2224)	1:A:968:TRP:HB2	1:A:969:VAL:H	14	0.34
(1,2201)	1:A:967:TRP:HA	1:A:968:TRP:HB3	6	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2196)	1:A:967:TRP:H	1:A:968:TRP:HA	9	0.34
(1,2196)	1:A:967:TRP:H	1:A:968:TRP:HA	11	0.34
(1,2196)	1:A:967:TRP:H	1:A:968:TRP:HA	13	0.34
(1,2196)	1:A:967:TRP:H	1:A:968:TRP:HA	19	0.34
(1,2166)	1:A:966:ILE:H	1:A:966:ILE:HG12	15	0.34
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD11	1	0.34
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD12	1	0.34
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD13	1	0.34
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD11	8	0.34
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD12	8	0.34
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD13	8	0.34
(1,2078)	1:A:988:TRP:H	2:B:719:ILE:HG12	16	0.34
(1,2060)	1:A:984:VAL:H	2:B:712:LEU:HA	18	0.34
(1,2047)	1:A:979:LEU:H	2:B:704:ILE:HB	4	0.34
(1,1890)	2:B:747:TYR:HB2	2:B:748:LYS:H	19	0.34
(1,141)	1:A:968:TRP:HB2	1:A:969:VAL:H	13	0.34
(1,141)	1:A:968:TRP:HB2	1:A:969:VAL:H	14	0.34
(1,118)	1:A:967:TRP:HA	1:A:968:TRP:HB3	6	0.34
(1,113)	1:A:967:TRP:H	1:A:968:TRP:HA	9	0.34
(1,113)	1:A:967:TRP:H	1:A:968:TRP:HA	11	0.34
(1,113)	1:A:967:TRP:H	1:A:968:TRP:HA	13	0.34
(1,113)	1:A:967:TRP:H	1:A:968:TRP:HA	19	0.34
(1,870)	2:B:693:ILE:H	2:B:693:ILE:HB	15	0.33
(1,843)	2:B:691:PRO:HB3	2:B:692:ASP:H	15	0.33
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD11	15	0.33
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD12	15	0.33
(1,79)	1:A:966:ILE:HA	1:A:966:ILE:HD13	15	0.33
(1,755)	1:A:997:ARG:H	1:A:997:ARG:HG3	8	0.33
(1,706)	1:A:994:LYS:H	1:A:994:LYS:HB3	4	0.33
(1,706)	1:A:994:LYS:H	1:A:994:LYS:HB3	19	0.33
(1,624)	1:A:990:VAL:HB	1:A:991:GLY:H	18	0.33
(1,602)	1:A:989:LYS:HA	1:A:991:GLY:H	2	0.33
(1,602)	1:A:989:LYS:HA	1:A:991:GLY:H	7	0.33
(1,602)	1:A:989:LYS:HA	1:A:991:GLY:H	13	0.33
(1,602)	1:A:989:LYS:HA	1:A:991:GLY:H	17	0.33
(1,590)	1:A:989:LYS:HB2	1:A:990:VAL:H	18	0.33
(1,577)	1:A:989:LYS:H	1:A:989:LYS:HB3	10	0.33
(1,547)	1:A:987:MET:HG3	1:A:989:LYS:H	20	0.33
(1,539)	1:A:987:MET:HB3	1:A:988:TRP:H	4	0.33
(1,539)	1:A:987:MET:HB3	1:A:988:TRP:H	9	0.33
(1,539)	1:A:987:MET:HB3	1:A:988:TRP:H	18	0.33
(1,516)	1:A:986:ALA:HA	1:A:988:TRP:H	11	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,516)	1:A:986:ALA:HA	1:A:988:TRP:H	18	0.33
(1,478)	1:A:985:LEU:HB3	1:A:986:ALA:HA	11	0.33
(1,460)	1:A:984:VAL:HA	1:A:988:TRP:HB3	2	0.33
(1,460)	1:A:984:VAL:HA	1:A:988:TRP:HB3	6	0.33
(1,4161)	1:A:988:TRP:H	2:B:719:ILE:HG12	1	0.33
(1,4161)	1:A:988:TRP:H	2:B:719:ILE:HG12	14	0.33
(1,416)	1:A:983:LEU:HB2	1:A:984:VAL:H	3	0.33
(1,416)	1:A:983:LEU:HB2	1:A:984:VAL:H	4	0.33
(1,416)	1:A:983:LEU:HB2	1:A:984:VAL:H	19	0.33
(1,4143)	1:A:984:VAL:H	2:B:712:LEU:HA	15	0.33
(1,4069)	2:B:759:TYR:H	2:B:759:TYR:HB3	19	0.33
(1,393)	1:A:982:ILE:H	1:A:984:VAL:H	17	0.33
(1,3860)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	7	0.33
(1,3684)	2:B:726:GLU:HA	2:B:729:LYS:HB3	7	0.33
(1,363)	1:A:981:THR:H	1:A:981:THR:HG21	10	0.33
(1,363)	1:A:981:THR:H	1:A:981:THR:HG22	10	0.33
(1,363)	1:A:981:THR:H	1:A:981:THR:HG23	10	0.33
(1,363)	1:A:981:THR:H	1:A:981:THR:HG21	12	0.33
(1,363)	1:A:981:THR:H	1:A:981:THR:HG22	12	0.33
(1,363)	1:A:981:THR:H	1:A:981:THR:HG23	12	0.33
(1,341)	1:A:979:LEU:HA	1:A:981:THR:H	16	0.33
(1,2953)	2:B:693:ILE:H	2:B:693:ILE:HB	15	0.33
(1,2926)	2:B:691:PRO:HB3	2:B:692:ASP:H	15	0.33
(1,2838)	1:A:997:ARG:H	1:A:997:ARG:HG3	8	0.33
(1,2789)	1:A:994:LYS:H	1:A:994:LYS:HB3	4	0.33
(1,2789)	1:A:994:LYS:H	1:A:994:LYS:HB3	19	0.33
(1,2707)	1:A:990:VAL:HB	1:A:991:GLY:H	18	0.33
(1,2685)	1:A:989:LYS:HA	1:A:991:GLY:H	2	0.33
(1,2685)	1:A:989:LYS:HA	1:A:991:GLY:H	7	0.33
(1,2685)	1:A:989:LYS:HA	1:A:991:GLY:H	13	0.33
(1,2685)	1:A:989:LYS:HA	1:A:991:GLY:H	17	0.33
(1,2673)	1:A:989:LYS:HB2	1:A:990:VAL:H	18	0.33
(1,2660)	1:A:989:LYS:H	1:A:989:LYS:HB3	10	0.33
(1,2630)	1:A:987:MET:HG3	1:A:989:LYS:H	20	0.33
(1,2622)	1:A:987:MET:HB3	1:A:988:TRP:H	4	0.33
(1,2622)	1:A:987:MET:HB3	1:A:988:TRP:H	9	0.33
(1,2622)	1:A:987:MET:HB3	1:A:988:TRP:H	18	0.33
(1,2599)	1:A:986:ALA:HA	1:A:988:TRP:H	11	0.33
(1,2599)	1:A:986:ALA:HA	1:A:988:TRP:H	18	0.33
(1,2561)	1:A:985:LEU:HB3	1:A:986:ALA:HA	11	0.33
(1,2543)	1:A:984:VAL:HA	1:A:988:TRP:HB3	2	0.33
(1,2543)	1:A:984:VAL:HA	1:A:988:TRP:HB3	6	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2499)	1:A:983:LEU:HB2	1:A:984:VAL:H	3	0.33
(1,2499)	1:A:983:LEU:HB2	1:A:984:VAL:H	4	0.33
(1,2499)	1:A:983:LEU:HB2	1:A:984:VAL:H	19	0.33
(1,2476)	1:A:982:ILE:H	1:A:984:VAL:H	17	0.33
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG21	10	0.33
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG22	10	0.33
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG23	10	0.33
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG21	12	0.33
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG22	12	0.33
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG23	12	0.33
(1,2424)	1:A:979:LEU:HA	1:A:981:THR:H	16	0.33
(1,2282)	1:A:970:LEU:HB2	1:A:971:VAL:H	1	0.33
(1,2224)	1:A:968:TRP:HB2	1:A:969:VAL:H	15	0.33
(1,2202)	1:A:967:TRP:HB2	1:A:968:TRP:H	3	0.33
(1,2196)	1:A:967:TRP:H	1:A:968:TRP:HA	5	0.33
(1,2196)	1:A:967:TRP:H	1:A:968:TRP:HA	17	0.33
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD11	15	0.33
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD12	15	0.33
(1,2162)	1:A:966:ILE:HA	1:A:966:ILE:HD13	15	0.33
(1,2078)	1:A:988:TRP:H	2:B:719:ILE:HG12	1	0.33
(1,2078)	1:A:988:TRP:H	2:B:719:ILE:HG12	14	0.33
(1,2060)	1:A:984:VAL:H	2:B:712:LEU:HA	15	0.33
(1,199)	1:A:970:LEU:HB2	1:A:971:VAL:H	1	0.33
(1,1986)	2:B:759:TYR:H	2:B:759:TYR:HB3	19	0.33
(1,1777)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	7	0.33
(1,1601)	2:B:726:GLU:HA	2:B:729:LYS:HB3	7	0.33
(1,141)	1:A:968:TRP:HB2	1:A:969:VAL:H	15	0.33
(1,119)	1:A:967:TRP:HB2	1:A:968:TRP:H	3	0.33
(1,113)	1:A:967:TRP:H	1:A:968:TRP:HA	5	0.33
(1,113)	1:A:967:TRP:H	1:A:968:TRP:HA	17	0.33
(1,83)	1:A:966:ILE:H	1:A:966:ILE:HG12	8	0.32
(1,811)	1:A:1006:GLU:H	1:A:1006:GLU:HB3	6	0.32
(1,803)	1:A:1004:ASP:HA	1:A:1005:GLU:H	2	0.32
(1,761)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	4	0.32
(1,706)	1:A:994:LYS:H	1:A:994:LYS:HB3	10	0.32
(1,706)	1:A:994:LYS:H	1:A:994:LYS:HB3	15	0.32
(1,602)	1:A:989:LYS:HA	1:A:991:GLY:H	8	0.32
(1,602)	1:A:989:LYS:HA	1:A:991:GLY:H	12	0.32
(1,577)	1:A:989:LYS:H	1:A:989:LYS:HB3	20	0.32
(1,547)	1:A:987:MET:HG3	1:A:989:LYS:H	9	0.32
(1,547)	1:A:987:MET:HG3	1:A:989:LYS:H	12	0.32
(1,547)	1:A:987:MET:HG3	1:A:989:LYS:H	14	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,547)	1:A:987:MET:HG3	1:A:989:LYS:H	17	0.32
(1,519)	1:A:986:ALA:HA	1:A:989:LYS:H	1	0.32
(1,519)	1:A:986:ALA:HA	1:A:989:LYS:H	3	0.32
(1,516)	1:A:986:ALA:HA	1:A:988:TRP:H	13	0.32
(1,499)	1:A:985:LEU:HA	1:A:989:LYS:H	14	0.32
(1,489)	1:A:985:LEU:HA	1:A:988:TRP:H	11	0.32
(1,489)	1:A:985:LEU:HA	1:A:988:TRP:H	15	0.32
(1,460)	1:A:984:VAL:HA	1:A:988:TRP:HB3	5	0.32
(1,45)	1:A:964:ILE:HB	1:A:965:PRO:HD3	9	0.32
(1,45)	1:A:964:ILE:HB	1:A:965:PRO:HD3	17	0.32
(1,4161)	1:A:988:TRP:H	2:B:719:ILE:HG12	4	0.32
(1,416)	1:A:983:LEU:HB2	1:A:984:VAL:H	6	0.32
(1,416)	1:A:983:LEU:HB2	1:A:984:VAL:H	7	0.32
(1,416)	1:A:983:LEU:HB2	1:A:984:VAL:H	8	0.32
(1,416)	1:A:983:LEU:HB2	1:A:984:VAL:H	16	0.32
(1,4130)	1:A:979:LEU:H	2:B:704:ILE:HB	3	0.32
(1,4130)	1:A:979:LEU:H	2:B:704:ILE:HB	15	0.32
(1,3893)	2:B:741:THR:HA	2:B:742:ALA:H	7	0.32
(1,3882)	2:B:739:TRP:HB2	2:B:740:ASP:H	12	0.32
(1,3852)	2:B:738:LYS:H	2:B:738:LYS:HG3	9	0.32
(1,3684)	2:B:726:GLU:HA	2:B:729:LYS:HB3	4	0.32
(1,3303)	2:B:708:GLY:H	2:B:710:ALA:H	6	0.32
(1,2894)	1:A:1006:GLU:H	1:A:1006:GLU:HB3	6	0.32
(1,2886)	1:A:1004:ASP:HA	1:A:1005:GLU:H	2	0.32
(1,285)	1:A:975:GLY:HA3	1:A:977:LEU:H	8	0.32
(1,285)	1:A:975:GLY:HA3	1:A:977:LEU:H	13	0.32
(1,2844)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	4	0.32
(1,2789)	1:A:994:LYS:H	1:A:994:LYS:HB3	10	0.32
(1,2789)	1:A:994:LYS:H	1:A:994:LYS:HB3	15	0.32
(1,2685)	1:A:989:LYS:HA	1:A:991:GLY:H	8	0.32
(1,2685)	1:A:989:LYS:HA	1:A:991:GLY:H	12	0.32
(1,2660)	1:A:989:LYS:H	1:A:989:LYS:HB3	20	0.32
(1,2630)	1:A:987:MET:HG3	1:A:989:LYS:H	9	0.32
(1,2630)	1:A:987:MET:HG3	1:A:989:LYS:H	12	0.32
(1,2630)	1:A:987:MET:HG3	1:A:989:LYS:H	14	0.32
(1,2630)	1:A:987:MET:HG3	1:A:989:LYS:H	17	0.32
(1,2602)	1:A:986:ALA:HA	1:A:989:LYS:H	1	0.32
(1,2602)	1:A:986:ALA:HA	1:A:989:LYS:H	3	0.32
(1,2599)	1:A:986:ALA:HA	1:A:988:TRP:H	13	0.32
(1,2582)	1:A:985:LEU:HA	1:A:989:LYS:H	14	0.32
(1,2572)	1:A:985:LEU:HA	1:A:988:TRP:H	11	0.32
(1,2572)	1:A:985:LEU:HA	1:A:988:TRP:H	15	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2543)	1:A:984:VAL:HA	1:A:988:TRP:HB3	5	0.32
(1,2499)	1:A:983:LEU:HB2	1:A:984:VAL:H	6	0.32
(1,2499)	1:A:983:LEU:HB2	1:A:984:VAL:H	7	0.32
(1,2499)	1:A:983:LEU:HB2	1:A:984:VAL:H	8	0.32
(1,2499)	1:A:983:LEU:HB2	1:A:984:VAL:H	16	0.32
(1,2368)	1:A:975:GLY:HA3	1:A:977:LEU:H	8	0.32
(1,2368)	1:A:975:GLY:HA3	1:A:977:LEU:H	13	0.32
(1,2298)	1:A:971:VAL:HA	1:A:972:GLY:HA3	7	0.32
(1,2298)	1:A:971:VAL:HA	1:A:972:GLY:HA3	20	0.32
(1,2224)	1:A:968:TRP:HB2	1:A:969:VAL:H	1	0.32
(1,2224)	1:A:968:TRP:HB2	1:A:969:VAL:H	5	0.32
(1,2224)	1:A:968:TRP:HB2	1:A:969:VAL:H	20	0.32
(1,2202)	1:A:967:TRP:HB2	1:A:968:TRP:H	1	0.32
(1,2202)	1:A:967:TRP:HB2	1:A:968:TRP:H	8	0.32
(1,2202)	1:A:967:TRP:HB2	1:A:968:TRP:H	17	0.32
(1,2196)	1:A:967:TRP:H	1:A:968:TRP:HA	7	0.32
(1,2196)	1:A:967:TRP:H	1:A:968:TRP:HA	8	0.32
(1,2196)	1:A:967:TRP:H	1:A:968:TRP:HA	20	0.32
(1,2166)	1:A:966:ILE:H	1:A:966:ILE:HG12	8	0.32
(1,215)	1:A:971:VAL:HA	1:A:972:GLY:HA3	7	0.32
(1,215)	1:A:971:VAL:HA	1:A:972:GLY:HA3	20	0.32
(1,2128)	1:A:964:ILE:HB	1:A:965:PRO:HD3	9	0.32
(1,2128)	1:A:964:ILE:HB	1:A:965:PRO:HD3	17	0.32
(1,2078)	1:A:988:TRP:H	2:B:719:ILE:HG12	4	0.32
(1,2047)	1:A:979:LEU:H	2:B:704:ILE:HB	3	0.32
(1,2047)	1:A:979:LEU:H	2:B:704:ILE:HB	15	0.32
(1,1810)	2:B:741:THR:HA	2:B:742:ALA:H	7	0.32
(1,1799)	2:B:739:TRP:HB2	2:B:740:ASP:H	12	0.32
(1,1769)	2:B:738:LYS:H	2:B:738:LYS:HG3	9	0.32
(1,1601)	2:B:726:GLU:HA	2:B:729:LYS:HB3	4	0.32
(1,141)	1:A:968:TRP:HB2	1:A:969:VAL:H	1	0.32
(1,141)	1:A:968:TRP:HB2	1:A:969:VAL:H	5	0.32
(1,141)	1:A:968:TRP:HB2	1:A:969:VAL:H	20	0.32
(1,1220)	2:B:708:GLY:H	2:B:710:ALA:H	6	0.32
(1,119)	1:A:967:TRP:HB2	1:A:968:TRP:H	1	0.32
(1,119)	1:A:967:TRP:HB2	1:A:968:TRP:H	8	0.32
(1,119)	1:A:967:TRP:HB2	1:A:968:TRP:H	17	0.32
(1,113)	1:A:967:TRP:H	1:A:968:TRP:HA	7	0.32
(1,113)	1:A:967:TRP:H	1:A:968:TRP:HA	8	0.32
(1,113)	1:A:967:TRP:H	1:A:968:TRP:HA	20	0.32
(1,809)	1:A:1005:GLU:HB2	1:A:1006:GLU:H	13	0.31
(1,807)	1:A:1005:GLU:H	1:A:1005:GLU:HB3	11	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,801)	1:A:1004:ASP:H	1:A:1004:ASP:HB3	7	0.31
(1,755)	1:A:997:ARG:H	1:A:997:ARG:HG3	1	0.31
(1,755)	1:A:997:ARG:H	1:A:997:ARG:HG3	9	0.31
(1,750)	1:A:996:ASN:HA	1:A:997:ARG:H	14	0.31
(1,750)	1:A:996:ASN:HA	1:A:997:ARG:H	15	0.31
(1,738)	1:A:995:ARG:HA	1:A:996:ASN:H	10	0.31
(1,737)	1:A:995:ARG:HB3	1:A:996:ASN:H	6	0.31
(1,706)	1:A:994:LYS:H	1:A:994:LYS:HB3	1	0.31
(1,706)	1:A:994:LYS:H	1:A:994:LYS:HB3	7	0.31
(1,706)	1:A:994:LYS:H	1:A:994:LYS:HB3	12	0.31
(1,624)	1:A:990:VAL:HB	1:A:991:GLY:H	14	0.31
(1,624)	1:A:990:VAL:HB	1:A:991:GLY:H	16	0.31
(1,602)	1:A:989:LYS:HA	1:A:991:GLY:H	1	0.31
(1,602)	1:A:989:LYS:HA	1:A:991:GLY:H	4	0.31
(1,602)	1:A:989:LYS:HA	1:A:991:GLY:H	10	0.31
(1,602)	1:A:989:LYS:HA	1:A:991:GLY:H	16	0.31
(1,602)	1:A:989:LYS:HA	1:A:991:GLY:H	19	0.31
(1,577)	1:A:989:LYS:H	1:A:989:LYS:HB3	4	0.31
(1,539)	1:A:987:MET:HB3	1:A:988:TRP:H	2	0.31
(1,539)	1:A:987:MET:HB3	1:A:988:TRP:H	6	0.31
(1,519)	1:A:986:ALA:HA	1:A:989:LYS:H	17	0.31
(1,516)	1:A:986:ALA:HA	1:A:988:TRP:H	9	0.31
(1,489)	1:A:985:LEU:HA	1:A:988:TRP:H	1	0.31
(1,489)	1:A:985:LEU:HA	1:A:988:TRP:H	8	0.31
(1,460)	1:A:984:VAL:HA	1:A:988:TRP:HB3	15	0.31
(1,45)	1:A:964:ILE:HB	1:A:965:PRO:HD3	19	0.31
(1,416)	1:A:983:LEU:HB2	1:A:984:VAL:H	5	0.31
(1,4143)	1:A:984:VAL:H	2:B:712:LEU:HA	20	0.31
(1,4010)	2:B:751:THR:H	2:B:751:THR:HG21	15	0.31
(1,4010)	2:B:751:THR:H	2:B:751:THR:HG22	15	0.31
(1,4010)	2:B:751:THR:H	2:B:751:THR:HG23	15	0.31
(1,3998)	2:B:749:GLU:H	2:B:749:GLU:HB3	12	0.31
(1,3945)	2:B:745:PRO:HA	2:B:746:LEU:H	12	0.31
(1,3945)	2:B:745:PRO:HA	2:B:746:LEU:H	15	0.31
(1,3945)	2:B:745:PRO:HA	2:B:746:LEU:H	18	0.31
(1,3945)	2:B:745:PRO:HA	2:B:746:LEU:H	19	0.31
(1,393)	1:A:982:ILE:H	1:A:984:VAL:H	1	0.31
(1,393)	1:A:982:ILE:H	1:A:984:VAL:H	16	0.31
(1,391)	1:A:982:ILE:H	1:A:983:LEU:HB3	9	0.31
(1,3852)	2:B:738:LYS:H	2:B:738:LYS:HG3	10	0.31
(1,3801)	2:B:734:ARG:HD2	2:B:734:ARG:HB2	9	0.31
(1,3684)	2:B:726:GLU:HA	2:B:729:LYS:HB3	15	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,363)	1:A:981:THR:H	1:A:981:THR:HG21	8	0.31
(1,363)	1:A:981:THR:H	1:A:981:THR:HG22	8	0.31
(1,363)	1:A:981:THR:H	1:A:981:THR:HG23	8	0.31
(1,363)	1:A:981:THR:H	1:A:981:THR:HG21	14	0.31
(1,363)	1:A:981:THR:H	1:A:981:THR:HG22	14	0.31
(1,363)	1:A:981:THR:H	1:A:981:THR:HG23	14	0.31
(1,3303)	2:B:708:GLY:H	2:B:710:ALA:H	1	0.31
(1,3303)	2:B:708:GLY:H	2:B:710:ALA:H	17	0.31
(1,2892)	1:A:1005:GLU:HB2	1:A:1006:GLU:H	13	0.31
(1,2890)	1:A:1005:GLU:H	1:A:1005:GLU:HB3	11	0.31
(1,2884)	1:A:1004:ASP:H	1:A:1004:ASP:HB3	7	0.31
(1,2838)	1:A:997:ARG:H	1:A:997:ARG:HG3	1	0.31
(1,2838)	1:A:997:ARG:H	1:A:997:ARG:HG3	9	0.31
(1,2833)	1:A:996:ASN:HA	1:A:997:ARG:H	14	0.31
(1,2833)	1:A:996:ASN:HA	1:A:997:ARG:H	15	0.31
(1,2821)	1:A:995:ARG:HA	1:A:996:ASN:H	10	0.31
(1,2820)	1:A:995:ARG:HB3	1:A:996:ASN:H	6	0.31
(1,2789)	1:A:994:LYS:H	1:A:994:LYS:HB3	1	0.31
(1,2789)	1:A:994:LYS:H	1:A:994:LYS:HB3	7	0.31
(1,2789)	1:A:994:LYS:H	1:A:994:LYS:HB3	12	0.31
(1,2707)	1:A:990:VAL:HB	1:A:991:GLY:H	14	0.31
(1,2707)	1:A:990:VAL:HB	1:A:991:GLY:H	16	0.31
(1,2685)	1:A:989:LYS:HA	1:A:991:GLY:H	1	0.31
(1,2685)	1:A:989:LYS:HA	1:A:991:GLY:H	4	0.31
(1,2685)	1:A:989:LYS:HA	1:A:991:GLY:H	10	0.31
(1,2685)	1:A:989:LYS:HA	1:A:991:GLY:H	16	0.31
(1,2685)	1:A:989:LYS:HA	1:A:991:GLY:H	19	0.31
(1,2660)	1:A:989:LYS:H	1:A:989:LYS:HB3	4	0.31
(1,2622)	1:A:987:MET:HB3	1:A:988:TRP:H	2	0.31
(1,2622)	1:A:987:MET:HB3	1:A:988:TRP:H	6	0.31
(1,2602)	1:A:986:ALA:HA	1:A:989:LYS:H	17	0.31
(1,2599)	1:A:986:ALA:HA	1:A:988:TRP:H	9	0.31
(1,2572)	1:A:985:LEU:HA	1:A:988:TRP:H	1	0.31
(1,2572)	1:A:985:LEU:HA	1:A:988:TRP:H	8	0.31
(1,2543)	1:A:984:VAL:HA	1:A:988:TRP:HB3	15	0.31
(1,2499)	1:A:983:LEU:HB2	1:A:984:VAL:H	5	0.31
(1,2476)	1:A:982:ILE:H	1:A:984:VAL:H	1	0.31
(1,2476)	1:A:982:ILE:H	1:A:984:VAL:H	16	0.31
(1,2474)	1:A:982:ILE:H	1:A:983:LEU:HB3	9	0.31
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG21	8	0.31
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG22	8	0.31
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG23	8	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG21	14	0.31
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG22	14	0.31
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG23	14	0.31
(1,2298)	1:A:971:VAL:HA	1:A:972:GLY:HA3	6	0.31
(1,2282)	1:A:970:LEU:HB2	1:A:971:VAL:H	20	0.31
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD21	19	0.31
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD22	19	0.31
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD23	19	0.31
(1,2224)	1:A:968:TRP:HB2	1:A:969:VAL:H	19	0.31
(1,2202)	1:A:967:TRP:HB2	1:A:968:TRP:H	18	0.31
(1,2202)	1:A:967:TRP:HB2	1:A:968:TRP:H	19	0.31
(1,2196)	1:A:967:TRP:H	1:A:968:TRP:HA	10	0.31
(1,215)	1:A:971:VAL:HA	1:A:972:GLY:HA3	6	0.31
(1,2128)	1:A:964:ILE:HB	1:A:965:PRO:HD3	19	0.31
(1,2060)	1:A:984:VAL:H	2:B:712:LEU:HA	20	0.31
(1,199)	1:A:970:LEU:HB2	1:A:971:VAL:H	20	0.31
(1,1927)	2:B:751:THR:H	2:B:751:THR:HG21	15	0.31
(1,1927)	2:B:751:THR:H	2:B:751:THR:HG22	15	0.31
(1,1927)	2:B:751:THR:H	2:B:751:THR:HG23	15	0.31
(1,1915)	2:B:749:GLU:H	2:B:749:GLU:HB3	12	0.31
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD21	19	0.31
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD22	19	0.31
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD23	19	0.31
(1,1862)	2:B:745:PRO:HA	2:B:746:LEU:H	12	0.31
(1,1862)	2:B:745:PRO:HA	2:B:746:LEU:H	15	0.31
(1,1862)	2:B:745:PRO:HA	2:B:746:LEU:H	18	0.31
(1,1862)	2:B:745:PRO:HA	2:B:746:LEU:H	19	0.31
(1,1769)	2:B:738:LYS:H	2:B:738:LYS:HG3	10	0.31
(1,1718)	2:B:734:ARG:HD2	2:B:734:ARG:HB2	9	0.31
(1,1601)	2:B:726:GLU:HA	2:B:729:LYS:HB3	15	0.31
(1,141)	1:A:968:TRP:HB2	1:A:969:VAL:H	19	0.31
(1,1220)	2:B:708:GLY:H	2:B:710:ALA:H	1	0.31
(1,1220)	2:B:708:GLY:H	2:B:710:ALA:H	17	0.31
(1,119)	1:A:967:TRP:HB2	1:A:968:TRP:H	18	0.31
(1,119)	1:A:967:TRP:HB2	1:A:968:TRP:H	19	0.31
(1,113)	1:A:967:TRP:H	1:A:968:TRP:HA	10	0.31
(1,809)	1:A:1005:GLU:HB2	1:A:1006:GLU:H	4	0.3
(1,741)	1:A:995:ARG:HB3	1:A:997:ARG:H	1	0.3
(1,741)	1:A:995:ARG:HB3	1:A:997:ARG:H	14	0.3
(1,602)	1:A:989:LYS:HA	1:A:991:GLY:H	11	0.3
(1,590)	1:A:989:LYS:HB2	1:A:990:VAL:H	19	0.3
(1,577)	1:A:989:LYS:H	1:A:989:LYS:HB3	1	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,577)	1:A:989:LYS:H	1:A:989:LYS:HB3	3	0.3
(1,577)	1:A:989:LYS:H	1:A:989:LYS:HB3	12	0.3
(1,547)	1:A:987:MET:HG3	1:A:989:LYS:H	3	0.3
(1,547)	1:A:987:MET:HG3	1:A:989:LYS:H	15	0.3
(1,539)	1:A:987:MET:HB3	1:A:988:TRP:H	7	0.3
(1,539)	1:A:987:MET:HB3	1:A:988:TRP:H	16	0.3
(1,519)	1:A:986:ALA:HA	1:A:989:LYS:H	12	0.3
(1,519)	1:A:986:ALA:HA	1:A:989:LYS:H	14	0.3
(1,519)	1:A:986:ALA:HA	1:A:989:LYS:H	20	0.3
(1,516)	1:A:986:ALA:HA	1:A:988:TRP:H	5	0.3
(1,516)	1:A:986:ALA:HA	1:A:988:TRP:H	12	0.3
(1,516)	1:A:986:ALA:HA	1:A:988:TRP:H	15	0.3
(1,5)	1:A:960:GLU:HA	1:A:961:GLU:H	12	0.3
(1,5)	1:A:960:GLU:HA	1:A:961:GLU:H	15	0.3
(1,5)	1:A:960:GLU:HA	1:A:961:GLU:H	16	0.3
(1,499)	1:A:985:LEU:HA	1:A:989:LYS:H	5	0.3
(1,489)	1:A:985:LEU:HA	1:A:988:TRP:H	5	0.3
(1,489)	1:A:985:LEU:HA	1:A:988:TRP:H	13	0.3
(1,489)	1:A:985:LEU:HA	1:A:988:TRP:H	18	0.3
(1,460)	1:A:984:VAL:HA	1:A:988:TRP:HB3	8	0.3
(1,460)	1:A:984:VAL:HA	1:A:988:TRP:HB3	14	0.3
(1,45)	1:A:964:ILE:HB	1:A:965:PRO:HD3	3	0.3
(1,45)	1:A:964:ILE:HB	1:A:965:PRO:HD3	5	0.3
(1,45)	1:A:964:ILE:HB	1:A:965:PRO:HD3	12	0.3
(1,45)	1:A:964:ILE:HB	1:A:965:PRO:HD3	14	0.3
(1,45)	1:A:964:ILE:HB	1:A:965:PRO:HD3	16	0.3
(1,45)	1:A:964:ILE:HB	1:A:965:PRO:HD3	20	0.3
(1,416)	1:A:983:LEU:HB2	1:A:984:VAL:H	17	0.3
(1,416)	1:A:983:LEU:HB2	1:A:984:VAL:H	18	0.3
(1,416)	1:A:983:LEU:HB2	1:A:984:VAL:H	20	0.3
(1,4130)	1:A:979:LEU:H	2:B:704:ILE:HB	7	0.3
(1,4130)	1:A:979:LEU:H	2:B:704:ILE:HB	13	0.3
(1,3998)	2:B:749:GLU:H	2:B:749:GLU:HB3	5	0.3
(1,3962)	2:B:746:LEU:HB3	2:B:747:TYR:H	11	0.3
(1,391)	1:A:982:ILE:H	1:A:983:LEU:HB3	2	0.3
(1,391)	1:A:982:ILE:H	1:A:983:LEU:HB3	10	0.3
(1,3903)	2:B:742:ALA:HB1	2:B:743:ASN:H	18	0.3
(1,3903)	2:B:742:ALA:HB2	2:B:743:ASN:H	18	0.3
(1,3903)	2:B:742:ALA:HB3	2:B:743:ASN:H	18	0.3
(1,3882)	2:B:739:TRP:HB2	2:B:740:ASP:H	20	0.3
(1,3863)	2:B:738:LYS:HB3	2:B:739:TRP:H	15	0.3
(1,3852)	2:B:738:LYS:H	2:B:738:LYS:HG3	2	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3852)	2:B:738:LYS:H	2:B:738:LYS:HG3	18	0.3
(1,3850)	2:B:738:LYS:HA	2:B:738:LYS:HD3	12	0.3
(1,3684)	2:B:726:GLU:HA	2:B:729:LYS:HB3	1	0.3
(1,3684)	2:B:726:GLU:HA	2:B:729:LYS:HB3	3	0.3
(1,3684)	2:B:726:GLU:HA	2:B:729:LYS:HB3	5	0.3
(1,3684)	2:B:726:GLU:HA	2:B:729:LYS:HB3	12	0.3
(1,363)	1:A:981:THR:H	1:A:981:THR:HG21	1	0.3
(1,363)	1:A:981:THR:H	1:A:981:THR:HG22	1	0.3
(1,363)	1:A:981:THR:H	1:A:981:THR:HG23	1	0.3
(1,356)	1:A:980:LEU:HB3	1:A:981:THR:HA	17	0.3
(1,3495)	2:B:718:LEU:HB3	2:B:719:ILE:HG12	18	0.3
(1,3319)	2:B:709:LEU:H	2:B:711:ALA:H	16	0.3
(1,3303)	2:B:708:GLY:H	2:B:710:ALA:H	16	0.3
(1,2892)	1:A:1005:GLU:HB2	1:A:1006:GLU:H	4	0.3
(1,285)	1:A:975:GLY:HA3	1:A:977:LEU:H	5	0.3
(1,285)	1:A:975:GLY:HA3	1:A:977:LEU:H	7	0.3
(1,285)	1:A:975:GLY:HA3	1:A:977:LEU:H	9	0.3
(1,285)	1:A:975:GLY:HA3	1:A:977:LEU:H	12	0.3
(1,2824)	1:A:995:ARG:HB3	1:A:997:ARG:H	1	0.3
(1,2824)	1:A:995:ARG:HB3	1:A:997:ARG:H	14	0.3
(1,2685)	1:A:989:LYS:HA	1:A:991:GLY:H	11	0.3
(1,2673)	1:A:989:LYS:HB2	1:A:990:VAL:H	19	0.3
(1,2660)	1:A:989:LYS:H	1:A:989:LYS:HB3	1	0.3
(1,2660)	1:A:989:LYS:H	1:A:989:LYS:HB3	3	0.3
(1,2660)	1:A:989:LYS:H	1:A:989:LYS:HB3	12	0.3
(1,2630)	1:A:987:MET:HG3	1:A:989:LYS:H	3	0.3
(1,2630)	1:A:987:MET:HG3	1:A:989:LYS:H	15	0.3
(1,2622)	1:A:987:MET:HB3	1:A:988:TRP:H	7	0.3
(1,2622)	1:A:987:MET:HB3	1:A:988:TRP:H	16	0.3
(1,2602)	1:A:986:ALA:HA	1:A:989:LYS:H	12	0.3
(1,2602)	1:A:986:ALA:HA	1:A:989:LYS:H	14	0.3
(1,2602)	1:A:986:ALA:HA	1:A:989:LYS:H	20	0.3
(1,2599)	1:A:986:ALA:HA	1:A:988:TRP:H	5	0.3
(1,2599)	1:A:986:ALA:HA	1:A:988:TRP:H	12	0.3
(1,2599)	1:A:986:ALA:HA	1:A:988:TRP:H	15	0.3
(1,2582)	1:A:985:LEU:HA	1:A:989:LYS:H	5	0.3
(1,2572)	1:A:985:LEU:HA	1:A:988:TRP:H	5	0.3
(1,2572)	1:A:985:LEU:HA	1:A:988:TRP:H	13	0.3
(1,2572)	1:A:985:LEU:HA	1:A:988:TRP:H	18	0.3
(1,2543)	1:A:984:VAL:HA	1:A:988:TRP:HB3	8	0.3
(1,2543)	1:A:984:VAL:HA	1:A:988:TRP:HB3	14	0.3
(1,2499)	1:A:983:LEU:HB2	1:A:984:VAL:H	17	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2499)	1:A:983:LEU:HB2	1:A:984:VAL:H	18	0.3
(1,2499)	1:A:983:LEU:HB2	1:A:984:VAL:H	20	0.3
(1,2474)	1:A:982:ILE:H	1:A:983:LEU:HB3	2	0.3
(1,2474)	1:A:982:ILE:H	1:A:983:LEU:HB3	10	0.3
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG21	1	0.3
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG22	1	0.3
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG23	1	0.3
(1,2439)	1:A:980:LEU:HB3	1:A:981:THR:HA	17	0.3
(1,2368)	1:A:975:GLY:HA3	1:A:977:LEU:H	5	0.3
(1,2368)	1:A:975:GLY:HA3	1:A:977:LEU:H	7	0.3
(1,2368)	1:A:975:GLY:HA3	1:A:977:LEU:H	9	0.3
(1,2368)	1:A:975:GLY:HA3	1:A:977:LEU:H	12	0.3
(1,2298)	1:A:971:VAL:HA	1:A:972:GLY:HA3	1	0.3
(1,2298)	1:A:971:VAL:HA	1:A:972:GLY:HA3	2	0.3
(1,2298)	1:A:971:VAL:HA	1:A:972:GLY:HA3	3	0.3
(1,2298)	1:A:971:VAL:HA	1:A:972:GLY:HA3	5	0.3
(1,2298)	1:A:971:VAL:HA	1:A:972:GLY:HA3	8	0.3
(1,2298)	1:A:971:VAL:HA	1:A:972:GLY:HA3	9	0.3
(1,2298)	1:A:971:VAL:HA	1:A:972:GLY:HA3	10	0.3
(1,2298)	1:A:971:VAL:HA	1:A:972:GLY:HA3	12	0.3
(1,2298)	1:A:971:VAL:HA	1:A:972:GLY:HA3	13	0.3
(1,2298)	1:A:971:VAL:HA	1:A:972:GLY:HA3	14	0.3
(1,2298)	1:A:971:VAL:HA	1:A:972:GLY:HA3	15	0.3
(1,2298)	1:A:971:VAL:HA	1:A:972:GLY:HA3	16	0.3
(1,2298)	1:A:971:VAL:HA	1:A:972:GLY:HA3	18	0.3
(1,2298)	1:A:971:VAL:HA	1:A:972:GLY:HA3	19	0.3
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD21	10	0.3
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD22	10	0.3
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD23	10	0.3
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD21	12	0.3
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD22	12	0.3
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD23	12	0.3
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD21	14	0.3
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD22	14	0.3
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD23	14	0.3
(1,2224)	1:A:968:TRP:HB2	1:A:969:VAL:H	10	0.3
(1,2202)	1:A:967:TRP:HB2	1:A:968:TRP:H	12	0.3
(1,2202)	1:A:967:TRP:HB2	1:A:968:TRP:H	15	0.3
(1,2196)	1:A:967:TRP:H	1:A:968:TRP:HA	4	0.3
(1,2196)	1:A:967:TRP:H	1:A:968:TRP:HA	14	0.3
(1,215)	1:A:971:VAL:HA	1:A:972:GLY:HA3	1	0.3
(1,215)	1:A:971:VAL:HA	1:A:972:GLY:HA3	2	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,215)	1:A:971:VAL:HA	1:A:972:GLY:HA3	3	0.3
(1,215)	1:A:971:VAL:HA	1:A:972:GLY:HA3	5	0.3
(1,215)	1:A:971:VAL:HA	1:A:972:GLY:HA3	8	0.3
(1,215)	1:A:971:VAL:HA	1:A:972:GLY:HA3	9	0.3
(1,215)	1:A:971:VAL:HA	1:A:972:GLY:HA3	10	0.3
(1,215)	1:A:971:VAL:HA	1:A:972:GLY:HA3	12	0.3
(1,215)	1:A:971:VAL:HA	1:A:972:GLY:HA3	13	0.3
(1,215)	1:A:971:VAL:HA	1:A:972:GLY:HA3	14	0.3
(1,215)	1:A:971:VAL:HA	1:A:972:GLY:HA3	15	0.3
(1,215)	1:A:971:VAL:HA	1:A:972:GLY:HA3	16	0.3
(1,215)	1:A:971:VAL:HA	1:A:972:GLY:HA3	18	0.3
(1,215)	1:A:971:VAL:HA	1:A:972:GLY:HA3	19	0.3
(1,2128)	1:A:964:ILE:HB	1:A:965:PRO:HD3	3	0.3
(1,2128)	1:A:964:ILE:HB	1:A:965:PRO:HD3	5	0.3
(1,2128)	1:A:964:ILE:HB	1:A:965:PRO:HD3	12	0.3
(1,2128)	1:A:964:ILE:HB	1:A:965:PRO:HD3	14	0.3
(1,2128)	1:A:964:ILE:HB	1:A:965:PRO:HD3	16	0.3
(1,2128)	1:A:964:ILE:HB	1:A:965:PRO:HD3	20	0.3
(1,2088)	1:A:960:GLU:HA	1:A:961:GLU:H	12	0.3
(1,2088)	1:A:960:GLU:HA	1:A:961:GLU:H	15	0.3
(1,2088)	1:A:960:GLU:HA	1:A:961:GLU:H	16	0.3
(1,2047)	1:A:979:LEU:H	2:B:704:ILE:HB	7	0.3
(1,2047)	1:A:979:LEU:H	2:B:704:ILE:HB	13	0.3
(1,1915)	2:B:749:GLU:H	2:B:749:GLU:HB3	5	0.3
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD21	10	0.3
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD22	10	0.3
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD23	10	0.3
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD21	12	0.3
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD22	12	0.3
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD23	12	0.3
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD21	14	0.3
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD22	14	0.3
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD23	14	0.3
(1,1879)	2:B:746:LEU:HB3	2:B:747:TYR:H	11	0.3
(1,1820)	2:B:742:ALA:HB1	2:B:743:ASN:H	18	0.3
(1,1820)	2:B:742:ALA:HB2	2:B:743:ASN:H	18	0.3
(1,1820)	2:B:742:ALA:HB3	2:B:743:ASN:H	18	0.3
(1,1799)	2:B:739:TRP:HB2	2:B:740:ASP:H	20	0.3
(1,1780)	2:B:738:LYS:HB3	2:B:739:TRP:H	15	0.3
(1,1769)	2:B:738:LYS:H	2:B:738:LYS:HG3	2	0.3
(1,1769)	2:B:738:LYS:H	2:B:738:LYS:HG3	18	0.3
(1,1767)	2:B:738:LYS:HA	2:B:738:LYS:HD3	12	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1601)	2:B:726:GLU:HA	2:B:729:LYS:HB3	1	0.3
(1,1601)	2:B:726:GLU:HA	2:B:729:LYS:HB3	3	0.3
(1,1601)	2:B:726:GLU:HA	2:B:729:LYS:HB3	5	0.3
(1,1601)	2:B:726:GLU:HA	2:B:729:LYS:HB3	12	0.3
(1,1412)	2:B:718:LEU:HB3	2:B:719:ILE:HG12	18	0.3
(1,141)	1:A:968:TRP:HB2	1:A:969:VAL:H	10	0.3
(1,1236)	2:B:709:LEU:H	2:B:711:ALA:H	16	0.3
(1,1220)	2:B:708:GLY:H	2:B:710:ALA:H	16	0.3
(1,119)	1:A:967:TRP:HB2	1:A:968:TRP:H	12	0.3
(1,119)	1:A:967:TRP:HB2	1:A:968:TRP:H	15	0.3
(1,113)	1:A:967:TRP:H	1:A:968:TRP:HA	4	0.3
(1,113)	1:A:967:TRP:H	1:A:968:TRP:HA	14	0.3
(1,755)	1:A:997:ARG:H	1:A:997:ARG:HG3	7	0.29
(1,750)	1:A:996:ASN:HA	1:A:997:ARG:H	20	0.29
(1,738)	1:A:995:ARG:HA	1:A:996:ASN:H	3	0.29
(1,706)	1:A:994:LYS:H	1:A:994:LYS:HB3	17	0.29
(1,602)	1:A:989:LYS:HA	1:A:991:GLY:H	5	0.29
(1,602)	1:A:989:LYS:HA	1:A:991:GLY:H	18	0.29
(1,602)	1:A:989:LYS:HA	1:A:991:GLY:H	20	0.29
(1,577)	1:A:989:LYS:H	1:A:989:LYS:HB3	2	0.29
(1,577)	1:A:989:LYS:H	1:A:989:LYS:HB3	13	0.29
(1,577)	1:A:989:LYS:H	1:A:989:LYS:HB3	18	0.29
(1,547)	1:A:987:MET:HG3	1:A:989:LYS:H	10	0.29
(1,547)	1:A:987:MET:HG3	1:A:989:LYS:H	13	0.29
(1,539)	1:A:987:MET:HB3	1:A:988:TRP:H	8	0.29
(1,519)	1:A:986:ALA:HA	1:A:989:LYS:H	13	0.29
(1,516)	1:A:986:ALA:HA	1:A:988:TRP:H	2	0.29
(1,516)	1:A:986:ALA:HA	1:A:988:TRP:H	10	0.29
(1,5)	1:A:960:GLU:HA	1:A:961:GLU:H	7	0.29
(1,499)	1:A:985:LEU:HA	1:A:989:LYS:H	11	0.29
(1,499)	1:A:985:LEU:HA	1:A:989:LYS:H	15	0.29
(1,499)	1:A:985:LEU:HA	1:A:989:LYS:H	19	0.29
(1,460)	1:A:984:VAL:HA	1:A:988:TRP:HB3	7	0.29
(1,45)	1:A:964:ILE:HB	1:A:965:PRO:HD3	1	0.29
(1,45)	1:A:964:ILE:HB	1:A:965:PRO:HD3	7	0.29
(1,45)	1:A:964:ILE:HB	1:A:965:PRO:HD3	13	0.29
(1,45)	1:A:964:ILE:HB	1:A:965:PRO:HD3	18	0.29
(1,416)	1:A:983:LEU:HB2	1:A:984:VAL:H	12	0.29
(1,4143)	1:A:984:VAL:H	2:B:712:LEU:HA	5	0.29
(1,4143)	1:A:984:VAL:H	2:B:712:LEU:HA	14	0.29
(1,4143)	1:A:984:VAL:H	2:B:712:LEU:HA	16	0.29
(1,4067)	2:B:758:THR:HA	2:B:759:TYR:H	16	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4033)	2:B:754:PHE:HA	2:B:755:THR:H	4	0.29
(1,4033)	2:B:754:PHE:HA	2:B:755:THR:H	14	0.29
(1,3998)	2:B:749:GLU:H	2:B:749:GLU:HB3	2	0.29
(1,3998)	2:B:749:GLU:H	2:B:749:GLU:HB3	19	0.29
(1,3893)	2:B:741:THR:HA	2:B:742:ALA:H	13	0.29
(1,3882)	2:B:739:TRP:HB2	2:B:740:ASP:H	8	0.29
(1,3852)	2:B:738:LYS:H	2:B:738:LYS:HG3	5	0.29
(1,3684)	2:B:726:GLU:HA	2:B:729:LYS:HB3	6	0.29
(1,3684)	2:B:726:GLU:HA	2:B:729:LYS:HB3	11	0.29
(1,3684)	2:B:726:GLU:HA	2:B:729:LYS:HB3	14	0.29
(1,3684)	2:B:726:GLU:HA	2:B:729:LYS:HB3	18	0.29
(1,363)	1:A:981:THR:H	1:A:981:THR:HG21	7	0.29
(1,363)	1:A:981:THR:H	1:A:981:THR:HG22	7	0.29
(1,363)	1:A:981:THR:H	1:A:981:THR:HG23	7	0.29
(1,363)	1:A:981:THR:H	1:A:981:THR:HG21	11	0.29
(1,363)	1:A:981:THR:H	1:A:981:THR:HG22	11	0.29
(1,363)	1:A:981:THR:H	1:A:981:THR:HG23	11	0.29
(1,363)	1:A:981:THR:H	1:A:981:THR:HG21	15	0.29
(1,363)	1:A:981:THR:H	1:A:981:THR:HG22	15	0.29
(1,363)	1:A:981:THR:H	1:A:981:THR:HG23	15	0.29
(1,363)	1:A:981:THR:H	1:A:981:THR:HG21	16	0.29
(1,363)	1:A:981:THR:H	1:A:981:THR:HG22	16	0.29
(1,363)	1:A:981:THR:H	1:A:981:THR:HG23	16	0.29
(1,3495)	2:B:718:LEU:HB3	2:B:719:ILE:HG12	20	0.29
(1,285)	1:A:975:GLY:HA3	1:A:977:LEU:H	2	0.29
(1,2838)	1:A:997:ARG:H	1:A:997:ARG:HG3	7	0.29
(1,2833)	1:A:996:ASN:HA	1:A:997:ARG:H	20	0.29
(1,2821)	1:A:995:ARG:HA	1:A:996:ASN:H	3	0.29
(1,2789)	1:A:994:LYS:H	1:A:994:LYS:HB3	17	0.29
(1,2685)	1:A:989:LYS:HA	1:A:991:GLY:H	5	0.29
(1,2685)	1:A:989:LYS:HA	1:A:991:GLY:H	18	0.29
(1,2685)	1:A:989:LYS:HA	1:A:991:GLY:H	20	0.29
(1,2660)	1:A:989:LYS:H	1:A:989:LYS:HB3	2	0.29
(1,2660)	1:A:989:LYS:H	1:A:989:LYS:HB3	13	0.29
(1,2660)	1:A:989:LYS:H	1:A:989:LYS:HB3	18	0.29
(1,2630)	1:A:987:MET:HG3	1:A:989:LYS:H	10	0.29
(1,2630)	1:A:987:MET:HG3	1:A:989:LYS:H	13	0.29
(1,2622)	1:A:987:MET:HB3	1:A:988:TRP:H	8	0.29
(1,2602)	1:A:986:ALA:HA	1:A:989:LYS:H	13	0.29
(1,2599)	1:A:986:ALA:HA	1:A:988:TRP:H	2	0.29
(1,2599)	1:A:986:ALA:HA	1:A:988:TRP:H	10	0.29
(1,2582)	1:A:985:LEU:HA	1:A:989:LYS:H	11	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2582)	1:A:985:LEU:HA	1:A:989:LYS:H	15	0.29
(1,2582)	1:A:985:LEU:HA	1:A:989:LYS:H	19	0.29
(1,2543)	1:A:984:VAL:HA	1:A:988:TRP:HB3	7	0.29
(1,2499)	1:A:983:LEU:HB2	1:A:984:VAL:H	12	0.29
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG21	7	0.29
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG22	7	0.29
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG23	7	0.29
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG21	11	0.29
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG22	11	0.29
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG23	11	0.29
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG21	15	0.29
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG22	15	0.29
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG23	15	0.29
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG21	16	0.29
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG22	16	0.29
(1,2446)	1:A:981:THR:H	1:A:981:THR:HG23	16	0.29
(1,2368)	1:A:975:GLY:HA3	1:A:977:LEU:H	2	0.29
(1,2298)	1:A:971:VAL:HA	1:A:972:GLY:HA3	4	0.29
(1,2298)	1:A:971:VAL:HA	1:A:972:GLY:HA3	11	0.29
(1,2298)	1:A:971:VAL:HA	1:A:972:GLY:HA3	17	0.29
(1,2224)	1:A:968:TRP:HB2	1:A:969:VAL:H	17	0.29
(1,2202)	1:A:967:TRP:HB2	1:A:968:TRP:H	4	0.29
(1,2202)	1:A:967:TRP:HB2	1:A:968:TRP:H	7	0.29
(1,2201)	1:A:967:TRP:HA	1:A:968:TRP:HB3	2	0.29
(1,2201)	1:A:967:TRP:HA	1:A:968:TRP:HB3	20	0.29
(1,215)	1:A:971:VAL:HA	1:A:972:GLY:HA3	4	0.29
(1,215)	1:A:971:VAL:HA	1:A:972:GLY:HA3	11	0.29
(1,215)	1:A:971:VAL:HA	1:A:972:GLY:HA3	17	0.29
(1,2128)	1:A:964:ILE:HB	1:A:965:PRO:HD3	1	0.29
(1,2128)	1:A:964:ILE:HB	1:A:965:PRO:HD3	7	0.29
(1,2128)	1:A:964:ILE:HB	1:A:965:PRO:HD3	13	0.29
(1,2128)	1:A:964:ILE:HB	1:A:965:PRO:HD3	18	0.29
(1,2088)	1:A:960:GLU:HA	1:A:961:GLU:H	7	0.29
(1,2060)	1:A:984:VAL:H	2:B:712:LEU:HA	5	0.29
(1,2060)	1:A:984:VAL:H	2:B:712:LEU:HA	14	0.29
(1,2060)	1:A:984:VAL:H	2:B:712:LEU:HA	16	0.29
(1,1984)	2:B:758:THR:HA	2:B:759:TYR:H	16	0.29
(1,1950)	2:B:754:PHE:HA	2:B:755:THR:H	4	0.29
(1,1950)	2:B:754:PHE:HA	2:B:755:THR:H	14	0.29
(1,1915)	2:B:749:GLU:H	2:B:749:GLU:HB3	2	0.29
(1,1915)	2:B:749:GLU:H	2:B:749:GLU:HB3	19	0.29
(1,1810)	2:B:741:THR:HA	2:B:742:ALA:H	13	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1799)	2:B:739:TRP:HB2	2:B:740:ASP:H	8	0.29
(1,1769)	2:B:738:LYS:H	2:B:738:LYS:HG3	5	0.29
(1,1601)	2:B:726:GLU:HA	2:B:729:LYS:HB3	6	0.29
(1,1601)	2:B:726:GLU:HA	2:B:729:LYS:HB3	11	0.29
(1,1601)	2:B:726:GLU:HA	2:B:729:LYS:HB3	14	0.29
(1,1601)	2:B:726:GLU:HA	2:B:729:LYS:HB3	18	0.29
(1,1412)	2:B:718:LEU:HB3	2:B:719:ILE:HG12	20	0.29
(1,141)	1:A:968:TRP:HB2	1:A:969:VAL:H	17	0.29
(1,119)	1:A:967:TRP:HB2	1:A:968:TRP:H	4	0.29
(1,119)	1:A:967:TRP:HB2	1:A:968:TRP:H	7	0.29
(1,118)	1:A:967:TRP:HA	1:A:968:TRP:HB3	2	0.29
(1,118)	1:A:967:TRP:HA	1:A:968:TRP:HB3	20	0.29
(1,862)	2:B:692:ASP:HB3	2:B:695:VAL:HA	8	0.28
(1,841)	2:B:691:PRO:HD3	2:B:692:ASP:H	4	0.28
(1,81)	1:A:966:ILE:H	1:A:966:ILE:HG13	18	0.28
(1,807)	1:A:1005:GLU:H	1:A:1005:GLU:HB3	16	0.28
(1,762)	1:A:997:ARG:HA	1:A:999:PRO:HD2	16	0.28
(1,762)	1:A:997:ARG:HA	1:A:999:PRO:HD2	20	0.28
(1,761)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	3	0.28
(1,761)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	5	0.28
(1,760)	1:A:997:ARG:HA	1:A:999:PRO:HD3	20	0.28
(1,738)	1:A:995:ARG:HA	1:A:996:ASN:H	19	0.28
(1,624)	1:A:990:VAL:HB	1:A:991:GLY:H	8	0.28
(1,624)	1:A:990:VAL:HB	1:A:991:GLY:H	11	0.28
(1,602)	1:A:989:LYS:HA	1:A:991:GLY:H	3	0.28
(1,602)	1:A:989:LYS:HA	1:A:991:GLY:H	15	0.28
(1,590)	1:A:989:LYS:HB2	1:A:990:VAL:H	5	0.28
(1,590)	1:A:989:LYS:HB2	1:A:990:VAL:H	15	0.28
(1,547)	1:A:987:MET:HG3	1:A:989:LYS:H	5	0.28
(1,539)	1:A:987:MET:HB3	1:A:988:TRP:H	10	0.28
(1,519)	1:A:986:ALA:HA	1:A:989:LYS:H	4	0.28
(1,519)	1:A:986:ALA:HA	1:A:989:LYS:H	5	0.28
(1,519)	1:A:986:ALA:HA	1:A:989:LYS:H	7	0.28
(1,519)	1:A:986:ALA:HA	1:A:989:LYS:H	9	0.28
(1,519)	1:A:986:ALA:HA	1:A:989:LYS:H	18	0.28
(1,516)	1:A:986:ALA:HA	1:A:988:TRP:H	7	0.28
(1,516)	1:A:986:ALA:HA	1:A:988:TRP:H	14	0.28
(1,516)	1:A:986:ALA:HA	1:A:988:TRP:H	17	0.28
(1,5)	1:A:960:GLU:HA	1:A:961:GLU:H	1	0.28
(1,5)	1:A:960:GLU:HA	1:A:961:GLU:H	9	0.28
(1,5)	1:A:960:GLU:HA	1:A:961:GLU:H	10	0.28
(1,5)	1:A:960:GLU:HA	1:A:961:GLU:H	14	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5)	1:A:960:GLU:HA	1:A:961:GLU:H	19	0.28
(1,5)	1:A:960:GLU:HA	1:A:961:GLU:H	20	0.28
(1,499)	1:A:985:LEU:HA	1:A:989:LYS:H	18	0.28
(1,480)	1:A:985:LEU:HA	1:A:986:ALA:H	1	0.28
(1,480)	1:A:985:LEU:HA	1:A:986:ALA:H	3	0.28
(1,480)	1:A:985:LEU:HA	1:A:986:ALA:H	4	0.28
(1,480)	1:A:985:LEU:HA	1:A:986:ALA:H	5	0.28
(1,480)	1:A:985:LEU:HA	1:A:986:ALA:H	6	0.28
(1,480)	1:A:985:LEU:HA	1:A:986:ALA:H	7	0.28
(1,480)	1:A:985:LEU:HA	1:A:986:ALA:H	8	0.28
(1,480)	1:A:985:LEU:HA	1:A:986:ALA:H	11	0.28
(1,480)	1:A:985:LEU:HA	1:A:986:ALA:H	14	0.28
(1,480)	1:A:985:LEU:HA	1:A:986:ALA:H	15	0.28
(1,480)	1:A:985:LEU:HA	1:A:986:ALA:H	16	0.28
(1,480)	1:A:985:LEU:HA	1:A:986:ALA:H	17	0.28
(1,480)	1:A:985:LEU:HA	1:A:986:ALA:H	18	0.28
(1,480)	1:A:985:LEU:HA	1:A:986:ALA:H	19	0.28
(1,480)	1:A:985:LEU:HA	1:A:986:ALA:H	20	0.28
(1,460)	1:A:984:VAL:HA	1:A:988:TRP:HB3	4	0.28
(1,450)	1:A:984:VAL:HA	1:A:987:MET:H	8	0.28
(1,45)	1:A:964:ILE:HB	1:A:965:PRO:HD3	4	0.28
(1,45)	1:A:964:ILE:HB	1:A:965:PRO:HD3	8	0.28
(1,45)	1:A:964:ILE:HB	1:A:965:PRO:HD3	10	0.28
(1,4130)	1:A:979:LEU:H	2:B:704:ILE:HB	16	0.28
(1,4067)	2:B:758:THR:HA	2:B:759:TYR:H	11	0.28
(1,4067)	2:B:758:THR:HA	2:B:759:TYR:H	20	0.28
(1,4033)	2:B:754:PHE:HA	2:B:755:THR:H	5	0.28
(1,4033)	2:B:754:PHE:HA	2:B:755:THR:H	6	0.28
(1,4033)	2:B:754:PHE:HA	2:B:755:THR:H	15	0.28
(1,4033)	2:B:754:PHE:HA	2:B:755:THR:H	20	0.28
(1,3998)	2:B:749:GLU:H	2:B:749:GLU:HB3	13	0.28
(1,3998)	2:B:749:GLU:H	2:B:749:GLU:HB3	18	0.28
(1,3973)	2:B:747:TYR:HB2	2:B:748:LYS:H	7	0.28
(1,3945)	2:B:745:PRO:HA	2:B:746:LEU:H	6	0.28
(1,3903)	2:B:742:ALA:HB1	2:B:743:ASN:H	7	0.28
(1,3903)	2:B:742:ALA:HB2	2:B:743:ASN:H	7	0.28
(1,3903)	2:B:742:ALA:HB3	2:B:743:ASN:H	7	0.28
(1,3888)	2:B:740:ASP:HA	2:B:741:THR:H	4	0.28
(1,3882)	2:B:739:TRP:HB2	2:B:740:ASP:H	2	0.28
(1,3882)	2:B:739:TRP:HB2	2:B:740:ASP:H	3	0.28
(1,3882)	2:B:739:TRP:HB2	2:B:740:ASP:H	7	0.28
(1,3882)	2:B:739:TRP:HB2	2:B:740:ASP:H	10	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3882)	2:B:739:TRP:HB2	2:B:740:ASP:H	11	0.28
(1,3882)	2:B:739:TRP:HB2	2:B:740:ASP:H	14	0.28
(1,3882)	2:B:739:TRP:HB2	2:B:740:ASP:H	17	0.28
(1,3859)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	9	0.28
(1,3859)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	16	0.28
(1,3859)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	19	0.28
(1,3852)	2:B:738:LYS:H	2:B:738:LYS:HG3	4	0.28
(1,3852)	2:B:738:LYS:H	2:B:738:LYS:HG3	17	0.28
(1,3852)	2:B:738:LYS:H	2:B:738:LYS:HG3	20	0.28
(1,3801)	2:B:734:ARG:HD2	2:B:734:ARG:HB2	12	0.28
(1,3684)	2:B:726:GLU:HA	2:B:729:LYS:HB3	2	0.28
(1,3684)	2:B:726:GLU:HA	2:B:729:LYS:HB3	9	0.28
(1,3684)	2:B:726:GLU:HA	2:B:729:LYS:HB3	10	0.28
(1,3684)	2:B:726:GLU:HA	2:B:729:LYS:HB3	13	0.28
(1,3684)	2:B:726:GLU:HA	2:B:729:LYS:HB3	20	0.28
(1,3495)	2:B:718:LEU:HB3	2:B:719:ILE:HG12	14	0.28
(1,341)	1:A:979:LEU:HA	1:A:981:THR:H	17	0.28
(1,2945)	2:B:692:ASP:HB3	2:B:695:VAL:HA	8	0.28
(1,2924)	2:B:691:PRO:HD3	2:B:692:ASP:H	4	0.28
(1,2890)	1:A:1005:GLU:H	1:A:1005:GLU:HB3	16	0.28
(1,285)	1:A:975:GLY:HA3	1:A:977:LEU:H	14	0.28
(1,2845)	1:A:997:ARG:HA	1:A:999:PRO:HD2	16	0.28
(1,2845)	1:A:997:ARG:HA	1:A:999:PRO:HD2	20	0.28
(1,2844)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	3	0.28
(1,2844)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	5	0.28
(1,2843)	1:A:997:ARG:HA	1:A:999:PRO:HD3	20	0.28
(1,2821)	1:A:995:ARG:HA	1:A:996:ASN:H	19	0.28
(1,2707)	1:A:990:VAL:HB	1:A:991:GLY:H	8	0.28
(1,2707)	1:A:990:VAL:HB	1:A:991:GLY:H	11	0.28
(1,2685)	1:A:989:LYS:HA	1:A:991:GLY:H	3	0.28
(1,2685)	1:A:989:LYS:HA	1:A:991:GLY:H	15	0.28
(1,2673)	1:A:989:LYS:HB2	1:A:990:VAL:H	5	0.28
(1,2673)	1:A:989:LYS:HB2	1:A:990:VAL:H	15	0.28
(1,2630)	1:A:987:MET:HG3	1:A:989:LYS:H	5	0.28
(1,2622)	1:A:987:MET:HB3	1:A:988:TRP:H	10	0.28
(1,2602)	1:A:986:ALA:HA	1:A:989:LYS:H	4	0.28
(1,2602)	1:A:986:ALA:HA	1:A:989:LYS:H	5	0.28
(1,2602)	1:A:986:ALA:HA	1:A:989:LYS:H	7	0.28
(1,2602)	1:A:986:ALA:HA	1:A:989:LYS:H	9	0.28
(1,2602)	1:A:986:ALA:HA	1:A:989:LYS:H	18	0.28
(1,2599)	1:A:986:ALA:HA	1:A:988:TRP:H	7	0.28
(1,2599)	1:A:986:ALA:HA	1:A:988:TRP:H	14	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2599)	1:A:986:ALA:HA	1:A:988:TRP:H	17	0.28
(1,2582)	1:A:985:LEU:HA	1:A:989:LYS:H	18	0.28
(1,2563)	1:A:985:LEU:HA	1:A:986:ALA:H	1	0.28
(1,2563)	1:A:985:LEU:HA	1:A:986:ALA:H	3	0.28
(1,2563)	1:A:985:LEU:HA	1:A:986:ALA:H	4	0.28
(1,2563)	1:A:985:LEU:HA	1:A:986:ALA:H	5	0.28
(1,2563)	1:A:985:LEU:HA	1:A:986:ALA:H	6	0.28
(1,2563)	1:A:985:LEU:HA	1:A:986:ALA:H	7	0.28
(1,2563)	1:A:985:LEU:HA	1:A:986:ALA:H	8	0.28
(1,2563)	1:A:985:LEU:HA	1:A:986:ALA:H	11	0.28
(1,2563)	1:A:985:LEU:HA	1:A:986:ALA:H	14	0.28
(1,2563)	1:A:985:LEU:HA	1:A:986:ALA:H	15	0.28
(1,2563)	1:A:985:LEU:HA	1:A:986:ALA:H	16	0.28
(1,2563)	1:A:985:LEU:HA	1:A:986:ALA:H	17	0.28
(1,2563)	1:A:985:LEU:HA	1:A:986:ALA:H	18	0.28
(1,2563)	1:A:985:LEU:HA	1:A:986:ALA:H	19	0.28
(1,2563)	1:A:985:LEU:HA	1:A:986:ALA:H	20	0.28
(1,2543)	1:A:984:VAL:HA	1:A:988:TRP:HB3	4	0.28
(1,2533)	1:A:984:VAL:HA	1:A:987:MET:H	8	0.28
(1,2424)	1:A:979:LEU:HA	1:A:981:THR:H	17	0.28
(1,2368)	1:A:975:GLY:HA3	1:A:977:LEU:H	14	0.28
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD21	8	0.28
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD22	8	0.28
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD23	8	0.28
(1,2224)	1:A:968:TRP:HB2	1:A:969:VAL:H	2	0.28
(1,2164)	1:A:966:ILE:H	1:A:966:ILE:HG13	18	0.28
(1,2128)	1:A:964:ILE:HB	1:A:965:PRO:HD3	4	0.28
(1,2128)	1:A:964:ILE:HB	1:A:965:PRO:HD3	8	0.28
(1,2128)	1:A:964:ILE:HB	1:A:965:PRO:HD3	10	0.28
(1,2088)	1:A:960:GLU:HA	1:A:961:GLU:H	1	0.28
(1,2088)	1:A:960:GLU:HA	1:A:961:GLU:H	9	0.28
(1,2088)	1:A:960:GLU:HA	1:A:961:GLU:H	10	0.28
(1,2088)	1:A:960:GLU:HA	1:A:961:GLU:H	14	0.28
(1,2088)	1:A:960:GLU:HA	1:A:961:GLU:H	19	0.28
(1,2088)	1:A:960:GLU:HA	1:A:961:GLU:H	20	0.28
(1,2047)	1:A:979:LEU:H	2:B:704:ILE:HB	16	0.28
(1,1984)	2:B:758:THR:HA	2:B:759:TYR:H	11	0.28
(1,1984)	2:B:758:THR:HA	2:B:759:TYR:H	20	0.28
(1,1950)	2:B:754:PHE:HA	2:B:755:THR:H	5	0.28
(1,1950)	2:B:754:PHE:HA	2:B:755:THR:H	6	0.28
(1,1950)	2:B:754:PHE:HA	2:B:755:THR:H	15	0.28
(1,1950)	2:B:754:PHE:HA	2:B:755:THR:H	20	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1915)	2:B:749:GLU:H	2:B:749:GLU:HB3	13	0.28
(1,1915)	2:B:749:GLU:H	2:B:749:GLU:HB3	18	0.28
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD21	8	0.28
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD22	8	0.28
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD23	8	0.28
(1,1890)	2:B:747:TYR:HB2	2:B:748:LYS:H	7	0.28
(1,1862)	2:B:745:PRO:HA	2:B:746:LEU:H	6	0.28
(1,1820)	2:B:742:ALA:HB1	2:B:743:ASN:H	7	0.28
(1,1820)	2:B:742:ALA:HB2	2:B:743:ASN:H	7	0.28
(1,1820)	2:B:742:ALA:HB3	2:B:743:ASN:H	7	0.28
(1,1805)	2:B:740:ASP:HA	2:B:741:THR:H	4	0.28
(1,1799)	2:B:739:TRP:HB2	2:B:740:ASP:H	2	0.28
(1,1799)	2:B:739:TRP:HB2	2:B:740:ASP:H	3	0.28
(1,1799)	2:B:739:TRP:HB2	2:B:740:ASP:H	7	0.28
(1,1799)	2:B:739:TRP:HB2	2:B:740:ASP:H	10	0.28
(1,1799)	2:B:739:TRP:HB2	2:B:740:ASP:H	11	0.28
(1,1799)	2:B:739:TRP:HB2	2:B:740:ASP:H	14	0.28
(1,1799)	2:B:739:TRP:HB2	2:B:740:ASP:H	17	0.28
(1,1776)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	9	0.28
(1,1776)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	16	0.28
(1,1776)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	19	0.28
(1,1769)	2:B:738:LYS:H	2:B:738:LYS:HG3	4	0.28
(1,1769)	2:B:738:LYS:H	2:B:738:LYS:HG3	17	0.28
(1,1769)	2:B:738:LYS:H	2:B:738:LYS:HG3	20	0.28
(1,1718)	2:B:734:ARG:HD2	2:B:734:ARG:HB2	12	0.28
(1,1601)	2:B:726:GLU:HA	2:B:729:LYS:HB3	2	0.28
(1,1601)	2:B:726:GLU:HA	2:B:729:LYS:HB3	9	0.28
(1,1601)	2:B:726:GLU:HA	2:B:729:LYS:HB3	10	0.28
(1,1601)	2:B:726:GLU:HA	2:B:729:LYS:HB3	13	0.28
(1,1601)	2:B:726:GLU:HA	2:B:729:LYS:HB3	20	0.28
(1,1412)	2:B:718:LEU:HB3	2:B:719:ILE:HG12	14	0.28
(1,141)	1:A:968:TRP:HB2	1:A:969:VAL:H	2	0.28
(1,851)	2:B:692:ASP:H	2:B:693:ILE:H	8	0.27
(1,841)	2:B:691:PRO:HD3	2:B:692:ASP:H	1	0.27
(1,841)	2:B:691:PRO:HD3	2:B:692:ASP:H	17	0.27
(1,81)	1:A:966:ILE:H	1:A:966:ILE:HG13	4	0.27
(1,81)	1:A:966:ILE:H	1:A:966:ILE:HG13	6	0.27
(1,807)	1:A:1005:GLU:H	1:A:1005:GLU:HB3	4	0.27
(1,755)	1:A:997:ARG:H	1:A:997:ARG:HG3	15	0.27
(1,750)	1:A:996:ASN:HA	1:A:997:ARG:H	19	0.27
(1,706)	1:A:994:LYS:H	1:A:994:LYS:HB3	2	0.27
(1,590)	1:A:989:LYS:HB2	1:A:990:VAL:H	3	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,590)	1:A:989:LYS:HB2	1:A:990:VAL:H	14	0.27
(1,577)	1:A:989:LYS:H	1:A:989:LYS:HB3	7	0.27
(1,577)	1:A:989:LYS:H	1:A:989:LYS:HB3	17	0.27
(1,519)	1:A:986:ALA:HA	1:A:989:LYS:H	2	0.27
(1,519)	1:A:986:ALA:HA	1:A:989:LYS:H	15	0.27
(1,519)	1:A:986:ALA:HA	1:A:989:LYS:H	19	0.27
(1,516)	1:A:986:ALA:HA	1:A:988:TRP:H	3	0.27
(1,516)	1:A:986:ALA:HA	1:A:988:TRP:H	19	0.27
(1,5)	1:A:960:GLU:HA	1:A:961:GLU:H	2	0.27
(1,5)	1:A:960:GLU:HA	1:A:961:GLU:H	11	0.27
(1,5)	1:A:960:GLU:HA	1:A:961:GLU:H	17	0.27
(1,499)	1:A:985:LEU:HA	1:A:989:LYS:H	6	0.27
(1,499)	1:A:985:LEU:HA	1:A:989:LYS:H	8	0.27
(1,499)	1:A:985:LEU:HA	1:A:989:LYS:H	9	0.27
(1,499)	1:A:985:LEU:HA	1:A:989:LYS:H	10	0.27
(1,499)	1:A:985:LEU:HA	1:A:989:LYS:H	16	0.27
(1,489)	1:A:985:LEU:HA	1:A:988:TRP:H	3	0.27
(1,489)	1:A:985:LEU:HA	1:A:988:TRP:H	12	0.27
(1,489)	1:A:985:LEU:HA	1:A:988:TRP:H	19	0.27
(1,487)	1:A:985:LEU:H	1:A:987:MET:HG2	8	0.27
(1,480)	1:A:985:LEU:HA	1:A:986:ALA:H	2	0.27
(1,480)	1:A:985:LEU:HA	1:A:986:ALA:H	9	0.27
(1,480)	1:A:985:LEU:HA	1:A:986:ALA:H	10	0.27
(1,480)	1:A:985:LEU:HA	1:A:986:ALA:H	12	0.27
(1,480)	1:A:985:LEU:HA	1:A:986:ALA:H	13	0.27
(1,460)	1:A:984:VAL:HA	1:A:988:TRP:HB3	20	0.27
(1,450)	1:A:984:VAL:HA	1:A:987:MET:H	1	0.27
(1,423)	1:A:983:LEU:H	1:A:985:LEU:H	1	0.27
(1,4161)	1:A:988:TRP:H	2:B:719:ILE:HG12	20	0.27
(1,416)	1:A:983:LEU:HB2	1:A:984:VAL:H	9	0.27
(1,416)	1:A:983:LEU:HB2	1:A:984:VAL:H	15	0.27
(1,4157)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	18	0.27
(1,4130)	1:A:979:LEU:H	2:B:704:ILE:HB	8	0.27
(1,4033)	2:B:754:PHE:HA	2:B:755:THR:H	7	0.27
(1,4033)	2:B:754:PHE:HA	2:B:755:THR:H	8	0.27
(1,4033)	2:B:754:PHE:HA	2:B:755:THR:H	13	0.27
(1,4033)	2:B:754:PHE:HA	2:B:755:THR:H	16	0.27
(1,4029)	2:B:754:PHE:H	2:B:754:PHE:HB3	19	0.27
(1,3973)	2:B:747:TYR:HB2	2:B:748:LYS:H	18	0.27
(1,391)	1:A:982:ILE:H	1:A:983:LEU:HB3	14	0.27
(1,3903)	2:B:742:ALA:HB1	2:B:743:ASN:H	16	0.27
(1,3903)	2:B:742:ALA:HB2	2:B:743:ASN:H	16	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3903)	2:B:742:ALA:HB3	2:B:743:ASN:H	16	0.27
(1,3894)	2:B:741:THR:HB	2:B:742:ALA:H	20	0.27
(1,3882)	2:B:739:TRP:HB2	2:B:740:ASP:H	1	0.27
(1,3882)	2:B:739:TRP:HB2	2:B:740:ASP:H	13	0.27
(1,3882)	2:B:739:TRP:HB2	2:B:740:ASP:H	15	0.27
(1,3882)	2:B:739:TRP:HB2	2:B:740:ASP:H	19	0.27
(1,3860)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	1	0.27
(1,3860)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	4	0.27
(1,3860)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	6	0.27
(1,3860)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	13	0.27
(1,3860)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	14	0.27
(1,3860)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	18	0.27
(1,3860)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	20	0.27
(1,3859)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	1	0.27
(1,3859)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	3	0.27
(1,3859)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	4	0.27
(1,3859)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	6	0.27
(1,3859)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	8	0.27
(1,3859)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	13	0.27
(1,3859)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	14	0.27
(1,3859)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	18	0.27
(1,3859)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	20	0.27
(1,3852)	2:B:738:LYS:H	2:B:738:LYS:HG3	1	0.27
(1,3852)	2:B:738:LYS:H	2:B:738:LYS:HG3	3	0.27
(1,3852)	2:B:738:LYS:H	2:B:738:LYS:HG3	6	0.27
(1,3852)	2:B:738:LYS:H	2:B:738:LYS:HG3	13	0.27
(1,3852)	2:B:738:LYS:H	2:B:738:LYS:HG3	14	0.27
(1,3852)	2:B:738:LYS:H	2:B:738:LYS:HG3	19	0.27
(1,3684)	2:B:726:GLU:HA	2:B:729:LYS:HB3	8	0.27
(1,3684)	2:B:726:GLU:HA	2:B:729:LYS:HB3	17	0.27
(1,3684)	2:B:726:GLU:HA	2:B:729:LYS:HB3	19	0.27
(1,3470)	2:B:717:LEU:H	2:B:719:ILE:H	17	0.27
(1,3303)	2:B:708:GLY:H	2:B:710:ALA:H	15	0.27
(1,2934)	2:B:692:ASP:H	2:B:693:ILE:H	8	0.27
(1,2924)	2:B:691:PRO:HD3	2:B:692:ASP:H	1	0.27
(1,2924)	2:B:691:PRO:HD3	2:B:692:ASP:H	17	0.27
(1,2890)	1:A:1005:GLU:H	1:A:1005:GLU:HB3	4	0.27
(1,285)	1:A:975:GLY:HA3	1:A:977:LEU:H	19	0.27
(1,2838)	1:A:997:ARG:H	1:A:997:ARG:HG3	15	0.27
(1,2833)	1:A:996:ASN:HA	1:A:997:ARG:H	19	0.27
(1,2789)	1:A:994:LYS:H	1:A:994:LYS:HB3	2	0.27
(1,2673)	1:A:989:LYS:HB2	1:A:990:VAL:H	3	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2673)	1:A:989:LYS:HB2	1:A:990:VAL:H	14	0.27
(1,2660)	1:A:989:LYS:H	1:A:989:LYS:HB3	7	0.27
(1,2660)	1:A:989:LYS:H	1:A:989:LYS:HB3	17	0.27
(1,2602)	1:A:986:ALA:HA	1:A:989:LYS:H	2	0.27
(1,2602)	1:A:986:ALA:HA	1:A:989:LYS:H	15	0.27
(1,2602)	1:A:986:ALA:HA	1:A:989:LYS:H	19	0.27
(1,2599)	1:A:986:ALA:HA	1:A:988:TRP:H	3	0.27
(1,2599)	1:A:986:ALA:HA	1:A:988:TRP:H	19	0.27
(1,2582)	1:A:985:LEU:HA	1:A:989:LYS:H	6	0.27
(1,2582)	1:A:985:LEU:HA	1:A:989:LYS:H	8	0.27
(1,2582)	1:A:985:LEU:HA	1:A:989:LYS:H	9	0.27
(1,2582)	1:A:985:LEU:HA	1:A:989:LYS:H	10	0.27
(1,2582)	1:A:985:LEU:HA	1:A:989:LYS:H	16	0.27
(1,2572)	1:A:985:LEU:HA	1:A:988:TRP:H	3	0.27
(1,2572)	1:A:985:LEU:HA	1:A:988:TRP:H	12	0.27
(1,2572)	1:A:985:LEU:HA	1:A:988:TRP:H	19	0.27
(1,2570)	1:A:985:LEU:H	1:A:987:MET:HG2	8	0.27
(1,2563)	1:A:985:LEU:HA	1:A:986:ALA:H	2	0.27
(1,2563)	1:A:985:LEU:HA	1:A:986:ALA:H	9	0.27
(1,2563)	1:A:985:LEU:HA	1:A:986:ALA:H	10	0.27
(1,2563)	1:A:985:LEU:HA	1:A:986:ALA:H	12	0.27
(1,2563)	1:A:985:LEU:HA	1:A:986:ALA:H	13	0.27
(1,2543)	1:A:984:VAL:HA	1:A:988:TRP:HB3	20	0.27
(1,2533)	1:A:984:VAL:HA	1:A:987:MET:H	1	0.27
(1,2506)	1:A:983:LEU:H	1:A:985:LEU:H	1	0.27
(1,2499)	1:A:983:LEU:HB2	1:A:984:VAL:H	9	0.27
(1,2499)	1:A:983:LEU:HB2	1:A:984:VAL:H	15	0.27
(1,2474)	1:A:982:ILE:H	1:A:983:LEU:HB3	14	0.27
(1,2368)	1:A:975:GLY:HA3	1:A:977:LEU:H	19	0.27
(1,2202)	1:A:967:TRP:HB2	1:A:968:TRP:H	14	0.27
(1,2202)	1:A:967:TRP:HB2	1:A:968:TRP:H	20	0.27
(1,2201)	1:A:967:TRP:HA	1:A:968:TRP:HB3	7	0.27
(1,2164)	1:A:966:ILE:H	1:A:966:ILE:HG13	4	0.27
(1,2164)	1:A:966:ILE:H	1:A:966:ILE:HG13	6	0.27
(1,2088)	1:A:960:GLU:HA	1:A:961:GLU:H	2	0.27
(1,2088)	1:A:960:GLU:HA	1:A:961:GLU:H	11	0.27
(1,2088)	1:A:960:GLU:HA	1:A:961:GLU:H	17	0.27
(1,2078)	1:A:988:TRP:H	2:B:719:ILE:HG12	20	0.27
(1,2074)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	18	0.27
(1,2047)	1:A:979:LEU:H	2:B:704:ILE:HB	8	0.27
(1,1950)	2:B:754:PHE:HA	2:B:755:THR:H	7	0.27
(1,1950)	2:B:754:PHE:HA	2:B:755:THR:H	8	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1950)	2:B:754:PHE:HA	2:B:755:THR:H	13	0.27
(1,1950)	2:B:754:PHE:HA	2:B:755:THR:H	16	0.27
(1,1946)	2:B:754:PHE:H	2:B:754:PHE:HB3	19	0.27
(1,1890)	2:B:747:TYR:HB2	2:B:748:LYS:H	18	0.27
(1,1820)	2:B:742:ALA:HB1	2:B:743:ASN:H	16	0.27
(1,1820)	2:B:742:ALA:HB2	2:B:743:ASN:H	16	0.27
(1,1820)	2:B:742:ALA:HB3	2:B:743:ASN:H	16	0.27
(1,1811)	2:B:741:THR:HB	2:B:742:ALA:H	20	0.27
(1,1799)	2:B:739:TRP:HB2	2:B:740:ASP:H	1	0.27
(1,1799)	2:B:739:TRP:HB2	2:B:740:ASP:H	13	0.27
(1,1799)	2:B:739:TRP:HB2	2:B:740:ASP:H	15	0.27
(1,1799)	2:B:739:TRP:HB2	2:B:740:ASP:H	19	0.27
(1,1777)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	1	0.27
(1,1777)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	4	0.27
(1,1777)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	6	0.27
(1,1777)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	13	0.27
(1,1777)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	14	0.27
(1,1777)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	18	0.27
(1,1777)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	20	0.27
(1,1776)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	1	0.27
(1,1776)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	3	0.27
(1,1776)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	4	0.27
(1,1776)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	6	0.27
(1,1776)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	8	0.27
(1,1776)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	13	0.27
(1,1776)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	14	0.27
(1,1776)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	18	0.27
(1,1776)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	20	0.27
(1,1769)	2:B:738:LYS:H	2:B:738:LYS:HG3	1	0.27
(1,1769)	2:B:738:LYS:H	2:B:738:LYS:HG3	3	0.27
(1,1769)	2:B:738:LYS:H	2:B:738:LYS:HG3	6	0.27
(1,1769)	2:B:738:LYS:H	2:B:738:LYS:HG3	13	0.27
(1,1769)	2:B:738:LYS:H	2:B:738:LYS:HG3	14	0.27
(1,1769)	2:B:738:LYS:H	2:B:738:LYS:HG3	19	0.27
(1,1601)	2:B:726:GLU:HA	2:B:729:LYS:HB3	8	0.27
(1,1601)	2:B:726:GLU:HA	2:B:729:LYS:HB3	17	0.27
(1,1601)	2:B:726:GLU:HA	2:B:729:LYS:HB3	19	0.27
(1,1387)	2:B:717:LEU:H	2:B:719:ILE:H	17	0.27
(1,1220)	2:B:708:GLY:H	2:B:710:ALA:H	15	0.27
(1,119)	1:A:967:TRP:HB2	1:A:968:TRP:H	14	0.27
(1,119)	1:A:967:TRP:HB2	1:A:968:TRP:H	20	0.27
(1,118)	1:A:967:TRP:HA	1:A:968:TRP:HB3	7	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,841)	2:B:691:PRO:HD3	2:B:692:ASP:H	16	0.26
(1,81)	1:A:966:ILE:H	1:A:966:ILE:HG13	2	0.26
(1,81)	1:A:966:ILE:H	1:A:966:ILE:HG13	3	0.26
(1,761)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	6	0.26
(1,761)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	16	0.26
(1,706)	1:A:994:LYS:H	1:A:994:LYS:HB3	9	0.26
(1,602)	1:A:989:LYS:HA	1:A:991:GLY:H	6	0.26
(1,590)	1:A:989:LYS:HB2	1:A:990:VAL:H	20	0.26
(1,577)	1:A:989:LYS:H	1:A:989:LYS:HB3	9	0.26
(1,577)	1:A:989:LYS:H	1:A:989:LYS:HB3	14	0.26
(1,576)	1:A:989:LYS:H	1:A:989:LYS:HD3	19	0.26
(1,547)	1:A:987:MET:HG3	1:A:989:LYS:H	11	0.26
(1,519)	1:A:986:ALA:HA	1:A:989:LYS:H	6	0.26
(1,519)	1:A:986:ALA:HA	1:A:989:LYS:H	16	0.26
(1,516)	1:A:986:ALA:HA	1:A:988:TRP:H	6	0.26
(1,5)	1:A:960:GLU:HA	1:A:961:GLU:H	4	0.26
(1,5)	1:A:960:GLU:HA	1:A:961:GLU:H	5	0.26
(1,5)	1:A:960:GLU:HA	1:A:961:GLU:H	6	0.26
(1,5)	1:A:960:GLU:HA	1:A:961:GLU:H	13	0.26
(1,499)	1:A:985:LEU:HA	1:A:989:LYS:H	2	0.26
(1,499)	1:A:985:LEU:HA	1:A:989:LYS:H	20	0.26
(1,489)	1:A:985:LEU:HA	1:A:988:TRP:H	9	0.26
(1,489)	1:A:985:LEU:HA	1:A:988:TRP:H	14	0.26
(1,460)	1:A:984:VAL:HA	1:A:988:TRP:HB3	11	0.26
(1,450)	1:A:984:VAL:HA	1:A:987:MET:H	15	0.26
(1,450)	1:A:984:VAL:HA	1:A:987:MET:H	18	0.26
(1,45)	1:A:964:ILE:HB	1:A:965:PRO:HD3	11	0.26
(1,45)	1:A:964:ILE:HB	1:A:965:PRO:HD3	15	0.26
(1,426)	1:A:983:LEU:HA	1:A:985:LEU:H	17	0.26
(1,416)	1:A:983:LEU:HB2	1:A:984:VAL:H	1	0.26
(1,416)	1:A:983:LEU:HB2	1:A:984:VAL:H	14	0.26
(1,4130)	1:A:979:LEU:H	2:B:704:ILE:HB	2	0.26
(1,4130)	1:A:979:LEU:H	2:B:704:ILE:HB	20	0.26
(1,4046)	2:B:756:ASN:HA	2:B:757:ILE:H	11	0.26
(1,4033)	2:B:754:PHE:HA	2:B:755:THR:H	18	0.26
(1,3998)	2:B:749:GLU:H	2:B:749:GLU:HB3	7	0.26
(1,3973)	2:B:747:TYR:HB2	2:B:748:LYS:H	1	0.26
(1,3973)	2:B:747:TYR:HB2	2:B:748:LYS:H	2	0.26
(1,3973)	2:B:747:TYR:HB2	2:B:748:LYS:H	12	0.26
(1,3973)	2:B:747:TYR:HB2	2:B:748:LYS:H	14	0.26
(1,3973)	2:B:747:TYR:HB2	2:B:748:LYS:H	15	0.26
(1,3968)	2:B:747:TYR:H	2:B:747:TYR:HB3	13	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3945)	2:B:745:PRO:HA	2:B:746:LEU:H	17	0.26
(1,393)	1:A:982:ILE:H	1:A:984:VAL:H	5	0.26
(1,391)	1:A:982:ILE:H	1:A:983:LEU:HB3	11	0.26
(1,3909)	2:B:743:ASN:HB2	2:B:743:ASN:H	1	0.26
(1,3897)	2:B:741:THR:HA	2:B:744:ASN:H	19	0.26
(1,3888)	2:B:740:ASP:HA	2:B:741:THR:H	11	0.26
(1,3882)	2:B:739:TRP:HB2	2:B:740:ASP:H	5	0.26
(1,3882)	2:B:739:TRP:HB2	2:B:740:ASP:H	6	0.26
(1,3882)	2:B:739:TRP:HB2	2:B:740:ASP:H	9	0.26
(1,3882)	2:B:739:TRP:HB2	2:B:740:ASP:H	18	0.26
(1,3860)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	3	0.26
(1,3860)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	8	0.26
(1,3860)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	9	0.26
(1,3860)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	16	0.26
(1,3860)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	19	0.26
(1,3852)	2:B:738:LYS:H	2:B:738:LYS:HG3	16	0.26
(1,3798)	2:B:734:ARG:HD3	2:B:734:ARG:HB2	2	0.26
(1,3303)	2:B:708:GLY:H	2:B:710:ALA:H	11	0.26
(1,3303)	2:B:708:GLY:H	2:B:710:ALA:H	18	0.26
(1,3303)	2:B:708:GLY:H	2:B:710:ALA:H	19	0.26
(1,3211)	2:B:704:ILE:HB	2:B:705:LEU:HB2	12	0.26
(1,2924)	2:B:691:PRO:HD3	2:B:692:ASP:H	16	0.26
(1,289)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	8	0.26
(1,285)	1:A:975:GLY:HA3	1:A:977:LEU:H	6	0.26
(1,2844)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	6	0.26
(1,2844)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	16	0.26
(1,2789)	1:A:994:LYS:H	1:A:994:LYS:HB3	9	0.26
(1,2685)	1:A:989:LYS:HA	1:A:991:GLY:H	6	0.26
(1,2673)	1:A:989:LYS:HB2	1:A:990:VAL:H	20	0.26
(1,2660)	1:A:989:LYS:H	1:A:989:LYS:HB3	9	0.26
(1,2660)	1:A:989:LYS:H	1:A:989:LYS:HB3	14	0.26
(1,2659)	1:A:989:LYS:H	1:A:989:LYS:HD3	19	0.26
(1,2630)	1:A:987:MET:HG3	1:A:989:LYS:H	11	0.26
(1,2602)	1:A:986:ALA:HA	1:A:989:LYS:H	6	0.26
(1,2602)	1:A:986:ALA:HA	1:A:989:LYS:H	16	0.26
(1,2599)	1:A:986:ALA:HA	1:A:988:TRP:H	6	0.26
(1,2582)	1:A:985:LEU:HA	1:A:989:LYS:H	2	0.26
(1,2582)	1:A:985:LEU:HA	1:A:989:LYS:H	20	0.26
(1,2572)	1:A:985:LEU:HA	1:A:988:TRP:H	9	0.26
(1,2572)	1:A:985:LEU:HA	1:A:988:TRP:H	14	0.26
(1,2543)	1:A:984:VAL:HA	1:A:988:TRP:HB3	11	0.26
(1,2533)	1:A:984:VAL:HA	1:A:987:MET:H	15	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2533)	1:A:984:VAL:HA	1:A:987:MET:H	18	0.26
(1,2509)	1:A:983:LEU:HA	1:A:985:LEU:H	17	0.26
(1,2499)	1:A:983:LEU:HB2	1:A:984:VAL:H	1	0.26
(1,2499)	1:A:983:LEU:HB2	1:A:984:VAL:H	14	0.26
(1,2476)	1:A:982:ILE:H	1:A:984:VAL:H	5	0.26
(1,2474)	1:A:982:ILE:H	1:A:983:LEU:HB3	11	0.26
(1,2372)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	8	0.26
(1,2368)	1:A:975:GLY:HA3	1:A:977:LEU:H	6	0.26
(1,2224)	1:A:968:TRP:HB2	1:A:969:VAL:H	6	0.26
(1,2202)	1:A:967:TRP:HB2	1:A:968:TRP:H	11	0.26
(1,2164)	1:A:966:ILE:H	1:A:966:ILE:HG13	2	0.26
(1,2164)	1:A:966:ILE:H	1:A:966:ILE:HG13	3	0.26
(1,2128)	1:A:964:ILE:HB	1:A:965:PRO:HD3	11	0.26
(1,2128)	1:A:964:ILE:HB	1:A:965:PRO:HD3	15	0.26
(1,2088)	1:A:960:GLU:HA	1:A:961:GLU:H	4	0.26
(1,2088)	1:A:960:GLU:HA	1:A:961:GLU:H	5	0.26
(1,2088)	1:A:960:GLU:HA	1:A:961:GLU:H	6	0.26
(1,2088)	1:A:960:GLU:HA	1:A:961:GLU:H	13	0.26
(1,2047)	1:A:979:LEU:H	2:B:704:ILE:HB	2	0.26
(1,2047)	1:A:979:LEU:H	2:B:704:ILE:HB	20	0.26
(1,1963)	2:B:756:ASN:HA	2:B:757:ILE:H	11	0.26
(1,1950)	2:B:754:PHE:HA	2:B:755:THR:H	18	0.26
(1,1915)	2:B:749:GLU:H	2:B:749:GLU:HB3	7	0.26
(1,1890)	2:B:747:TYR:HB2	2:B:748:LYS:H	1	0.26
(1,1890)	2:B:747:TYR:HB2	2:B:748:LYS:H	2	0.26
(1,1890)	2:B:747:TYR:HB2	2:B:748:LYS:H	12	0.26
(1,1890)	2:B:747:TYR:HB2	2:B:748:LYS:H	14	0.26
(1,1890)	2:B:747:TYR:HB2	2:B:748:LYS:H	15	0.26
(1,1885)	2:B:747:TYR:H	2:B:747:TYR:HB3	13	0.26
(1,1862)	2:B:745:PRO:HA	2:B:746:LEU:H	17	0.26
(1,1826)	2:B:743:ASN:HB2	2:B:743:ASN:H	1	0.26
(1,1814)	2:B:741:THR:HA	2:B:744:ASN:H	19	0.26
(1,1805)	2:B:740:ASP:HA	2:B:741:THR:H	11	0.26
(1,1799)	2:B:739:TRP:HB2	2:B:740:ASP:H	5	0.26
(1,1799)	2:B:739:TRP:HB2	2:B:740:ASP:H	6	0.26
(1,1799)	2:B:739:TRP:HB2	2:B:740:ASP:H	9	0.26
(1,1799)	2:B:739:TRP:HB2	2:B:740:ASP:H	18	0.26
(1,1777)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	3	0.26
(1,1777)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	8	0.26
(1,1777)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	9	0.26
(1,1777)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	16	0.26
(1,1777)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	19	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1769)	2:B:738:LYS:H	2:B:738:LYS:HG3	16	0.26
(1,1715)	2:B:734:ARG:HD3	2:B:734:ARG:HB2	2	0.26
(1,141)	1:A:968:TRP:HB2	1:A:969:VAL:H	6	0.26
(1,1220)	2:B:708:GLY:H	2:B:710:ALA:H	11	0.26
(1,1220)	2:B:708:GLY:H	2:B:710:ALA:H	18	0.26
(1,1220)	2:B:708:GLY:H	2:B:710:ALA:H	19	0.26
(1,119)	1:A:967:TRP:HB2	1:A:968:TRP:H	11	0.26
(1,1128)	2:B:704:ILE:HB	2:B:705:LEU:HB2	12	0.26
(1,846)	2:B:691:PRO:HA	2:B:692:ASP:HB3	8	0.25
(1,841)	2:B:691:PRO:HD3	2:B:692:ASP:H	5	0.25
(1,841)	2:B:691:PRO:HD3	2:B:692:ASP:H	11	0.25
(1,776)	1:A:999:PRO:HA	1:A:1000:LEU:H	6	0.25
(1,761)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	11	0.25
(1,738)	1:A:995:ARG:HA	1:A:996:ASN:H	2	0.25
(1,737)	1:A:995:ARG:HB3	1:A:996:ASN:H	4	0.25
(1,723)	1:A:994:LYS:HD3	1:A:995:ARG:H	20	0.25
(1,645)	1:A:990:VAL:HB	1:A:993:PHE:H	16	0.25
(1,590)	1:A:989:LYS:HB2	1:A:990:VAL:H	4	0.25
(1,590)	1:A:989:LYS:HB2	1:A:990:VAL:H	6	0.25
(1,590)	1:A:989:LYS:HB2	1:A:990:VAL:H	7	0.25
(1,590)	1:A:989:LYS:HB2	1:A:990:VAL:H	11	0.25
(1,590)	1:A:989:LYS:HB2	1:A:990:VAL:H	13	0.25
(1,5)	1:A:960:GLU:HA	1:A:961:GLU:H	8	0.25
(1,499)	1:A:985:LEU:HA	1:A:989:LYS:H	7	0.25
(1,489)	1:A:985:LEU:HA	1:A:988:TRP:H	2	0.25
(1,489)	1:A:985:LEU:HA	1:A:988:TRP:H	6	0.25
(1,485)	1:A:985:LEU:HA	1:A:987:MET:H	12	0.25
(1,460)	1:A:984:VAL:HA	1:A:988:TRP:HB3	12	0.25
(1,450)	1:A:984:VAL:HA	1:A:987:MET:H	3	0.25
(1,450)	1:A:984:VAL:HA	1:A:987:MET:H	5	0.25
(1,450)	1:A:984:VAL:HA	1:A:987:MET:H	7	0.25
(1,450)	1:A:984:VAL:HA	1:A:987:MET:H	17	0.25
(1,450)	1:A:984:VAL:HA	1:A:987:MET:H	20	0.25
(1,426)	1:A:983:LEU:HA	1:A:985:LEU:H	3	0.25
(1,426)	1:A:983:LEU:HA	1:A:985:LEU:H	15	0.25
(1,4130)	1:A:979:LEU:H	2:B:704:ILE:HB	6	0.25
(1,4101)	1:A:973:VAL:H	2:B:700:VAL:HA	14	0.25
(1,4046)	2:B:756:ASN:HA	2:B:757:ILE:H	2	0.25
(1,3998)	2:B:749:GLU:H	2:B:749:GLU:HB3	1	0.25
(1,3998)	2:B:749:GLU:H	2:B:749:GLU:HB3	20	0.25
(1,3973)	2:B:747:TYR:HB2	2:B:748:LYS:H	5	0.25
(1,3973)	2:B:747:TYR:HB2	2:B:748:LYS:H	6	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3945)	2:B:745:PRO:HA	2:B:746:LEU:H	13	0.25
(1,393)	1:A:982:ILE:H	1:A:984:VAL:H	8	0.25
(1,393)	1:A:982:ILE:H	1:A:984:VAL:H	15	0.25
(1,393)	1:A:982:ILE:H	1:A:984:VAL:H	18	0.25
(1,3911)	2:B:743:ASN:HB3	2:B:743:ASN:H	14	0.25
(1,391)	1:A:982:ILE:H	1:A:983:LEU:HB3	4	0.25
(1,3902)	2:B:742:ALA:HA	2:B:743:ASN:H	8	0.25
(1,3870)	2:B:738:LYS:HA	2:B:740:ASP:H	1	0.25
(1,3870)	2:B:738:LYS:HA	2:B:740:ASP:H	4	0.25
(1,3870)	2:B:738:LYS:HA	2:B:740:ASP:H	5	0.25
(1,3870)	2:B:738:LYS:HA	2:B:740:ASP:H	6	0.25
(1,3870)	2:B:738:LYS:HA	2:B:740:ASP:H	12	0.25
(1,3870)	2:B:738:LYS:HA	2:B:740:ASP:H	19	0.25
(1,3303)	2:B:708:GLY:H	2:B:710:ALA:H	2	0.25
(1,3303)	2:B:708:GLY:H	2:B:710:ALA:H	10	0.25
(1,3303)	2:B:708:GLY:H	2:B:710:ALA:H	13	0.25
(1,2929)	2:B:691:PRO:HA	2:B:692:ASP:HB3	8	0.25
(1,2924)	2:B:691:PRO:HD3	2:B:692:ASP:H	5	0.25
(1,2924)	2:B:691:PRO:HD3	2:B:692:ASP:H	11	0.25
(1,289)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	13	0.25
(1,2859)	1:A:999:PRO:HA	1:A:1000:LEU:H	6	0.25
(1,2844)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	11	0.25
(1,2821)	1:A:995:ARG:HA	1:A:996:ASN:H	2	0.25
(1,2820)	1:A:995:ARG:HB3	1:A:996:ASN:H	4	0.25
(1,2806)	1:A:994:LYS:HD3	1:A:995:ARG:H	20	0.25
(1,2728)	1:A:990:VAL:HB	1:A:993:PHE:H	16	0.25
(1,2673)	1:A:989:LYS:HB2	1:A:990:VAL:H	4	0.25
(1,2673)	1:A:989:LYS:HB2	1:A:990:VAL:H	6	0.25
(1,2673)	1:A:989:LYS:HB2	1:A:990:VAL:H	7	0.25
(1,2673)	1:A:989:LYS:HB2	1:A:990:VAL:H	11	0.25
(1,2673)	1:A:989:LYS:HB2	1:A:990:VAL:H	13	0.25
(1,2582)	1:A:985:LEU:HA	1:A:989:LYS:H	7	0.25
(1,2572)	1:A:985:LEU:HA	1:A:988:TRP:H	2	0.25
(1,2572)	1:A:985:LEU:HA	1:A:988:TRP:H	6	0.25
(1,2568)	1:A:985:LEU:HA	1:A:987:MET:H	12	0.25
(1,2543)	1:A:984:VAL:HA	1:A:988:TRP:HB3	12	0.25
(1,2533)	1:A:984:VAL:HA	1:A:987:MET:H	3	0.25
(1,2533)	1:A:984:VAL:HA	1:A:987:MET:H	5	0.25
(1,2533)	1:A:984:VAL:HA	1:A:987:MET:H	7	0.25
(1,2533)	1:A:984:VAL:HA	1:A:987:MET:H	17	0.25
(1,2533)	1:A:984:VAL:HA	1:A:987:MET:H	20	0.25
(1,2509)	1:A:983:LEU:HA	1:A:985:LEU:H	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2509)	1:A:983:LEU:HA	1:A:985:LEU:H	15	0.25
(1,2476)	1:A:982:ILE:H	1:A:984:VAL:H	8	0.25
(1,2476)	1:A:982:ILE:H	1:A:984:VAL:H	15	0.25
(1,2476)	1:A:982:ILE:H	1:A:984:VAL:H	18	0.25
(1,2474)	1:A:982:ILE:H	1:A:983:LEU:HB3	4	0.25
(1,243)	1:A:972:GLY:H	1:A:976:GLY:H	18	0.25
(1,2372)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	13	0.25
(1,2326)	1:A:972:GLY:H	1:A:976:GLY:H	18	0.25
(1,2202)	1:A:967:TRP:HB2	1:A:968:TRP:H	9	0.25
(1,2201)	1:A:967:TRP:HA	1:A:968:TRP:HB3	1	0.25
(1,2097)	1:A:962:ARG:H	1:A:962:ARG:HB2	2	0.25
(1,2097)	1:A:962:ARG:H	1:A:962:ARG:HB2	18	0.25
(1,2088)	1:A:960:GLU:HA	1:A:961:GLU:H	8	0.25
(1,2047)	1:A:979:LEU:H	2:B:704:ILE:HB	6	0.25
(1,2018)	1:A:973:VAL:H	2:B:700:VAL:HA	14	0.25
(1,1963)	2:B:756:ASN:HA	2:B:757:ILE:H	2	0.25
(1,1915)	2:B:749:GLU:H	2:B:749:GLU:HB3	1	0.25
(1,1915)	2:B:749:GLU:H	2:B:749:GLU:HB3	20	0.25
(1,1890)	2:B:747:TYR:HB2	2:B:748:LYS:H	5	0.25
(1,1890)	2:B:747:TYR:HB2	2:B:748:LYS:H	6	0.25
(1,1862)	2:B:745:PRO:HA	2:B:746:LEU:H	13	0.25
(1,1828)	2:B:743:ASN:HB3	2:B:743:ASN:H	14	0.25
(1,1819)	2:B:742:ALA:HA	2:B:743:ASN:H	8	0.25
(1,1787)	2:B:738:LYS:HA	2:B:740:ASP:H	1	0.25
(1,1787)	2:B:738:LYS:HA	2:B:740:ASP:H	4	0.25
(1,1787)	2:B:738:LYS:HA	2:B:740:ASP:H	5	0.25
(1,1787)	2:B:738:LYS:HA	2:B:740:ASP:H	6	0.25
(1,1787)	2:B:738:LYS:HA	2:B:740:ASP:H	12	0.25
(1,1787)	2:B:738:LYS:HA	2:B:740:ASP:H	19	0.25
(1,14)	1:A:962:ARG:H	1:A:962:ARG:HB2	2	0.25
(1,14)	1:A:962:ARG:H	1:A:962:ARG:HB2	18	0.25
(1,1220)	2:B:708:GLY:H	2:B:710:ALA:H	2	0.25
(1,1220)	2:B:708:GLY:H	2:B:710:ALA:H	10	0.25
(1,1220)	2:B:708:GLY:H	2:B:710:ALA:H	13	0.25
(1,119)	1:A:967:TRP:HB2	1:A:968:TRP:H	9	0.25
(1,118)	1:A:967:TRP:HA	1:A:968:TRP:HB3	1	0.25
(1,841)	2:B:691:PRO:HD3	2:B:692:ASP:H	13	0.24
(1,81)	1:A:966:ILE:H	1:A:966:ILE:HG13	10	0.24
(1,81)	1:A:966:ILE:H	1:A:966:ILE:HG13	16	0.24
(1,81)	1:A:966:ILE:H	1:A:966:ILE:HG13	17	0.24
(1,762)	1:A:997:ARG:HA	1:A:999:PRO:HD2	13	0.24
(1,761)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	13	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,750)	1:A:996:ASN:HA	1:A:997:ARG:H	9	0.24
(1,741)	1:A:995:ARG:HB3	1:A:997:ARG:H	10	0.24
(1,741)	1:A:995:ARG:HB3	1:A:997:ARG:H	16	0.24
(1,645)	1:A:990:VAL:HB	1:A:993:PHE:H	14	0.24
(1,590)	1:A:989:LYS:HB2	1:A:990:VAL:H	1	0.24
(1,590)	1:A:989:LYS:HB2	1:A:990:VAL:H	2	0.24
(1,590)	1:A:989:LYS:HB2	1:A:990:VAL:H	16	0.24
(1,577)	1:A:989:LYS:H	1:A:989:LYS:HB3	19	0.24
(1,576)	1:A:989:LYS:H	1:A:989:LYS:HD3	9	0.24
(1,576)	1:A:989:LYS:H	1:A:989:LYS:HD3	14	0.24
(1,519)	1:A:986:ALA:HA	1:A:989:LYS:H	10	0.24
(1,519)	1:A:986:ALA:HA	1:A:989:LYS:H	11	0.24
(1,5)	1:A:960:GLU:HA	1:A:961:GLU:H	18	0.24
(1,499)	1:A:985:LEU:HA	1:A:989:LYS:H	1	0.24
(1,499)	1:A:985:LEU:HA	1:A:989:LYS:H	3	0.24
(1,499)	1:A:985:LEU:HA	1:A:989:LYS:H	4	0.24
(1,499)	1:A:985:LEU:HA	1:A:989:LYS:H	13	0.24
(1,489)	1:A:985:LEU:HA	1:A:988:TRP:H	7	0.24
(1,489)	1:A:985:LEU:HA	1:A:988:TRP:H	20	0.24
(1,488)	1:A:985:LEU:H	1:A:987:MET:HG3	1	0.24
(1,460)	1:A:984:VAL:HA	1:A:988:TRP:HB3	16	0.24
(1,437)	1:A:984:VAL:H	1:A:984:VAL:HG11	3	0.24
(1,437)	1:A:984:VAL:H	1:A:984:VAL:HG12	3	0.24
(1,437)	1:A:984:VAL:H	1:A:984:VAL:HG13	3	0.24
(1,437)	1:A:984:VAL:H	1:A:984:VAL:HG11	13	0.24
(1,437)	1:A:984:VAL:H	1:A:984:VAL:HG12	13	0.24
(1,437)	1:A:984:VAL:H	1:A:984:VAL:HG13	13	0.24
(1,426)	1:A:983:LEU:HA	1:A:985:LEU:H	13	0.24
(1,423)	1:A:983:LEU:H	1:A:985:LEU:H	2	0.24
(1,4151)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	8	0.24
(1,4130)	1:A:979:LEU:H	2:B:704:ILE:HB	1	0.24
(1,4130)	1:A:979:LEU:H	2:B:704:ILE:HB	10	0.24
(1,4130)	1:A:979:LEU:H	2:B:704:ILE:HB	17	0.24
(1,4130)	1:A:979:LEU:H	2:B:704:ILE:HB	19	0.24
(1,4033)	2:B:754:PHE:HA	2:B:755:THR:H	10	0.24
(1,3998)	2:B:749:GLU:H	2:B:749:GLU:HB3	3	0.24
(1,3998)	2:B:749:GLU:H	2:B:749:GLU:HB3	9	0.24
(1,3998)	2:B:749:GLU:H	2:B:749:GLU:HB3	17	0.24
(1,3973)	2:B:747:TYR:HB2	2:B:748:LYS:H	17	0.24
(1,3945)	2:B:745:PRO:HA	2:B:746:LEU:H	1	0.24
(1,3945)	2:B:745:PRO:HA	2:B:746:LEU:H	5	0.24
(1,393)	1:A:982:ILE:H	1:A:984:VAL:H	3	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,393)	1:A:982:ILE:H	1:A:984:VAL:H	13	0.24
(1,393)	1:A:982:ILE:H	1:A:984:VAL:H	20	0.24
(1,3918)	2:B:743:ASN:HA	2:B:744:ASN:H	2	0.24
(1,3918)	2:B:743:ASN:HA	2:B:744:ASN:H	19	0.24
(1,391)	1:A:982:ILE:H	1:A:983:LEU:HB3	3	0.24
(1,391)	1:A:982:ILE:H	1:A:983:LEU:HB3	6	0.24
(1,391)	1:A:982:ILE:H	1:A:983:LEU:HB3	13	0.24
(1,3902)	2:B:742:ALA:HA	2:B:743:ASN:H	1	0.24
(1,3902)	2:B:742:ALA:HA	2:B:743:ASN:H	10	0.24
(1,3897)	2:B:741:THR:HA	2:B:744:ASN:H	3	0.24
(1,3888)	2:B:740:ASP:HA	2:B:741:THR:H	2	0.24
(1,3888)	2:B:740:ASP:HA	2:B:741:THR:H	20	0.24
(1,3870)	2:B:738:LYS:HA	2:B:740:ASP:H	2	0.24
(1,3870)	2:B:738:LYS:HA	2:B:740:ASP:H	3	0.24
(1,3870)	2:B:738:LYS:HA	2:B:740:ASP:H	10	0.24
(1,3870)	2:B:738:LYS:HA	2:B:740:ASP:H	14	0.24
(1,3870)	2:B:738:LYS:HA	2:B:740:ASP:H	17	0.24
(1,3870)	2:B:738:LYS:HA	2:B:740:ASP:H	20	0.24
(1,3646)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	8	0.24
(1,3579)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	6	0.24
(1,3303)	2:B:708:GLY:H	2:B:710:ALA:H	14	0.24
(1,2924)	2:B:691:PRO:HD3	2:B:692:ASP:H	13	0.24
(1,2845)	1:A:997:ARG:HA	1:A:999:PRO:HD2	13	0.24
(1,2844)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	13	0.24
(1,2833)	1:A:996:ASN:HA	1:A:997:ARG:H	9	0.24
(1,2824)	1:A:995:ARG:HB3	1:A:997:ARG:H	10	0.24
(1,2824)	1:A:995:ARG:HB3	1:A:997:ARG:H	16	0.24
(1,273)	1:A:974:LEU:H	1:A:975:GLY:HA2	7	0.24
(1,2728)	1:A:990:VAL:HB	1:A:993:PHE:H	14	0.24
(1,2673)	1:A:989:LYS:HB2	1:A:990:VAL:H	1	0.24
(1,2673)	1:A:989:LYS:HB2	1:A:990:VAL:H	2	0.24
(1,2673)	1:A:989:LYS:HB2	1:A:990:VAL:H	16	0.24
(1,2660)	1:A:989:LYS:H	1:A:989:LYS:HB3	19	0.24
(1,2659)	1:A:989:LYS:H	1:A:989:LYS:HD3	9	0.24
(1,2659)	1:A:989:LYS:H	1:A:989:LYS:HD3	14	0.24
(1,2602)	1:A:986:ALA:HA	1:A:989:LYS:H	10	0.24
(1,2602)	1:A:986:ALA:HA	1:A:989:LYS:H	11	0.24
(1,2582)	1:A:985:LEU:HA	1:A:989:LYS:H	1	0.24
(1,2582)	1:A:985:LEU:HA	1:A:989:LYS:H	3	0.24
(1,2582)	1:A:985:LEU:HA	1:A:989:LYS:H	4	0.24
(1,2582)	1:A:985:LEU:HA	1:A:989:LYS:H	13	0.24
(1,2572)	1:A:985:LEU:HA	1:A:988:TRP:H	7	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2572)	1:A:985:LEU:HA	1:A:988:TRP:H	20	0.24
(1,2571)	1:A:985:LEU:H	1:A:987:MET:HG3	1	0.24
(1,2543)	1:A:984:VAL:HA	1:A:988:TRP:HB3	16	0.24
(1,2520)	1:A:984:VAL:H	1:A:984:VAL:HG11	3	0.24
(1,2520)	1:A:984:VAL:H	1:A:984:VAL:HG12	3	0.24
(1,2520)	1:A:984:VAL:H	1:A:984:VAL:HG13	3	0.24
(1,2520)	1:A:984:VAL:H	1:A:984:VAL:HG11	13	0.24
(1,2520)	1:A:984:VAL:H	1:A:984:VAL:HG12	13	0.24
(1,2520)	1:A:984:VAL:H	1:A:984:VAL:HG13	13	0.24
(1,2509)	1:A:983:LEU:HA	1:A:985:LEU:H	13	0.24
(1,2506)	1:A:983:LEU:H	1:A:985:LEU:H	2	0.24
(1,2476)	1:A:982:ILE:H	1:A:984:VAL:H	3	0.24
(1,2476)	1:A:982:ILE:H	1:A:984:VAL:H	13	0.24
(1,2476)	1:A:982:ILE:H	1:A:984:VAL:H	20	0.24
(1,2474)	1:A:982:ILE:H	1:A:983:LEU:HB3	3	0.24
(1,2474)	1:A:982:ILE:H	1:A:983:LEU:HB3	6	0.24
(1,2474)	1:A:982:ILE:H	1:A:983:LEU:HB3	13	0.24
(1,2356)	1:A:974:LEU:H	1:A:975:GLY:HA2	7	0.24
(1,2308)	1:A:971:VAL:H	1:A:973:VAL:H	11	0.24
(1,2278)	1:A:970:LEU:HD11	1:A:970:LEU:HA	8	0.24
(1,2278)	1:A:970:LEU:HD12	1:A:970:LEU:HA	8	0.24
(1,2278)	1:A:970:LEU:HD13	1:A:970:LEU:HA	8	0.24
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD21	1	0.24
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD22	1	0.24
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD23	1	0.24
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD21	4	0.24
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD22	4	0.24
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD23	4	0.24
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD21	18	0.24
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD22	18	0.24
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD23	18	0.24
(1,225)	1:A:971:VAL:H	1:A:973:VAL:H	11	0.24
(1,2224)	1:A:968:TRP:HB2	1:A:969:VAL:H	7	0.24
(1,2202)	1:A:967:TRP:HB2	1:A:968:TRP:H	10	0.24
(1,2202)	1:A:967:TRP:HB2	1:A:968:TRP:H	16	0.24
(1,2201)	1:A:967:TRP:HA	1:A:968:TRP:HB3	18	0.24
(1,2164)	1:A:966:ILE:H	1:A:966:ILE:HG13	10	0.24
(1,2164)	1:A:966:ILE:H	1:A:966:ILE:HG13	16	0.24
(1,2164)	1:A:966:ILE:H	1:A:966:ILE:HG13	17	0.24
(1,2088)	1:A:960:GLU:HA	1:A:961:GLU:H	18	0.24
(1,2068)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	8	0.24
(1,2047)	1:A:979:LEU:H	2:B:704:ILE:HB	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2047)	1:A:979:LEU:H	2:B:704:ILE:HB	10	0.24
(1,2047)	1:A:979:LEU:H	2:B:704:ILE:HB	17	0.24
(1,2047)	1:A:979:LEU:H	2:B:704:ILE:HB	19	0.24
(1,1950)	2:B:754:PHE:HA	2:B:755:THR:H	10	0.24
(1,195)	1:A:970:LEU:HD11	1:A:970:LEU:HA	8	0.24
(1,195)	1:A:970:LEU:HD12	1:A:970:LEU:HA	8	0.24
(1,195)	1:A:970:LEU:HD13	1:A:970:LEU:HA	8	0.24
(1,1915)	2:B:749:GLU:H	2:B:749:GLU:HB3	3	0.24
(1,1915)	2:B:749:GLU:H	2:B:749:GLU:HB3	9	0.24
(1,1915)	2:B:749:GLU:H	2:B:749:GLU:HB3	17	0.24
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD21	1	0.24
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD22	1	0.24
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD23	1	0.24
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD21	4	0.24
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD22	4	0.24
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD23	4	0.24
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD21	18	0.24
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD22	18	0.24
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD23	18	0.24
(1,1890)	2:B:747:TYR:HB2	2:B:748:LYS:H	17	0.24
(1,1862)	2:B:745:PRO:HA	2:B:746:LEU:H	1	0.24
(1,1862)	2:B:745:PRO:HA	2:B:746:LEU:H	5	0.24
(1,1835)	2:B:743:ASN:HA	2:B:744:ASN:H	2	0.24
(1,1835)	2:B:743:ASN:HA	2:B:744:ASN:H	19	0.24
(1,1819)	2:B:742:ALA:HA	2:B:743:ASN:H	1	0.24
(1,1819)	2:B:742:ALA:HA	2:B:743:ASN:H	10	0.24
(1,1814)	2:B:741:THR:HA	2:B:744:ASN:H	3	0.24
(1,1805)	2:B:740:ASP:HA	2:B:741:THR:H	2	0.24
(1,1805)	2:B:740:ASP:HA	2:B:741:THR:H	20	0.24
(1,1787)	2:B:738:LYS:HA	2:B:740:ASP:H	2	0.24
(1,1787)	2:B:738:LYS:HA	2:B:740:ASP:H	3	0.24
(1,1787)	2:B:738:LYS:HA	2:B:740:ASP:H	10	0.24
(1,1787)	2:B:738:LYS:HA	2:B:740:ASP:H	14	0.24
(1,1787)	2:B:738:LYS:HA	2:B:740:ASP:H	17	0.24
(1,1787)	2:B:738:LYS:HA	2:B:740:ASP:H	20	0.24
(1,1563)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	8	0.24
(1,1496)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	6	0.24
(1,141)	1:A:968:TRP:HB2	1:A:969:VAL:H	7	0.24
(1,1220)	2:B:708:GLY:H	2:B:710:ALA:H	14	0.24
(1,119)	1:A:967:TRP:HB2	1:A:968:TRP:H	10	0.24
(1,119)	1:A:967:TRP:HB2	1:A:968:TRP:H	16	0.24
(1,118)	1:A:967:TRP:HA	1:A:968:TRP:HB3	18	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,848)	2:B:692:ASP:H	2:B:692:ASP:HB3	8	0.23
(1,843)	2:B:691:PRO:HB3	2:B:692:ASP:H	20	0.23
(1,81)	1:A:966:ILE:H	1:A:966:ILE:HG13	9	0.23
(1,81)	1:A:966:ILE:H	1:A:966:ILE:HG13	14	0.23
(1,762)	1:A:997:ARG:HA	1:A:999:PRO:HD2	5	0.23
(1,762)	1:A:997:ARG:HA	1:A:999:PRO:HD2	6	0.23
(1,761)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	17	0.23
(1,741)	1:A:995:ARG:HB3	1:A:997:ARG:H	5	0.23
(1,684)	1:A:993:PHE:HB3	1:A:993:PHE:H	18	0.23
(1,672)	1:A:992:PHE:HB3	1:A:993:PHE:H	1	0.23
(1,645)	1:A:990:VAL:HB	1:A:993:PHE:H	11	0.23
(1,590)	1:A:989:LYS:HB2	1:A:990:VAL:H	8	0.23
(1,590)	1:A:989:LYS:HB2	1:A:990:VAL:H	17	0.23
(1,533)	1:A:987:MET:H	1:A:987:MET:HG2	8	0.23
(1,519)	1:A:986:ALA:HA	1:A:989:LYS:H	8	0.23
(1,516)	1:A:986:ALA:HA	1:A:988:TRP:H	4	0.23
(1,516)	1:A:986:ALA:HA	1:A:988:TRP:H	20	0.23
(1,489)	1:A:985:LEU:HA	1:A:988:TRP:H	4	0.23
(1,489)	1:A:985:LEU:HA	1:A:988:TRP:H	10	0.23
(1,460)	1:A:984:VAL:HA	1:A:988:TRP:HB3	13	0.23
(1,460)	1:A:984:VAL:HA	1:A:988:TRP:HB3	18	0.23
(1,450)	1:A:984:VAL:HA	1:A:987:MET:H	13	0.23
(1,423)	1:A:983:LEU:H	1:A:985:LEU:H	7	0.23
(1,423)	1:A:983:LEU:H	1:A:985:LEU:H	15	0.23
(1,4162)	1:A:988:TRP:HE1	2:B:719:ILE:HB	7	0.23
(1,4143)	1:A:984:VAL:H	2:B:712:LEU:HA	7	0.23
(1,4143)	1:A:984:VAL:H	2:B:712:LEU:HA	8	0.23
(1,4143)	1:A:984:VAL:H	2:B:712:LEU:HA	9	0.23
(1,4130)	1:A:979:LEU:H	2:B:704:ILE:HB	9	0.23
(1,4033)	2:B:754:PHE:HA	2:B:755:THR:H	2	0.23
(1,4000)	2:B:749:GLU:H	2:B:749:GLU:HG3	4	0.23
(1,4000)	2:B:749:GLU:H	2:B:749:GLU:HG3	15	0.23
(1,3998)	2:B:749:GLU:H	2:B:749:GLU:HB3	4	0.23
(1,3998)	2:B:749:GLU:H	2:B:749:GLU:HB3	14	0.23
(1,3998)	2:B:749:GLU:H	2:B:749:GLU:HB3	16	0.23
(1,3973)	2:B:747:TYR:HB2	2:B:748:LYS:H	13	0.23
(1,3973)	2:B:747:TYR:HB2	2:B:748:LYS:H	20	0.23
(1,393)	1:A:982:ILE:H	1:A:984:VAL:H	10	0.23
(1,391)	1:A:982:ILE:H	1:A:983:LEU:HB3	1	0.23
(1,391)	1:A:982:ILE:H	1:A:983:LEU:HB3	7	0.23
(1,391)	1:A:982:ILE:H	1:A:983:LEU:HB3	15	0.23
(1,391)	1:A:982:ILE:H	1:A:983:LEU:HB3	20	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3902)	2:B:742:ALA:HA	2:B:743:ASN:H	11	0.23
(1,3902)	2:B:742:ALA:HA	2:B:743:ASN:H	20	0.23
(1,3897)	2:B:741:THR:HA	2:B:744:ASN:H	13	0.23
(1,3888)	2:B:740:ASP:HA	2:B:741:THR:H	13	0.23
(1,3870)	2:B:738:LYS:HA	2:B:740:ASP:H	11	0.23
(1,3870)	2:B:738:LYS:HA	2:B:740:ASP:H	13	0.23
(1,3870)	2:B:738:LYS:HA	2:B:740:ASP:H	16	0.23
(1,3852)	2:B:738:LYS:H	2:B:738:LYS:HG3	8	0.23
(1,3646)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	1	0.23
(1,3646)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	19	0.23
(1,3579)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	16	0.23
(1,356)	1:A:980:LEU:HB3	1:A:981:THR:HA	14	0.23
(1,3470)	2:B:717:LEU:H	2:B:719:ILE:H	3	0.23
(1,342)	1:A:979:LEU:HA	1:A:982:ILE:HB	12	0.23
(1,312)	1:A:977:LEU:HD11	1:A:977:LEU:HA	14	0.23
(1,312)	1:A:977:LEU:HD12	1:A:977:LEU:HA	14	0.23
(1,312)	1:A:977:LEU:HD13	1:A:977:LEU:HA	14	0.23
(1,2931)	2:B:692:ASP:H	2:B:692:ASP:HB3	8	0.23
(1,2926)	2:B:691:PRO:HB3	2:B:692:ASP:H	20	0.23
(1,2845)	1:A:997:ARG:HA	1:A:999:PRO:HD2	5	0.23
(1,2845)	1:A:997:ARG:HA	1:A:999:PRO:HD2	6	0.23
(1,2844)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	17	0.23
(1,2824)	1:A:995:ARG:HB3	1:A:997:ARG:H	5	0.23
(1,2767)	1:A:993:PHE:HB3	1:A:993:PHE:H	18	0.23
(1,2755)	1:A:992:PHE:HB3	1:A:993:PHE:H	1	0.23
(1,273)	1:A:974:LEU:H	1:A:975:GLY:HA2	20	0.23
(1,2728)	1:A:990:VAL:HB	1:A:993:PHE:H	11	0.23
(1,2673)	1:A:989:LYS:HB2	1:A:990:VAL:H	8	0.23
(1,2673)	1:A:989:LYS:HB2	1:A:990:VAL:H	17	0.23
(1,2616)	1:A:987:MET:H	1:A:987:MET:HG2	8	0.23
(1,2602)	1:A:986:ALA:HA	1:A:989:LYS:H	8	0.23
(1,2599)	1:A:986:ALA:HA	1:A:988:TRP:H	4	0.23
(1,2599)	1:A:986:ALA:HA	1:A:988:TRP:H	20	0.23
(1,2572)	1:A:985:LEU:HA	1:A:988:TRP:H	4	0.23
(1,2572)	1:A:985:LEU:HA	1:A:988:TRP:H	10	0.23
(1,2543)	1:A:984:VAL:HA	1:A:988:TRP:HB3	13	0.23
(1,2543)	1:A:984:VAL:HA	1:A:988:TRP:HB3	18	0.23
(1,2533)	1:A:984:VAL:HA	1:A:987:MET:H	13	0.23
(1,2506)	1:A:983:LEU:H	1:A:985:LEU:H	7	0.23
(1,2506)	1:A:983:LEU:H	1:A:985:LEU:H	15	0.23
(1,2476)	1:A:982:ILE:H	1:A:984:VAL:H	10	0.23
(1,2474)	1:A:982:ILE:H	1:A:983:LEU:HB3	1	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2474)	1:A:982:ILE:H	1:A:983:LEU:HB3	7	0.23
(1,2474)	1:A:982:ILE:H	1:A:983:LEU:HB3	15	0.23
(1,2474)	1:A:982:ILE:H	1:A:983:LEU:HB3	20	0.23
(1,2439)	1:A:980:LEU:HB3	1:A:981:THR:HA	14	0.23
(1,2425)	1:A:979:LEU:HA	1:A:982:ILE:HB	12	0.23
(1,2395)	1:A:977:LEU:HD11	1:A:977:LEU:HA	14	0.23
(1,2395)	1:A:977:LEU:HD12	1:A:977:LEU:HA	14	0.23
(1,2395)	1:A:977:LEU:HD13	1:A:977:LEU:HA	14	0.23
(1,2356)	1:A:974:LEU:H	1:A:975:GLY:HA2	20	0.23
(1,2278)	1:A:970:LEU:HD11	1:A:970:LEU:HA	12	0.23
(1,2278)	1:A:970:LEU:HD12	1:A:970:LEU:HA	12	0.23
(1,2278)	1:A:970:LEU:HD13	1:A:970:LEU:HA	12	0.23
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD21	20	0.23
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD22	20	0.23
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD23	20	0.23
(1,2224)	1:A:968:TRP:HB2	1:A:969:VAL:H	12	0.23
(1,2208)	1:A:967:TRP:H	1:A:970:LEU:H	14	0.23
(1,2202)	1:A:967:TRP:HB2	1:A:968:TRP:H	6	0.23
(1,2201)	1:A:967:TRP:HA	1:A:968:TRP:HB3	16	0.23
(1,2164)	1:A:966:ILE:H	1:A:966:ILE:HG13	9	0.23
(1,2164)	1:A:966:ILE:H	1:A:966:ILE:HG13	14	0.23
(1,2097)	1:A:962:ARG:H	1:A:962:ARG:HB2	17	0.23
(1,2079)	1:A:988:TRP:HE1	2:B:719:ILE:HB	7	0.23
(1,2060)	1:A:984:VAL:H	2:B:712:LEU:HA	7	0.23
(1,2060)	1:A:984:VAL:H	2:B:712:LEU:HA	8	0.23
(1,2060)	1:A:984:VAL:H	2:B:712:LEU:HA	9	0.23
(1,2047)	1:A:979:LEU:H	2:B:704:ILE:HB	9	0.23
(1,1950)	2:B:754:PHE:HA	2:B:755:THR:H	2	0.23
(1,195)	1:A:970:LEU:HD11	1:A:970:LEU:HA	12	0.23
(1,195)	1:A:970:LEU:HD12	1:A:970:LEU:HA	12	0.23
(1,195)	1:A:970:LEU:HD13	1:A:970:LEU:HA	12	0.23
(1,1917)	2:B:749:GLU:H	2:B:749:GLU:HG3	4	0.23
(1,1917)	2:B:749:GLU:H	2:B:749:GLU:HG3	15	0.23
(1,1915)	2:B:749:GLU:H	2:B:749:GLU:HB3	4	0.23
(1,1915)	2:B:749:GLU:H	2:B:749:GLU:HB3	14	0.23
(1,1915)	2:B:749:GLU:H	2:B:749:GLU:HB3	16	0.23
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD21	20	0.23
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD22	20	0.23
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD23	20	0.23
(1,1890)	2:B:747:TYR:HB2	2:B:748:LYS:H	13	0.23
(1,1890)	2:B:747:TYR:HB2	2:B:748:LYS:H	20	0.23
(1,1819)	2:B:742:ALA:HA	2:B:743:ASN:H	11	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1819)	2:B:742:ALA:HA	2:B:743:ASN:H	20	0.23
(1,1814)	2:B:741:THR:HA	2:B:744:ASN:H	13	0.23
(1,1805)	2:B:740:ASP:HA	2:B:741:THR:H	13	0.23
(1,1787)	2:B:738:LYS:HA	2:B:740:ASP:H	11	0.23
(1,1787)	2:B:738:LYS:HA	2:B:740:ASP:H	13	0.23
(1,1787)	2:B:738:LYS:HA	2:B:740:ASP:H	16	0.23
(1,1769)	2:B:738:LYS:H	2:B:738:LYS:HG3	8	0.23
(1,1563)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	1	0.23
(1,1563)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	19	0.23
(1,1496)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	16	0.23
(1,141)	1:A:968:TRP:HB2	1:A:969:VAL:H	12	0.23
(1,14)	1:A:962:ARG:H	1:A:962:ARG:HB2	17	0.23
(1,1387)	2:B:717:LEU:H	2:B:719:ILE:H	3	0.23
(1,125)	1:A:967:TRP:H	1:A:970:LEU:H	14	0.23
(1,119)	1:A:967:TRP:HB2	1:A:968:TRP:H	6	0.23
(1,118)	1:A:967:TRP:HA	1:A:968:TRP:HB3	16	0.23
(1,870)	2:B:693:ILE:H	2:B:693:ILE:HB	14	0.22
(1,850)	2:B:692:ASP:HA	2:B:693:ILE:H	6	0.22
(1,843)	2:B:691:PRO:HB3	2:B:692:ASP:H	2	0.22
(1,81)	1:A:966:ILE:H	1:A:966:ILE:HG13	11	0.22
(1,8)	1:A:961:GLU:H	1:A:961:GLU:HB3	12	0.22
(1,787)	1:A:1000:LEU:HA	1:A:1001:GLU:H	16	0.22
(1,762)	1:A:997:ARG:HA	1:A:999:PRO:HD2	18	0.22
(1,761)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	12	0.22
(1,751)	1:A:996:ASN:H	1:A:997:ARG:H	5	0.22
(1,740)	1:A:995:ARG:H	1:A:996:ASN:H	18	0.22
(1,725)	1:A:994:LYS:HB3	1:A:995:ARG:HG3	20	0.22
(1,672)	1:A:992:PHE:HB3	1:A:993:PHE:H	19	0.22
(1,645)	1:A:990:VAL:HB	1:A:993:PHE:H	10	0.22
(1,590)	1:A:989:LYS:HB2	1:A:990:VAL:H	9	0.22
(1,590)	1:A:989:LYS:HB2	1:A:990:VAL:H	10	0.22
(1,590)	1:A:989:LYS:HB2	1:A:990:VAL:H	12	0.22
(1,499)	1:A:985:LEU:HA	1:A:989:LYS:H	12	0.22
(1,499)	1:A:985:LEU:HA	1:A:989:LYS:H	17	0.22
(1,489)	1:A:985:LEU:HA	1:A:988:TRP:H	17	0.22
(1,450)	1:A:984:VAL:HA	1:A:987:MET:H	4	0.22
(1,450)	1:A:984:VAL:HA	1:A:987:MET:H	11	0.22
(1,450)	1:A:984:VAL:HA	1:A:987:MET:H	16	0.22
(1,45)	1:A:964:ILE:HB	1:A:965:PRO:HD3	2	0.22
(1,45)	1:A:964:ILE:HB	1:A:965:PRO:HD3	6	0.22
(1,44)	1:A:964:ILE:H	1:A:965:PRO:HB2	13	0.22
(1,426)	1:A:983:LEU:HA	1:A:985:LEU:H	5	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,426)	1:A:983:LEU:HA	1:A:985:LEU:H	20	0.22
(1,423)	1:A:983:LEU:H	1:A:985:LEU:H	5	0.22
(1,423)	1:A:983:LEU:H	1:A:985:LEU:H	9	0.22
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG21	15	0.22
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG22	15	0.22
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG23	15	0.22
(1,4151)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	12	0.22
(1,4151)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	14	0.22
(1,4143)	1:A:984:VAL:H	2:B:712:LEU:HA	6	0.22
(1,4143)	1:A:984:VAL:H	2:B:712:LEU:HA	10	0.22
(1,4143)	1:A:984:VAL:H	2:B:712:LEU:HA	19	0.22
(1,4077)	2:B:760:ARG:H	2:B:760:ARG:HB2	9	0.22
(1,4004)	2:B:749:GLU:HB2	2:B:750:ALA:H	10	0.22
(1,4000)	2:B:749:GLU:H	2:B:749:GLU:HG3	14	0.22
(1,3998)	2:B:749:GLU:H	2:B:749:GLU:HB3	15	0.22
(1,3973)	2:B:747:TYR:HB2	2:B:748:LYS:H	4	0.22
(1,3973)	2:B:747:TYR:HB2	2:B:748:LYS:H	11	0.22
(1,393)	1:A:982:ILE:H	1:A:984:VAL:H	9	0.22
(1,393)	1:A:982:ILE:H	1:A:984:VAL:H	11	0.22
(1,393)	1:A:982:ILE:H	1:A:984:VAL:H	14	0.22
(1,393)	1:A:982:ILE:H	1:A:984:VAL:H	19	0.22
(1,391)	1:A:982:ILE:H	1:A:983:LEU:HB3	18	0.22
(1,3902)	2:B:742:ALA:HA	2:B:743:ASN:H	4	0.22
(1,3897)	2:B:741:THR:HA	2:B:744:ASN:H	8	0.22
(1,3897)	2:B:741:THR:HA	2:B:744:ASN:H	11	0.22
(1,3863)	2:B:738:LYS:HB3	2:B:739:TRP:H	9	0.22
(1,3859)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	2	0.22
(1,3859)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	17	0.22
(1,3742)	2:B:730:PHE:HB3	2:B:731:GLU:HG2	11	0.22
(1,3742)	2:B:730:PHE:HB3	2:B:731:GLU:HG2	13	0.22
(1,3646)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	13	0.22
(1,3579)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	14	0.22
(1,356)	1:A:980:LEU:HB3	1:A:981:THR:HA	16	0.22
(1,341)	1:A:979:LEU:HA	1:A:981:THR:H	14	0.22
(1,3319)	2:B:709:LEU:H	2:B:711:ALA:H	10	0.22
(1,3319)	2:B:709:LEU:H	2:B:711:ALA:H	17	0.22
(1,3303)	2:B:708:GLY:H	2:B:710:ALA:H	5	0.22
(1,3303)	2:B:708:GLY:H	2:B:710:ALA:H	8	0.22
(1,3303)	2:B:708:GLY:H	2:B:710:ALA:H	9	0.22
(1,3211)	2:B:704:ILE:HB	2:B:705:LEU:HB2	8	0.22
(1,3211)	2:B:704:ILE:HB	2:B:705:LEU:HB2	10	0.22
(1,3211)	2:B:704:ILE:HB	2:B:705:LEU:HB2	13	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3211)	2:B:704:ILE:HB	2:B:705:LEU:HB2	15	0.22
(1,2953)	2:B:693:ILE:H	2:B:693:ILE:HB	14	0.22
(1,2933)	2:B:692:ASP:HA	2:B:693:ILE:H	6	0.22
(1,2926)	2:B:691:PRO:HB3	2:B:692:ASP:H	2	0.22
(1,289)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	1	0.22
(1,2870)	1:A:1000:LEU:HA	1:A:1001:GLU:H	16	0.22
(1,2845)	1:A:997:ARG:HA	1:A:999:PRO:HD2	18	0.22
(1,2844)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	12	0.22
(1,2834)	1:A:996:ASN:H	1:A:997:ARG:H	5	0.22
(1,2823)	1:A:995:ARG:H	1:A:996:ASN:H	18	0.22
(1,2808)	1:A:994:LYS:HB3	1:A:995:ARG:HG3	20	0.22
(1,2755)	1:A:992:PHE:HB3	1:A:993:PHE:H	19	0.22
(1,273)	1:A:974:LEU:H	1:A:975:GLY:HA2	14	0.22
(1,2728)	1:A:990:VAL:HB	1:A:993:PHE:H	10	0.22
(1,2673)	1:A:989:LYS:HB2	1:A:990:VAL:H	9	0.22
(1,2673)	1:A:989:LYS:HB2	1:A:990:VAL:H	10	0.22
(1,2673)	1:A:989:LYS:HB2	1:A:990:VAL:H	12	0.22
(1,2582)	1:A:985:LEU:HA	1:A:989:LYS:H	12	0.22
(1,2582)	1:A:985:LEU:HA	1:A:989:LYS:H	17	0.22
(1,2572)	1:A:985:LEU:HA	1:A:988:TRP:H	17	0.22
(1,2533)	1:A:984:VAL:HA	1:A:987:MET:H	4	0.22
(1,2533)	1:A:984:VAL:HA	1:A:987:MET:H	11	0.22
(1,2533)	1:A:984:VAL:HA	1:A:987:MET:H	16	0.22
(1,2509)	1:A:983:LEU:HA	1:A:985:LEU:H	5	0.22
(1,2509)	1:A:983:LEU:HA	1:A:985:LEU:H	20	0.22
(1,2506)	1:A:983:LEU:H	1:A:985:LEU:H	5	0.22
(1,2506)	1:A:983:LEU:H	1:A:985:LEU:H	9	0.22
(1,2476)	1:A:982:ILE:H	1:A:984:VAL:H	9	0.22
(1,2476)	1:A:982:ILE:H	1:A:984:VAL:H	11	0.22
(1,2476)	1:A:982:ILE:H	1:A:984:VAL:H	14	0.22
(1,2476)	1:A:982:ILE:H	1:A:984:VAL:H	19	0.22
(1,2474)	1:A:982:ILE:H	1:A:983:LEU:HB3	18	0.22
(1,2439)	1:A:980:LEU:HB3	1:A:981:THR:HA	16	0.22
(1,243)	1:A:972:GLY:H	1:A:976:GLY:H	14	0.22
(1,2424)	1:A:979:LEU:HA	1:A:981:THR:H	14	0.22
(1,2372)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	1	0.22
(1,2356)	1:A:974:LEU:H	1:A:975:GLY:HA2	14	0.22
(1,2326)	1:A:972:GLY:H	1:A:976:GLY:H	14	0.22
(1,2278)	1:A:970:LEU:HD11	1:A:970:LEU:HA	10	0.22
(1,2278)	1:A:970:LEU:HD12	1:A:970:LEU:HA	10	0.22
(1,2278)	1:A:970:LEU:HD13	1:A:970:LEU:HA	10	0.22
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD21	3	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD22	3	0.22
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD23	3	0.22
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD21	5	0.22
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD22	5	0.22
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD23	5	0.22
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD21	9	0.22
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD22	9	0.22
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD23	9	0.22
(1,2258)	1:A:969:VAL:H	1:A:970:LEU:HB3	4	0.22
(1,2208)	1:A:967:TRP:H	1:A:970:LEU:H	9	0.22
(1,2202)	1:A:967:TRP:HB2	1:A:968:TRP:H	13	0.22
(1,2201)	1:A:967:TRP:HA	1:A:968:TRP:HB3	12	0.22
(1,2201)	1:A:967:TRP:HA	1:A:968:TRP:HB3	13	0.22
(1,2201)	1:A:967:TRP:HA	1:A:968:TRP:HB3	17	0.22
(1,2201)	1:A:967:TRP:HA	1:A:968:TRP:HB3	19	0.22
(1,2164)	1:A:966:ILE:H	1:A:966:ILE:HG13	11	0.22
(1,2128)	1:A:964:ILE:HB	1:A:965:PRO:HD3	2	0.22
(1,2128)	1:A:964:ILE:HB	1:A:965:PRO:HD3	6	0.22
(1,2127)	1:A:964:ILE:H	1:A:965:PRO:HB2	13	0.22
(1,2091)	1:A:961:GLU:H	1:A:961:GLU:HB3	12	0.22
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG21	15	0.22
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG22	15	0.22
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG23	15	0.22
(1,2068)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	12	0.22
(1,2068)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	14	0.22
(1,2060)	1:A:984:VAL:H	2:B:712:LEU:HA	6	0.22
(1,2060)	1:A:984:VAL:H	2:B:712:LEU:HA	10	0.22
(1,2060)	1:A:984:VAL:H	2:B:712:LEU:HA	19	0.22
(1,1994)	2:B:760:ARG:H	2:B:760:ARG:HB2	9	0.22
(1,195)	1:A:970:LEU:HD11	1:A:970:LEU:HA	10	0.22
(1,195)	1:A:970:LEU:HD12	1:A:970:LEU:HA	10	0.22
(1,195)	1:A:970:LEU:HD13	1:A:970:LEU:HA	10	0.22
(1,1921)	2:B:749:GLU:HB2	2:B:750:ALA:H	10	0.22
(1,1917)	2:B:749:GLU:H	2:B:749:GLU:HG3	14	0.22
(1,1915)	2:B:749:GLU:H	2:B:749:GLU:HB3	15	0.22
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD21	3	0.22
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD22	3	0.22
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD23	3	0.22
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD21	5	0.22
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD22	5	0.22
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD23	5	0.22
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD21	9	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD22	9	0.22
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD23	9	0.22
(1,1890)	2:B:747:TYR:HB2	2:B:748:LYS:H	4	0.22
(1,1890)	2:B:747:TYR:HB2	2:B:748:LYS:H	11	0.22
(1,1819)	2:B:742:ALA:HA	2:B:743:ASN:H	4	0.22
(1,1814)	2:B:741:THR:HA	2:B:744:ASN:H	8	0.22
(1,1814)	2:B:741:THR:HA	2:B:744:ASN:H	11	0.22
(1,1780)	2:B:738:LYS:HB3	2:B:739:TRP:H	9	0.22
(1,1776)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	2	0.22
(1,1776)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	17	0.22
(1,175)	1:A:969:VAL:H	1:A:970:LEU:HB3	4	0.22
(1,1659)	2:B:730:PHE:HB3	2:B:731:GLU:HG2	11	0.22
(1,1659)	2:B:730:PHE:HB3	2:B:731:GLU:HG2	13	0.22
(1,1563)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	13	0.22
(1,1496)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	14	0.22
(1,125)	1:A:967:TRP:H	1:A:970:LEU:H	9	0.22
(1,1236)	2:B:709:LEU:H	2:B:711:ALA:H	10	0.22
(1,1236)	2:B:709:LEU:H	2:B:711:ALA:H	17	0.22
(1,1220)	2:B:708:GLY:H	2:B:710:ALA:H	5	0.22
(1,1220)	2:B:708:GLY:H	2:B:710:ALA:H	8	0.22
(1,1220)	2:B:708:GLY:H	2:B:710:ALA:H	9	0.22
(1,119)	1:A:967:TRP:HB2	1:A:968:TRP:H	13	0.22
(1,118)	1:A:967:TRP:HA	1:A:968:TRP:HB3	12	0.22
(1,118)	1:A:967:TRP:HA	1:A:968:TRP:HB3	13	0.22
(1,118)	1:A:967:TRP:HA	1:A:968:TRP:HB3	17	0.22
(1,118)	1:A:967:TRP:HA	1:A:968:TRP:HB3	19	0.22
(1,1128)	2:B:704:ILE:HB	2:B:705:LEU:HB2	8	0.22
(1,1128)	2:B:704:ILE:HB	2:B:705:LEU:HB2	10	0.22
(1,1128)	2:B:704:ILE:HB	2:B:705:LEU:HB2	13	0.22
(1,1128)	2:B:704:ILE:HB	2:B:705:LEU:HB2	15	0.22
(3,270)	2:B:710:ALA:O	2:B:714:ILE:H	16	0.21
(3,111)	2:B:710:ALA:O	2:B:714:ILE:H	16	0.21
(1,850)	2:B:692:ASP:HA	2:B:693:ILE:H	17	0.21
(1,843)	2:B:691:PRO:HB3	2:B:692:ASP:H	3	0.21
(1,843)	2:B:691:PRO:HB3	2:B:692:ASP:H	14	0.21
(1,843)	2:B:691:PRO:HB3	2:B:692:ASP:H	18	0.21
(1,843)	2:B:691:PRO:HB3	2:B:692:ASP:H	19	0.21
(1,841)	2:B:691:PRO:HD3	2:B:692:ASP:H	14	0.21
(1,802)	1:A:1004:ASP:H	1:A:1004:ASP:HB2	2	0.21
(1,755)	1:A:997:ARG:H	1:A:997:ARG:HG3	2	0.21
(1,755)	1:A:997:ARG:H	1:A:997:ARG:HG3	10	0.21
(1,750)	1:A:996:ASN:HA	1:A:997:ARG:H	8	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,742)	1:A:996:ASN:H	1:A:996:ASN:HB2	15	0.21
(1,738)	1:A:995:ARG:HA	1:A:996:ASN:H	8	0.21
(1,738)	1:A:995:ARG:HA	1:A:996:ASN:H	12	0.21
(1,737)	1:A:995:ARG:HB3	1:A:996:ASN:H	11	0.21
(1,712)	1:A:994:LYS:HB2	1:A:994:LYS:HD3	20	0.21
(1,684)	1:A:993:PHE:HB3	1:A:993:PHE:H	11	0.21
(1,672)	1:A:992:PHE:HB3	1:A:993:PHE:H	18	0.21
(1,645)	1:A:990:VAL:HB	1:A:993:PHE:H	8	0.21
(1,576)	1:A:989:LYS:H	1:A:989:LYS:HD3	7	0.21
(1,576)	1:A:989:LYS:H	1:A:989:LYS:HD3	17	0.21
(1,533)	1:A:987:MET:H	1:A:987:MET:HG2	16	0.21
(1,450)	1:A:984:VAL:HA	1:A:987:MET:H	19	0.21
(1,423)	1:A:983:LEU:H	1:A:985:LEU:H	4	0.21
(1,423)	1:A:983:LEU:H	1:A:985:LEU:H	10	0.21
(1,4163)	1:A:988:TRP:HE1	2:B:719:ILE:HG21	15	0.21
(1,4163)	1:A:988:TRP:HE1	2:B:719:ILE:HG22	15	0.21
(1,4163)	1:A:988:TRP:HE1	2:B:719:ILE:HG23	15	0.21
(1,4151)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	6	0.21
(1,4130)	1:A:979:LEU:H	2:B:704:ILE:HB	11	0.21
(1,4102)	1:A:973:VAL:H	2:B:701:MET:HE1	16	0.21
(1,4102)	1:A:973:VAL:H	2:B:701:MET:HE2	16	0.21
(1,4102)	1:A:973:VAL:H	2:B:701:MET:HE3	16	0.21
(1,4101)	1:A:973:VAL:H	2:B:700:VAL:HA	19	0.21
(1,4000)	2:B:749:GLU:H	2:B:749:GLU:HG3	16	0.21
(1,3973)	2:B:747:TYR:HB2	2:B:748:LYS:H	9	0.21
(1,3973)	2:B:747:TYR:HB2	2:B:748:LYS:H	10	0.21
(1,3945)	2:B:745:PRO:HA	2:B:746:LEU:H	8	0.21
(1,3945)	2:B:745:PRO:HA	2:B:746:LEU:H	9	0.21
(1,3945)	2:B:745:PRO:HA	2:B:746:LEU:H	14	0.21
(1,3945)	2:B:745:PRO:HA	2:B:746:LEU:H	16	0.21
(1,391)	1:A:982:ILE:H	1:A:983:LEU:HB3	5	0.21
(1,391)	1:A:982:ILE:H	1:A:983:LEU:HB3	12	0.21
(1,391)	1:A:982:ILE:H	1:A:983:LEU:HB3	16	0.21
(1,391)	1:A:982:ILE:H	1:A:983:LEU:HB3	17	0.21
(1,3909)	2:B:743:ASN:HB2	2:B:743:ASN:H	7	0.21
(1,3909)	2:B:743:ASN:HB2	2:B:743:ASN:H	18	0.21
(1,3902)	2:B:742:ALA:HA	2:B:743:ASN:H	3	0.21
(1,3902)	2:B:742:ALA:HA	2:B:743:ASN:H	13	0.21
(1,3902)	2:B:742:ALA:HA	2:B:743:ASN:H	14	0.21
(1,3897)	2:B:741:THR:HA	2:B:744:ASN:H	9	0.21
(1,3870)	2:B:738:LYS:HA	2:B:740:ASP:H	8	0.21
(1,3870)	2:B:738:LYS:HA	2:B:740:ASP:H	9	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3859)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	5	0.21
(1,3859)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	10	0.21
(1,3852)	2:B:738:LYS:H	2:B:738:LYS:HG3	7	0.21
(1,3850)	2:B:738:LYS:HA	2:B:738:LYS:HD3	7	0.21
(1,3801)	2:B:734:ARG:HD2	2:B:734:ARG:HB2	17	0.21
(1,3801)	2:B:734:ARG:HD2	2:B:734:ARG:HB2	20	0.21
(1,3798)	2:B:734:ARG:HD3	2:B:734:ARG:HB2	6	0.21
(1,3744)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	20	0.21
(1,3718)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	11	0.21
(1,3718)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	12	0.21
(1,3646)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	4	0.21
(1,3646)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	6	0.21
(1,3646)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	20	0.21
(1,3579)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	9	0.21
(1,3495)	2:B:718:LEU:HB3	2:B:719:ILE:HG12	7	0.21
(1,3319)	2:B:709:LEU:H	2:B:711:ALA:H	12	0.21
(1,3319)	2:B:709:LEU:H	2:B:711:ALA:H	20	0.21
(1,3303)	2:B:708:GLY:H	2:B:710:ALA:H	3	0.21
(1,3303)	2:B:708:GLY:H	2:B:710:ALA:H	7	0.21
(1,3303)	2:B:708:GLY:H	2:B:710:ALA:H	20	0.21
(1,3211)	2:B:704:ILE:HB	2:B:705:LEU:HB2	2	0.21
(1,3211)	2:B:704:ILE:HB	2:B:705:LEU:HB2	3	0.21
(1,3211)	2:B:704:ILE:HB	2:B:705:LEU:HB2	4	0.21
(1,3211)	2:B:704:ILE:HB	2:B:705:LEU:HB2	7	0.21
(1,2933)	2:B:692:ASP:HA	2:B:693:ILE:H	17	0.21
(1,2926)	2:B:691:PRO:HB3	2:B:692:ASP:H	3	0.21
(1,2926)	2:B:691:PRO:HB3	2:B:692:ASP:H	14	0.21
(1,2926)	2:B:691:PRO:HB3	2:B:692:ASP:H	18	0.21
(1,2926)	2:B:691:PRO:HB3	2:B:692:ASP:H	19	0.21
(1,2924)	2:B:691:PRO:HD3	2:B:692:ASP:H	14	0.21
(1,2885)	1:A:1004:ASP:H	1:A:1004:ASP:HB2	2	0.21
(1,2838)	1:A:997:ARG:H	1:A:997:ARG:HG3	2	0.21
(1,2838)	1:A:997:ARG:H	1:A:997:ARG:HG3	10	0.21
(1,2833)	1:A:996:ASN:HA	1:A:997:ARG:H	8	0.21
(1,2825)	1:A:996:ASN:H	1:A:996:ASN:HB2	15	0.21
(1,2821)	1:A:995:ARG:HA	1:A:996:ASN:H	8	0.21
(1,2821)	1:A:995:ARG:HA	1:A:996:ASN:H	12	0.21
(1,2820)	1:A:995:ARG:HB3	1:A:996:ASN:H	11	0.21
(1,2795)	1:A:994:LYS:HB2	1:A:994:LYS:HD3	20	0.21
(1,2767)	1:A:993:PHE:HB3	1:A:993:PHE:H	11	0.21
(1,2755)	1:A:992:PHE:HB3	1:A:993:PHE:H	18	0.21
(1,275)	1:A:974:LEU:HB2	1:A:975:GLY:H	18	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,273)	1:A:974:LEU:H	1:A:975:GLY:HA2	1	0.21
(1,2728)	1:A:990:VAL:HB	1:A:993:PHE:H	8	0.21
(1,2659)	1:A:989:LYS:H	1:A:989:LYS:HD3	7	0.21
(1,2659)	1:A:989:LYS:H	1:A:989:LYS:HD3	17	0.21
(1,2616)	1:A:987:MET:H	1:A:987:MET:HG2	16	0.21
(1,2533)	1:A:984:VAL:HA	1:A:987:MET:H	19	0.21
(1,2506)	1:A:983:LEU:H	1:A:985:LEU:H	4	0.21
(1,2506)	1:A:983:LEU:H	1:A:985:LEU:H	10	0.21
(1,2474)	1:A:982:ILE:H	1:A:983:LEU:HB3	5	0.21
(1,2474)	1:A:982:ILE:H	1:A:983:LEU:HB3	12	0.21
(1,2474)	1:A:982:ILE:H	1:A:983:LEU:HB3	16	0.21
(1,2474)	1:A:982:ILE:H	1:A:983:LEU:HB3	17	0.21
(1,243)	1:A:972:GLY:H	1:A:976:GLY:H	11	0.21
(1,243)	1:A:972:GLY:H	1:A:976:GLY:H	13	0.21
(1,2358)	1:A:974:LEU:HB2	1:A:975:GLY:H	18	0.21
(1,2356)	1:A:974:LEU:H	1:A:975:GLY:HA2	1	0.21
(1,2326)	1:A:972:GLY:H	1:A:976:GLY:H	11	0.21
(1,2326)	1:A:972:GLY:H	1:A:976:GLY:H	13	0.21
(1,2308)	1:A:971:VAL:H	1:A:973:VAL:H	14	0.21
(1,2278)	1:A:970:LEU:HD11	1:A:970:LEU:HA	14	0.21
(1,2278)	1:A:970:LEU:HD12	1:A:970:LEU:HA	14	0.21
(1,2278)	1:A:970:LEU:HD13	1:A:970:LEU:HA	14	0.21
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD21	15	0.21
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD22	15	0.21
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD23	15	0.21
(1,2258)	1:A:969:VAL:H	1:A:970:LEU:HB3	18	0.21
(1,225)	1:A:971:VAL:H	1:A:973:VAL:H	14	0.21
(1,2208)	1:A:967:TRP:H	1:A:970:LEU:H	3	0.21
(1,2208)	1:A:967:TRP:H	1:A:970:LEU:H	4	0.21
(1,2208)	1:A:967:TRP:H	1:A:970:LEU:H	8	0.21
(1,2208)	1:A:967:TRP:H	1:A:970:LEU:H	13	0.21
(1,2202)	1:A:967:TRP:HB2	1:A:968:TRP:H	2	0.21
(1,2202)	1:A:967:TRP:HB2	1:A:968:TRP:H	5	0.21
(1,2201)	1:A:967:TRP:HA	1:A:968:TRP:HB3	10	0.21
(1,2201)	1:A:967:TRP:HA	1:A:968:TRP:HB3	15	0.21
(1,2196)	1:A:967:TRP:H	1:A:968:TRP:HA	6	0.21
(1,2080)	1:A:988:TRP:HE1	2:B:719:ILE:HG21	15	0.21
(1,2080)	1:A:988:TRP:HE1	2:B:719:ILE:HG22	15	0.21
(1,2080)	1:A:988:TRP:HE1	2:B:719:ILE:HG23	15	0.21
(1,2068)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	6	0.21
(1,2047)	1:A:979:LEU:H	2:B:704:ILE:HB	11	0.21
(1,2019)	1:A:973:VAL:H	2:B:701:MET:HE1	16	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2019)	1:A:973:VAL:H	2:B:701:MET:HE2	16	0.21
(1,2019)	1:A:973:VAL:H	2:B:701:MET:HE3	16	0.21
(1,2018)	1:A:973:VAL:H	2:B:700:VAL:HA	19	0.21
(1,195)	1:A:970:LEU:HD11	1:A:970:LEU:HA	14	0.21
(1,195)	1:A:970:LEU:HD12	1:A:970:LEU:HA	14	0.21
(1,195)	1:A:970:LEU:HD13	1:A:970:LEU:HA	14	0.21
(1,1917)	2:B:749:GLU:H	2:B:749:GLU:HG3	16	0.21
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD21	15	0.21
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD22	15	0.21
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD23	15	0.21
(1,1890)	2:B:747:TYR:HB2	2:B:748:LYS:H	9	0.21
(1,1890)	2:B:747:TYR:HB2	2:B:748:LYS:H	10	0.21
(1,1862)	2:B:745:PRO:HA	2:B:746:LEU:H	8	0.21
(1,1862)	2:B:745:PRO:HA	2:B:746:LEU:H	9	0.21
(1,1862)	2:B:745:PRO:HA	2:B:746:LEU:H	14	0.21
(1,1862)	2:B:745:PRO:HA	2:B:746:LEU:H	16	0.21
(1,1826)	2:B:743:ASN:HB2	2:B:743:ASN:H	7	0.21
(1,1826)	2:B:743:ASN:HB2	2:B:743:ASN:H	18	0.21
(1,1819)	2:B:742:ALA:HA	2:B:743:ASN:H	3	0.21
(1,1819)	2:B:742:ALA:HA	2:B:743:ASN:H	13	0.21
(1,1819)	2:B:742:ALA:HA	2:B:743:ASN:H	14	0.21
(1,1814)	2:B:741:THR:HA	2:B:744:ASN:H	9	0.21
(1,1787)	2:B:738:LYS:HA	2:B:740:ASP:H	8	0.21
(1,1787)	2:B:738:LYS:HA	2:B:740:ASP:H	9	0.21
(1,1776)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	5	0.21
(1,1776)	2:B:738:LYS:HE3	2:B:738:LYS:HG2	10	0.21
(1,1769)	2:B:738:LYS:H	2:B:738:LYS:HG3	7	0.21
(1,1767)	2:B:738:LYS:HA	2:B:738:LYS:HD3	7	0.21
(1,175)	1:A:969:VAL:H	1:A:970:LEU:HB3	18	0.21
(1,1718)	2:B:734:ARG:HD2	2:B:734:ARG:HB2	17	0.21
(1,1718)	2:B:734:ARG:HD2	2:B:734:ARG:HB2	20	0.21
(1,1715)	2:B:734:ARG:HD3	2:B:734:ARG:HB2	6	0.21
(1,1661)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	20	0.21
(1,1635)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	11	0.21
(1,1635)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	12	0.21
(1,1563)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	4	0.21
(1,1563)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	6	0.21
(1,1563)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	20	0.21
(1,1496)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	9	0.21
(1,1412)	2:B:718:LEU:HB3	2:B:719:ILE:HG12	7	0.21
(1,125)	1:A:967:TRP:H	1:A:970:LEU:H	3	0.21
(1,125)	1:A:967:TRP:H	1:A:970:LEU:H	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,125)	1:A:967:TRP:H	1:A:970:LEU:H	8	0.21
(1,125)	1:A:967:TRP:H	1:A:970:LEU:H	13	0.21
(1,1236)	2:B:709:LEU:H	2:B:711:ALA:H	12	0.21
(1,1236)	2:B:709:LEU:H	2:B:711:ALA:H	20	0.21
(1,1220)	2:B:708:GLY:H	2:B:710:ALA:H	3	0.21
(1,1220)	2:B:708:GLY:H	2:B:710:ALA:H	7	0.21
(1,1220)	2:B:708:GLY:H	2:B:710:ALA:H	20	0.21
(1,119)	1:A:967:TRP:HB2	1:A:968:TRP:H	2	0.21
(1,119)	1:A:967:TRP:HB2	1:A:968:TRP:H	5	0.21
(1,118)	1:A:967:TRP:HA	1:A:968:TRP:HB3	10	0.21
(1,118)	1:A:967:TRP:HA	1:A:968:TRP:HB3	15	0.21
(1,113)	1:A:967:TRP:H	1:A:968:TRP:HA	6	0.21
(1,1128)	2:B:704:ILE:HB	2:B:705:LEU:HB2	2	0.21
(1,1128)	2:B:704:ILE:HB	2:B:705:LEU:HB2	3	0.21
(1,1128)	2:B:704:ILE:HB	2:B:705:LEU:HB2	4	0.21
(1,1128)	2:B:704:ILE:HB	2:B:705:LEU:HB2	7	0.21
(1,870)	2:B:693:ILE:H	2:B:693:ILE:HB	7	0.2
(1,870)	2:B:693:ILE:H	2:B:693:ILE:HB	19	0.2
(1,869)	2:B:693:ILE:H	2:B:693:ILE:HG12	11	0.2
(1,851)	2:B:692:ASP:H	2:B:693:ILE:H	9	0.2
(1,850)	2:B:692:ASP:HA	2:B:693:ILE:H	13	0.2
(1,850)	2:B:692:ASP:HA	2:B:693:ILE:H	15	0.2
(1,849)	2:B:692:ASP:HB3	2:B:693:ILE:H	8	0.2
(1,841)	2:B:691:PRO:HD3	2:B:692:ASP:H	3	0.2
(1,841)	2:B:691:PRO:HD3	2:B:692:ASP:H	18	0.2
(1,761)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	1	0.2
(1,755)	1:A:997:ARG:H	1:A:997:ARG:HG3	19	0.2
(1,740)	1:A:995:ARG:H	1:A:996:ASN:H	11	0.2
(1,737)	1:A:995:ARG:HB3	1:A:996:ASN:H	18	0.2
(1,718)	1:A:994:LYS:HB2	1:A:995:ARG:H	17	0.2
(1,704)	1:A:994:LYS:H	1:A:994:LYS:HG3	20	0.2
(1,690)	1:A:993:PHE:HB2	1:A:994:LYS:H	1	0.2
(1,690)	1:A:993:PHE:HB2	1:A:994:LYS:H	5	0.2
(1,690)	1:A:993:PHE:HB2	1:A:994:LYS:H	13	0.2
(1,684)	1:A:993:PHE:HB3	1:A:993:PHE:H	2	0.2
(1,684)	1:A:993:PHE:HB3	1:A:993:PHE:H	8	0.2
(1,684)	1:A:993:PHE:HB3	1:A:993:PHE:H	10	0.2
(1,684)	1:A:993:PHE:HB3	1:A:993:PHE:H	15	0.2
(1,684)	1:A:993:PHE:HB3	1:A:993:PHE:H	16	0.2
(1,684)	1:A:993:PHE:HB3	1:A:993:PHE:H	17	0.2
(1,672)	1:A:992:PHE:HB3	1:A:993:PHE:H	10	0.2
(1,672)	1:A:992:PHE:HB3	1:A:993:PHE:H	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,672)	1:A:992:PHE:HB3	1:A:993:PHE:H	12	0.2
(1,645)	1:A:990:VAL:HB	1:A:993:PHE:H	15	0.2
(1,548)	1:A:987:MET:HA	1:A:990:VAL:H	16	0.2
(1,485)	1:A:985:LEU:HA	1:A:987:MET:H	11	0.2
(1,485)	1:A:985:LEU:HA	1:A:987:MET:H	13	0.2
(1,460)	1:A:984:VAL:HA	1:A:988:TRP:HB3	17	0.2
(1,450)	1:A:984:VAL:HA	1:A:987:MET:H	14	0.2
(1,426)	1:A:983:LEU:HA	1:A:985:LEU:H	7	0.2
(1,426)	1:A:983:LEU:HA	1:A:985:LEU:H	14	0.2
(1,423)	1:A:983:LEU:H	1:A:985:LEU:H	6	0.2
(1,423)	1:A:983:LEU:H	1:A:985:LEU:H	11	0.2
(1,423)	1:A:983:LEU:H	1:A:985:LEU:H	12	0.2
(1,423)	1:A:983:LEU:H	1:A:985:LEU:H	17	0.2
(1,423)	1:A:983:LEU:H	1:A:985:LEU:H	19	0.2
(1,423)	1:A:983:LEU:H	1:A:985:LEU:H	20	0.2
(1,4162)	1:A:988:TRP:HE1	2:B:719:ILE:HB	2	0.2
(1,4162)	1:A:988:TRP:HE1	2:B:719:ILE:HB	4	0.2
(1,4151)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	4	0.2
(1,4151)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	7	0.2
(1,4151)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	10	0.2
(1,4151)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	16	0.2
(1,4143)	1:A:984:VAL:H	2:B:712:LEU:HA	3	0.2
(1,4130)	1:A:979:LEU:H	2:B:704:ILE:HB	14	0.2
(1,4007)	2:B:750:ALA:H	2:B:751:THR:H	10	0.2
(1,4000)	2:B:749:GLU:H	2:B:749:GLU:HG3	3	0.2
(1,4000)	2:B:749:GLU:H	2:B:749:GLU:HG3	9	0.2
(1,4000)	2:B:749:GLU:H	2:B:749:GLU:HG3	17	0.2
(1,3973)	2:B:747:TYR:HB2	2:B:748:LYS:H	8	0.2
(1,3963)	2:B:746:LEU:HB2	2:B:747:TYR:H	16	0.2
(1,395)	1:A:982:ILE:HA	1:A:985:LEU:HB3	1	0.2
(1,3945)	2:B:745:PRO:HA	2:B:746:LEU:H	11	0.2
(1,393)	1:A:982:ILE:H	1:A:984:VAL:H	7	0.2
(1,393)	1:A:982:ILE:H	1:A:984:VAL:H	12	0.2
(1,391)	1:A:982:ILE:H	1:A:983:LEU:HB3	8	0.2
(1,391)	1:A:982:ILE:H	1:A:983:LEU:HB3	19	0.2
(1,3909)	2:B:743:ASN:HB2	2:B:743:ASN:H	17	0.2
(1,3902)	2:B:742:ALA:HA	2:B:743:ASN:H	17	0.2
(1,3897)	2:B:741:THR:HA	2:B:744:ASN:H	10	0.2
(1,3893)	2:B:741:THR:HA	2:B:742:ALA:H	18	0.2
(1,3870)	2:B:738:LYS:HA	2:B:740:ASP:H	18	0.2
(1,3863)	2:B:738:LYS:HB3	2:B:739:TRP:H	18	0.2
(1,3742)	2:B:730:PHE:HB3	2:B:731:GLU:HG2	3	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3742)	2:B:730:PHE:HB3	2:B:731:GLU:HG2	10	0.2
(1,3742)	2:B:730:PHE:HB3	2:B:731:GLU:HG2	14	0.2
(1,3718)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	1	0.2
(1,3718)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	2	0.2
(1,3718)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	3	0.2
(1,3718)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	5	0.2
(1,3718)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	6	0.2
(1,3718)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	8	0.2
(1,3718)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	10	0.2
(1,3718)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	13	0.2
(1,3718)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	14	0.2
(1,3718)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	15	0.2
(1,3718)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	18	0.2
(1,3718)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	19	0.2
(1,3718)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	20	0.2
(1,3646)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	5	0.2
(1,3646)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	7	0.2
(1,3646)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	10	0.2
(1,3646)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	14	0.2
(1,3646)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	15	0.2
(1,3579)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	17	0.2
(1,3495)	2:B:718:LEU:HB3	2:B:719:ILE:HG12	2	0.2
(1,3495)	2:B:718:LEU:HB3	2:B:719:ILE:HG12	4	0.2
(1,3495)	2:B:718:LEU:HB3	2:B:719:ILE:HG12	5	0.2
(1,3495)	2:B:718:LEU:HB3	2:B:719:ILE:HG12	19	0.2
(1,3319)	2:B:709:LEU:H	2:B:711:ALA:H	6	0.2
(1,3319)	2:B:709:LEU:H	2:B:711:ALA:H	13	0.2
(1,3303)	2:B:708:GLY:H	2:B:710:ALA:H	4	0.2
(1,3211)	2:B:704:ILE:HB	2:B:705:LEU:HB2	1	0.2
(1,3211)	2:B:704:ILE:HB	2:B:705:LEU:HB2	5	0.2
(1,3211)	2:B:704:ILE:HB	2:B:705:LEU:HB2	16	0.2
(1,2953)	2:B:693:ILE:H	2:B:693:ILE:HB	7	0.2
(1,2953)	2:B:693:ILE:H	2:B:693:ILE:HB	19	0.2
(1,2952)	2:B:693:ILE:H	2:B:693:ILE:HG12	11	0.2
(1,2934)	2:B:692:ASP:H	2:B:693:ILE:H	9	0.2
(1,2933)	2:B:692:ASP:HA	2:B:693:ILE:H	13	0.2
(1,2933)	2:B:692:ASP:HA	2:B:693:ILE:H	15	0.2
(1,2932)	2:B:692:ASP:HB3	2:B:693:ILE:H	8	0.2
(1,2924)	2:B:691:PRO:HD3	2:B:692:ASP:H	3	0.2
(1,2924)	2:B:691:PRO:HD3	2:B:692:ASP:H	18	0.2
(1,289)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	14	0.2
(1,2844)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	1	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2838)	1:A:997:ARG:H	1:A:997:ARG:HG3	19	0.2
(1,2823)	1:A:995:ARG:H	1:A:996:ASN:H	11	0.2
(1,2820)	1:A:995:ARG:HB3	1:A:996:ASN:H	18	0.2
(1,2801)	1:A:994:LYS:HB2	1:A:995:ARG:H	17	0.2
(1,2787)	1:A:994:LYS:H	1:A:994:LYS:HG3	20	0.2
(1,2773)	1:A:993:PHE:HB2	1:A:994:LYS:H	1	0.2
(1,2773)	1:A:993:PHE:HB2	1:A:994:LYS:H	5	0.2
(1,2773)	1:A:993:PHE:HB2	1:A:994:LYS:H	13	0.2
(1,2767)	1:A:993:PHE:HB3	1:A:993:PHE:H	2	0.2
(1,2767)	1:A:993:PHE:HB3	1:A:993:PHE:H	8	0.2
(1,2767)	1:A:993:PHE:HB3	1:A:993:PHE:H	10	0.2
(1,2767)	1:A:993:PHE:HB3	1:A:993:PHE:H	15	0.2
(1,2767)	1:A:993:PHE:HB3	1:A:993:PHE:H	16	0.2
(1,2767)	1:A:993:PHE:HB3	1:A:993:PHE:H	17	0.2
(1,2755)	1:A:992:PHE:HB3	1:A:993:PHE:H	10	0.2
(1,2755)	1:A:992:PHE:HB3	1:A:993:PHE:H	11	0.2
(1,2755)	1:A:992:PHE:HB3	1:A:993:PHE:H	12	0.2
(1,275)	1:A:974:LEU:HB2	1:A:975:GLY:H	11	0.2
(1,273)	1:A:974:LEU:H	1:A:975:GLY:HA2	12	0.2
(1,2728)	1:A:990:VAL:HB	1:A:993:PHE:H	15	0.2
(1,2631)	1:A:987:MET:HA	1:A:990:VAL:H	16	0.2
(1,2568)	1:A:985:LEU:HA	1:A:987:MET:H	11	0.2
(1,2568)	1:A:985:LEU:HA	1:A:987:MET:H	13	0.2
(1,2543)	1:A:984:VAL:HA	1:A:988:TRP:HB3	17	0.2
(1,2533)	1:A:984:VAL:HA	1:A:987:MET:H	14	0.2
(1,2509)	1:A:983:LEU:HA	1:A:985:LEU:H	7	0.2
(1,2509)	1:A:983:LEU:HA	1:A:985:LEU:H	14	0.2
(1,2506)	1:A:983:LEU:H	1:A:985:LEU:H	6	0.2
(1,2506)	1:A:983:LEU:H	1:A:985:LEU:H	11	0.2
(1,2506)	1:A:983:LEU:H	1:A:985:LEU:H	12	0.2
(1,2506)	1:A:983:LEU:H	1:A:985:LEU:H	17	0.2
(1,2506)	1:A:983:LEU:H	1:A:985:LEU:H	19	0.2
(1,2506)	1:A:983:LEU:H	1:A:985:LEU:H	20	0.2
(1,2478)	1:A:982:ILE:HA	1:A:985:LEU:HB3	1	0.2
(1,2476)	1:A:982:ILE:H	1:A:984:VAL:H	7	0.2
(1,2476)	1:A:982:ILE:H	1:A:984:VAL:H	12	0.2
(1,2474)	1:A:982:ILE:H	1:A:983:LEU:HB3	8	0.2
(1,2474)	1:A:982:ILE:H	1:A:983:LEU:HB3	19	0.2
(1,243)	1:A:972:GLY:H	1:A:976:GLY:H	9	0.2
(1,243)	1:A:972:GLY:H	1:A:976:GLY:H	16	0.2
(1,2372)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	14	0.2
(1,2358)	1:A:974:LEU:HB2	1:A:975:GLY:H	11	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2356)	1:A:974:LEU:H	1:A:975:GLY:HA2	12	0.2
(1,2326)	1:A:972:GLY:H	1:A:976:GLY:H	9	0.2
(1,2326)	1:A:972:GLY:H	1:A:976:GLY:H	16	0.2
(1,2308)	1:A:971:VAL:H	1:A:973:VAL:H	9	0.2
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD21	6	0.2
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD22	6	0.2
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD23	6	0.2
(1,2258)	1:A:969:VAL:H	1:A:970:LEU:HB3	20	0.2
(1,225)	1:A:971:VAL:H	1:A:973:VAL:H	9	0.2
(1,2208)	1:A:967:TRP:H	1:A:970:LEU:H	11	0.2
(1,2208)	1:A:967:TRP:H	1:A:970:LEU:H	12	0.2
(1,2208)	1:A:967:TRP:H	1:A:970:LEU:H	15	0.2
(1,2208)	1:A:967:TRP:H	1:A:970:LEU:H	16	0.2
(1,2208)	1:A:967:TRP:H	1:A:970:LEU:H	17	0.2
(1,2208)	1:A:967:TRP:H	1:A:970:LEU:H	18	0.2
(1,2208)	1:A:967:TRP:H	1:A:970:LEU:H	19	0.2
(1,2203)	1:A:967:TRP:HB3	1:A:968:TRP:HB3	5	0.2
(1,2196)	1:A:967:TRP:H	1:A:968:TRP:HA	2	0.2
(1,2079)	1:A:988:TRP:HE1	2:B:719:ILE:HB	2	0.2
(1,2079)	1:A:988:TRP:HE1	2:B:719:ILE:HB	4	0.2
(1,2068)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	4	0.2
(1,2068)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	7	0.2
(1,2068)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	10	0.2
(1,2068)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	16	0.2
(1,2060)	1:A:984:VAL:H	2:B:712:LEU:HA	3	0.2
(1,2047)	1:A:979:LEU:H	2:B:704:ILE:HB	14	0.2
(1,1924)	2:B:750:ALA:H	2:B:751:THR:H	10	0.2
(1,1917)	2:B:749:GLU:H	2:B:749:GLU:HG3	3	0.2
(1,1917)	2:B:749:GLU:H	2:B:749:GLU:HG3	9	0.2
(1,1917)	2:B:749:GLU:H	2:B:749:GLU:HG3	17	0.2
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD21	6	0.2
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD22	6	0.2
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD23	6	0.2
(1,1890)	2:B:747:TYR:HB2	2:B:748:LYS:H	8	0.2
(1,1880)	2:B:746:LEU:HB2	2:B:747:TYR:H	16	0.2
(1,1862)	2:B:745:PRO:HA	2:B:746:LEU:H	11	0.2
(1,1826)	2:B:743:ASN:HB2	2:B:743:ASN:H	17	0.2
(1,1819)	2:B:742:ALA:HA	2:B:743:ASN:H	17	0.2
(1,1814)	2:B:741:THR:HA	2:B:744:ASN:H	10	0.2
(1,1810)	2:B:741:THR:HA	2:B:742:ALA:H	18	0.2
(1,1787)	2:B:738:LYS:HA	2:B:740:ASP:H	18	0.2
(1,1780)	2:B:738:LYS:HB3	2:B:739:TRP:H	18	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:A:969:VAL:H	1:A:970:LEU:HB3	20	0.2
(1,1659)	2:B:730:PHE:HB3	2:B:731:GLU:HG2	3	0.2
(1,1659)	2:B:730:PHE:HB3	2:B:731:GLU:HG2	10	0.2
(1,1659)	2:B:730:PHE:HB3	2:B:731:GLU:HG2	14	0.2
(1,1635)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	1	0.2
(1,1635)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	2	0.2
(1,1635)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	3	0.2
(1,1635)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	5	0.2
(1,1635)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	6	0.2
(1,1635)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	8	0.2
(1,1635)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	10	0.2
(1,1635)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	13	0.2
(1,1635)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	14	0.2
(1,1635)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	15	0.2
(1,1635)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	18	0.2
(1,1635)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	19	0.2
(1,1635)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	20	0.2
(1,1563)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	5	0.2
(1,1563)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	7	0.2
(1,1563)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	10	0.2
(1,1563)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	14	0.2
(1,1563)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	15	0.2
(1,1496)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	17	0.2
(1,1412)	2:B:718:LEU:HB3	2:B:719:ILE:HG12	2	0.2
(1,1412)	2:B:718:LEU:HB3	2:B:719:ILE:HG12	4	0.2
(1,1412)	2:B:718:LEU:HB3	2:B:719:ILE:HG12	5	0.2
(1,1412)	2:B:718:LEU:HB3	2:B:719:ILE:HG12	19	0.2
(1,125)	1:A:967:TRP:H	1:A:970:LEU:H	11	0.2
(1,125)	1:A:967:TRP:H	1:A:970:LEU:H	12	0.2
(1,125)	1:A:967:TRP:H	1:A:970:LEU:H	15	0.2
(1,125)	1:A:967:TRP:H	1:A:970:LEU:H	16	0.2
(1,125)	1:A:967:TRP:H	1:A:970:LEU:H	17	0.2
(1,125)	1:A:967:TRP:H	1:A:970:LEU:H	18	0.2
(1,125)	1:A:967:TRP:H	1:A:970:LEU:H	19	0.2
(1,1236)	2:B:709:LEU:H	2:B:711:ALA:H	6	0.2
(1,1236)	2:B:709:LEU:H	2:B:711:ALA:H	13	0.2
(1,1220)	2:B:708:GLY:H	2:B:710:ALA:H	4	0.2
(1,120)	1:A:967:TRP:HB3	1:A:968:TRP:HB3	5	0.2
(1,113)	1:A:967:TRP:H	1:A:968:TRP:HA	2	0.2
(1,1128)	2:B:704:ILE:HB	2:B:705:LEU:HB2	1	0.2
(1,1128)	2:B:704:ILE:HB	2:B:705:LEU:HB2	5	0.2
(1,1128)	2:B:704:ILE:HB	2:B:705:LEU:HB2	16	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,870)	2:B:693:ILE:H	2:B:693:ILE:HB	6	0.19
(1,869)	2:B:693:ILE:H	2:B:693:ILE:HG12	1	0.19
(1,843)	2:B:691:PRO:HB3	2:B:692:ASP:H	9	0.19
(1,841)	2:B:691:PRO:HD3	2:B:692:ASP:H	2	0.19
(1,841)	2:B:691:PRO:HD3	2:B:692:ASP:H	19	0.19
(1,841)	2:B:691:PRO:HD3	2:B:692:ASP:H	20	0.19
(1,813)	1:A:1006:GLU:H	1:A:1006:GLU:HB2	2	0.19
(1,811)	1:A:1006:GLU:H	1:A:1006:GLU:HB3	5	0.19
(1,807)	1:A:1005:GLU:H	1:A:1005:GLU:HB3	15	0.19
(1,798)	1:A:1003:ASP:H	1:A:1003:ASP:HB2	14	0.19
(1,792)	1:A:1002:GLU:H	1:A:1002:GLU:HG3	8	0.19
(1,762)	1:A:997:ARG:HA	1:A:999:PRO:HD2	17	0.19
(1,742)	1:A:996:ASN:H	1:A:996:ASN:HB2	19	0.19
(1,724)	1:A:994:LYS:HB2	1:A:995:ARG:HG3	17	0.19
(1,7)	1:A:960:GLU:HB2	1:A:961:GLU:H	18	0.19
(1,690)	1:A:993:PHE:HB2	1:A:994:LYS:H	14	0.19
(1,684)	1:A:993:PHE:HB3	1:A:993:PHE:H	1	0.19
(1,684)	1:A:993:PHE:HB3	1:A:993:PHE:H	5	0.19
(1,684)	1:A:993:PHE:HB3	1:A:993:PHE:H	6	0.19
(1,684)	1:A:993:PHE:HB3	1:A:993:PHE:H	7	0.19
(1,672)	1:A:992:PHE:HB3	1:A:993:PHE:H	8	0.19
(1,645)	1:A:990:VAL:HB	1:A:993:PHE:H	20	0.19
(1,557)	1:A:988:TRP:H	1:A:988:TRP:HB3	16	0.19
(1,548)	1:A:987:MET:HA	1:A:990:VAL:H	8	0.19
(1,548)	1:A:987:MET:HA	1:A:990:VAL:H	11	0.19
(1,485)	1:A:985:LEU:HA	1:A:987:MET:H	1	0.19
(1,485)	1:A:985:LEU:HA	1:A:987:MET:H	3	0.19
(1,450)	1:A:984:VAL:HA	1:A:987:MET:H	2	0.19
(1,450)	1:A:984:VAL:HA	1:A:987:MET:H	6	0.19
(1,423)	1:A:983:LEU:H	1:A:985:LEU:H	14	0.19
(1,4163)	1:A:988:TRP:HE1	2:B:719:ILE:HG21	16	0.19
(1,4163)	1:A:988:TRP:HE1	2:B:719:ILE:HG22	16	0.19
(1,4163)	1:A:988:TRP:HE1	2:B:719:ILE:HG23	16	0.19
(1,4162)	1:A:988:TRP:HE1	2:B:719:ILE:HB	5	0.19
(1,4162)	1:A:988:TRP:HE1	2:B:719:ILE:HB	6	0.19
(1,4162)	1:A:988:TRP:HE1	2:B:719:ILE:HB	19	0.19
(1,4162)	1:A:988:TRP:HE1	2:B:719:ILE:HB	20	0.19
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG21	11	0.19
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG22	11	0.19
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG23	11	0.19
(1,4157)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	3	0.19
(1,4157)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	19	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4151)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	1	0.19
(1,4151)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	5	0.19
(1,4151)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	9	0.19
(1,4143)	1:A:984:VAL:H	2:B:712:LEU:HA	2	0.19
(1,4138)	1:A:980:LEU:HA	2:B:708:GLY:H	16	0.19
(1,4131)	1:A:979:LEU:H	2:B:707:ILE:HB	12	0.19
(1,4121)	1:A:976:GLY:H	2:B:707:ILE:HB	17	0.19
(1,4032)	2:B:754:PHE:HB3	2:B:755:THR:H	2	0.19
(1,4000)	2:B:749:GLU:H	2:B:749:GLU:HG3	20	0.19
(1,3968)	2:B:747:TYR:H	2:B:747:TYR:HB3	6	0.19
(1,3968)	2:B:747:TYR:H	2:B:747:TYR:HB3	15	0.19
(1,3945)	2:B:745:PRO:HA	2:B:746:LEU:H	2	0.19
(1,3945)	2:B:745:PRO:HA	2:B:746:LEU:H	4	0.19
(1,393)	1:A:982:ILE:H	1:A:984:VAL:H	2	0.19
(1,393)	1:A:982:ILE:H	1:A:984:VAL:H	6	0.19
(1,3913)	2:B:743:ASN:H	2:B:743:ASN:HD22	6	0.19
(1,3902)	2:B:742:ALA:HA	2:B:743:ASN:H	2	0.19
(1,3897)	2:B:741:THR:HA	2:B:744:ASN:H	4	0.19
(1,3893)	2:B:741:THR:HA	2:B:742:ALA:H	3	0.19
(1,3893)	2:B:741:THR:HA	2:B:742:ALA:H	4	0.19
(1,3893)	2:B:741:THR:HA	2:B:742:ALA:H	8	0.19
(1,3893)	2:B:741:THR:HA	2:B:742:ALA:H	20	0.19
(1,3888)	2:B:740:ASP:HA	2:B:741:THR:H	9	0.19
(1,3870)	2:B:738:LYS:HA	2:B:740:ASP:H	15	0.19
(1,3863)	2:B:738:LYS:HB3	2:B:739:TRP:H	2	0.19
(1,3863)	2:B:738:LYS:HB3	2:B:739:TRP:H	11	0.19
(1,3852)	2:B:738:LYS:H	2:B:738:LYS:HG3	12	0.19
(1,3801)	2:B:734:ARG:HD2	2:B:734:ARG:HB2	11	0.19
(1,3718)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	9	0.19
(1,3718)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	17	0.19
(1,3646)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	2	0.19
(1,3646)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	11	0.19
(1,3646)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	18	0.19
(1,3644)	2:B:725:LYS:H	2:B:725:LYS:HG3	4	0.19
(1,3620)	2:B:724:ARG:HD3	2:B:724:ARG:HB3	4	0.19
(1,3620)	2:B:724:ARG:HD3	2:B:724:ARG:HB3	8	0.19
(1,3579)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	10	0.19
(1,3579)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	11	0.19
(1,3579)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	20	0.19
(1,3508)	2:B:718:LEU:HD21	2:B:721:ILE:HB	7	0.19
(1,3508)	2:B:718:LEU:HD22	2:B:721:ILE:HB	7	0.19
(1,3508)	2:B:718:LEU:HD23	2:B:721:ILE:HB	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3470)	2:B:717:LEU:H	2:B:719:ILE:H	1	0.19
(1,3454)	2:B:716:LYS:HE3	2:B:719:ILE:HG12	7	0.19
(1,341)	1:A:979:LEU:HA	1:A:981:THR:H	12	0.19
(1,341)	1:A:979:LEU:HA	1:A:981:THR:H	20	0.19
(1,3319)	2:B:709:LEU:H	2:B:711:ALA:H	19	0.19
(1,2953)	2:B:693:ILE:H	2:B:693:ILE:HB	6	0.19
(1,2952)	2:B:693:ILE:H	2:B:693:ILE:HG12	1	0.19
(1,2926)	2:B:691:PRO:HB3	2:B:692:ASP:H	9	0.19
(1,2924)	2:B:691:PRO:HD3	2:B:692:ASP:H	2	0.19
(1,2924)	2:B:691:PRO:HD3	2:B:692:ASP:H	19	0.19
(1,2924)	2:B:691:PRO:HD3	2:B:692:ASP:H	20	0.19
(1,2896)	1:A:1006:GLU:H	1:A:1006:GLU:HB2	2	0.19
(1,2894)	1:A:1006:GLU:H	1:A:1006:GLU:HB3	5	0.19
(1,2890)	1:A:1005:GLU:H	1:A:1005:GLU:HB3	15	0.19
(1,289)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	7	0.19
(1,289)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	9	0.19
(1,2881)	1:A:1003:ASP:H	1:A:1003:ASP:HB2	14	0.19
(1,2875)	1:A:1002:GLU:H	1:A:1002:GLU:HG3	8	0.19
(1,2845)	1:A:997:ARG:HA	1:A:999:PRO:HD2	17	0.19
(1,2825)	1:A:996:ASN:H	1:A:996:ASN:HB2	19	0.19
(1,2807)	1:A:994:LYS:HB2	1:A:995:ARG:HG3	17	0.19
(1,2773)	1:A:993:PHE:HB2	1:A:994:LYS:H	14	0.19
(1,2767)	1:A:993:PHE:HB3	1:A:993:PHE:H	1	0.19
(1,2767)	1:A:993:PHE:HB3	1:A:993:PHE:H	5	0.19
(1,2767)	1:A:993:PHE:HB3	1:A:993:PHE:H	6	0.19
(1,2767)	1:A:993:PHE:HB3	1:A:993:PHE:H	7	0.19
(1,2755)	1:A:992:PHE:HB3	1:A:993:PHE:H	8	0.19
(1,273)	1:A:974:LEU:H	1:A:975:GLY:HA2	2	0.19
(1,273)	1:A:974:LEU:H	1:A:975:GLY:HA2	10	0.19
(1,273)	1:A:974:LEU:H	1:A:975:GLY:HA2	19	0.19
(1,2728)	1:A:990:VAL:HB	1:A:993:PHE:H	20	0.19
(1,2640)	1:A:988:TRP:H	1:A:988:TRP:HB3	16	0.19
(1,2631)	1:A:987:MET:HA	1:A:990:VAL:H	8	0.19
(1,2631)	1:A:987:MET:HA	1:A:990:VAL:H	11	0.19
(1,2568)	1:A:985:LEU:HA	1:A:987:MET:H	1	0.19
(1,2568)	1:A:985:LEU:HA	1:A:987:MET:H	3	0.19
(1,2533)	1:A:984:VAL:HA	1:A:987:MET:H	2	0.19
(1,2533)	1:A:984:VAL:HA	1:A:987:MET:H	6	0.19
(1,2506)	1:A:983:LEU:H	1:A:985:LEU:H	14	0.19
(1,2476)	1:A:982:ILE:H	1:A:984:VAL:H	2	0.19
(1,2476)	1:A:982:ILE:H	1:A:984:VAL:H	6	0.19
(1,2424)	1:A:979:LEU:HA	1:A:981:THR:H	12	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2424)	1:A:979:LEU:HA	1:A:981:THR:H	20	0.19
(1,24)	1:A:963:ALA:H	1:A:964:ILE:H	13	0.19
(1,2372)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	7	0.19
(1,2372)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	9	0.19
(1,2356)	1:A:974:LEU:H	1:A:975:GLY:HA2	2	0.19
(1,2356)	1:A:974:LEU:H	1:A:975:GLY:HA2	10	0.19
(1,2356)	1:A:974:LEU:H	1:A:975:GLY:HA2	19	0.19
(1,2308)	1:A:971:VAL:H	1:A:973:VAL:H	8	0.19
(1,2258)	1:A:969:VAL:H	1:A:970:LEU:HB3	1	0.19
(1,2258)	1:A:969:VAL:H	1:A:970:LEU:HB3	9	0.19
(1,2258)	1:A:969:VAL:H	1:A:970:LEU:HB3	11	0.19
(1,2258)	1:A:969:VAL:H	1:A:970:LEU:HB3	13	0.19
(1,2258)	1:A:969:VAL:H	1:A:970:LEU:HB3	16	0.19
(1,225)	1:A:971:VAL:H	1:A:973:VAL:H	8	0.19
(1,2208)	1:A:967:TRP:H	1:A:970:LEU:H	1	0.19
(1,2208)	1:A:967:TRP:H	1:A:970:LEU:H	5	0.19
(1,2208)	1:A:967:TRP:H	1:A:970:LEU:H	7	0.19
(1,2208)	1:A:967:TRP:H	1:A:970:LEU:H	10	0.19
(1,2208)	1:A:967:TRP:H	1:A:970:LEU:H	20	0.19
(1,2201)	1:A:967:TRP:HA	1:A:968:TRP:HB3	14	0.19
(1,2107)	1:A:963:ALA:H	1:A:964:ILE:H	13	0.19
(1,2090)	1:A:960:GLU:HB2	1:A:961:GLU:H	18	0.19
(1,2080)	1:A:988:TRP:HE1	2:B:719:ILE:HG21	16	0.19
(1,2080)	1:A:988:TRP:HE1	2:B:719:ILE:HG22	16	0.19
(1,2080)	1:A:988:TRP:HE1	2:B:719:ILE:HG23	16	0.19
(1,2079)	1:A:988:TRP:HE1	2:B:719:ILE:HB	5	0.19
(1,2079)	1:A:988:TRP:HE1	2:B:719:ILE:HB	6	0.19
(1,2079)	1:A:988:TRP:HE1	2:B:719:ILE:HB	19	0.19
(1,2079)	1:A:988:TRP:HE1	2:B:719:ILE:HB	20	0.19
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG21	11	0.19
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG22	11	0.19
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG23	11	0.19
(1,2074)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	3	0.19
(1,2074)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	19	0.19
(1,2068)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	1	0.19
(1,2068)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	5	0.19
(1,2068)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	9	0.19
(1,2060)	1:A:984:VAL:H	2:B:712:LEU:HA	2	0.19
(1,2055)	1:A:980:LEU:HA	2:B:708:GLY:H	16	0.19
(1,2048)	1:A:979:LEU:H	2:B:707:ILE:HB	12	0.19
(1,2038)	1:A:976:GLY:H	2:B:707:ILE:HB	17	0.19
(1,1949)	2:B:754:PHE:HB3	2:B:755:THR:H	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1917)	2:B:749:GLU:H	2:B:749:GLU:HG3	20	0.19
(1,1885)	2:B:747:TYR:H	2:B:747:TYR:HB3	6	0.19
(1,1885)	2:B:747:TYR:H	2:B:747:TYR:HB3	15	0.19
(1,1862)	2:B:745:PRO:HA	2:B:746:LEU:H	2	0.19
(1,1862)	2:B:745:PRO:HA	2:B:746:LEU:H	4	0.19
(1,1830)	2:B:743:ASN:H	2:B:743:ASN:HD22	6	0.19
(1,1819)	2:B:742:ALA:HA	2:B:743:ASN:H	2	0.19
(1,1814)	2:B:741:THR:HA	2:B:744:ASN:H	4	0.19
(1,1810)	2:B:741:THR:HA	2:B:742:ALA:H	3	0.19
(1,1810)	2:B:741:THR:HA	2:B:742:ALA:H	4	0.19
(1,1810)	2:B:741:THR:HA	2:B:742:ALA:H	8	0.19
(1,1810)	2:B:741:THR:HA	2:B:742:ALA:H	20	0.19
(1,1805)	2:B:740:ASP:HA	2:B:741:THR:H	9	0.19
(1,1787)	2:B:738:LYS:HA	2:B:740:ASP:H	15	0.19
(1,1780)	2:B:738:LYS:HB3	2:B:739:TRP:H	2	0.19
(1,1780)	2:B:738:LYS:HB3	2:B:739:TRP:H	11	0.19
(1,1769)	2:B:738:LYS:H	2:B:738:LYS:HG3	12	0.19
(1,175)	1:A:969:VAL:H	1:A:970:LEU:HB3	1	0.19
(1,175)	1:A:969:VAL:H	1:A:970:LEU:HB3	9	0.19
(1,175)	1:A:969:VAL:H	1:A:970:LEU:HB3	11	0.19
(1,175)	1:A:969:VAL:H	1:A:970:LEU:HB3	13	0.19
(1,175)	1:A:969:VAL:H	1:A:970:LEU:HB3	16	0.19
(1,1718)	2:B:734:ARG:HD2	2:B:734:ARG:HB2	11	0.19
(1,1635)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	9	0.19
(1,1635)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	17	0.19
(1,1563)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	2	0.19
(1,1563)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	11	0.19
(1,1563)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	18	0.19
(1,1561)	2:B:725:LYS:H	2:B:725:LYS:HG3	4	0.19
(1,1537)	2:B:724:ARG:HD3	2:B:724:ARG:HB3	4	0.19
(1,1537)	2:B:724:ARG:HD3	2:B:724:ARG:HB3	8	0.19
(1,1496)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	10	0.19
(1,1496)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	11	0.19
(1,1496)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	20	0.19
(1,1425)	2:B:718:LEU:HD21	2:B:721:ILE:HB	7	0.19
(1,1425)	2:B:718:LEU:HD22	2:B:721:ILE:HB	7	0.19
(1,1425)	2:B:718:LEU:HD23	2:B:721:ILE:HB	7	0.19
(1,1387)	2:B:717:LEU:H	2:B:719:ILE:H	1	0.19
(1,1371)	2:B:716:LYS:HE3	2:B:719:ILE:HG12	7	0.19
(1,125)	1:A:967:TRP:H	1:A:970:LEU:H	1	0.19
(1,125)	1:A:967:TRP:H	1:A:970:LEU:H	5	0.19
(1,125)	1:A:967:TRP:H	1:A:970:LEU:H	7	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,125)	1:A:967:TRP:H	1:A:970:LEU:H	10	0.19
(1,125)	1:A:967:TRP:H	1:A:970:LEU:H	20	0.19
(1,1236)	2:B:709:LEU:H	2:B:711:ALA:H	19	0.19
(1,118)	1:A:967:TRP:HA	1:A:968:TRP:HB3	14	0.19
(1,870)	2:B:693:ILE:H	2:B:693:ILE:HB	20	0.18
(1,850)	2:B:692:ASP:HA	2:B:693:ILE:H	1	0.18
(1,850)	2:B:692:ASP:HA	2:B:693:ILE:H	4	0.18
(1,850)	2:B:692:ASP:HA	2:B:693:ILE:H	7	0.18
(1,850)	2:B:692:ASP:HA	2:B:693:ILE:H	20	0.18
(1,841)	2:B:691:PRO:HD3	2:B:692:ASP:H	9	0.18
(1,8)	1:A:961:GLU:H	1:A:961:GLU:HB3	3	0.18
(1,750)	1:A:996:ASN:HA	1:A:997:ARG:H	1	0.18
(1,729)	1:A:995:ARG:H	1:A:995:ARG:HB3	6	0.18
(1,729)	1:A:995:ARG:H	1:A:995:ARG:HB3	11	0.18
(1,725)	1:A:994:LYS:HB3	1:A:995:ARG:HG3	4	0.18
(1,693)	1:A:993:PHE:H	1:A:994:LYS:HD3	1	0.18
(1,672)	1:A:992:PHE:HB3	1:A:993:PHE:H	16	0.18
(1,645)	1:A:990:VAL:HB	1:A:993:PHE:H	3	0.18
(1,645)	1:A:990:VAL:HB	1:A:993:PHE:H	5	0.18
(1,576)	1:A:989:LYS:H	1:A:989:LYS:HD3	18	0.18
(1,557)	1:A:988:TRP:H	1:A:988:TRP:HB3	12	0.18
(1,547)	1:A:987:MET:HG3	1:A:989:LYS:H	16	0.18
(1,485)	1:A:985:LEU:HA	1:A:987:MET:H	4	0.18
(1,485)	1:A:985:LEU:HA	1:A:987:MET:H	14	0.18
(1,485)	1:A:985:LEU:HA	1:A:987:MET:H	17	0.18
(1,460)	1:A:984:VAL:HA	1:A:988:TRP:HB3	3	0.18
(1,450)	1:A:984:VAL:HA	1:A:987:MET:H	12	0.18
(1,426)	1:A:983:LEU:HA	1:A:985:LEU:H	8	0.18
(1,426)	1:A:983:LEU:HA	1:A:985:LEU:H	18	0.18
(1,423)	1:A:983:LEU:H	1:A:985:LEU:H	8	0.18
(1,423)	1:A:983:LEU:H	1:A:985:LEU:H	18	0.18
(1,4162)	1:A:988:TRP:HE1	2:B:719:ILE:HB	9	0.18
(1,4162)	1:A:988:TRP:HE1	2:B:719:ILE:HB	14	0.18
(1,4157)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	9	0.18
(1,4151)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	19	0.18
(1,4151)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	20	0.18
(1,4143)	1:A:984:VAL:H	2:B:712:LEU:HA	4	0.18
(1,4130)	1:A:979:LEU:H	2:B:704:ILE:HB	18	0.18
(1,4101)	1:A:973:VAL:H	2:B:700:VAL:HA	9	0.18
(1,4034)	2:B:755:THR:H	2:B:755:THR:HB	18	0.18
(1,4007)	2:B:750:ALA:H	2:B:751:THR:H	6	0.18
(1,4000)	2:B:749:GLU:H	2:B:749:GLU:HG3	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3973)	2:B:747:TYR:HB2	2:B:748:LYS:H	3	0.18
(1,3968)	2:B:747:TYR:H	2:B:747:TYR:HB3	16	0.18
(1,395)	1:A:982:ILE:HA	1:A:985:LEU:HB3	12	0.18
(1,395)	1:A:982:ILE:HA	1:A:985:LEU:HB3	14	0.18
(1,3913)	2:B:743:ASN:H	2:B:743:ASN:HD22	16	0.18
(1,3911)	2:B:743:ASN:HB3	2:B:743:ASN:H	2	0.18
(1,3909)	2:B:743:ASN:HB2	2:B:743:ASN:H	12	0.18
(1,3893)	2:B:741:THR:HA	2:B:742:ALA:H	16	0.18
(1,3888)	2:B:740:ASP:HA	2:B:741:THR:H	7	0.18
(1,3888)	2:B:740:ASP:HA	2:B:741:THR:H	14	0.18
(1,3882)	2:B:739:TRP:HB2	2:B:740:ASP:H	4	0.18
(1,3881)	2:B:739:TRP:HB3	2:B:740:ASP:H	4	0.18
(1,3881)	2:B:739:TRP:HB3	2:B:740:ASP:H	16	0.18
(1,3870)	2:B:738:LYS:HA	2:B:740:ASP:H	7	0.18
(1,3863)	2:B:738:LYS:HB3	2:B:739:TRP:H	8	0.18
(1,3863)	2:B:738:LYS:HB3	2:B:739:TRP:H	10	0.18
(1,3863)	2:B:738:LYS:HB3	2:B:739:TRP:H	12	0.18
(1,3852)	2:B:738:LYS:H	2:B:738:LYS:HG3	11	0.18
(1,3852)	2:B:738:LYS:H	2:B:738:LYS:HG3	15	0.18
(1,3741)	2:B:730:PHE:HB3	2:B:731:GLU:HG3	9	0.18
(1,3646)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	17	0.18
(1,3644)	2:B:725:LYS:H	2:B:725:LYS:HG3	1	0.18
(1,3644)	2:B:725:LYS:H	2:B:725:LYS:HG3	11	0.18
(1,3644)	2:B:725:LYS:H	2:B:725:LYS:HG3	13	0.18
(1,3644)	2:B:725:LYS:H	2:B:725:LYS:HG3	15	0.18
(1,3644)	2:B:725:LYS:H	2:B:725:LYS:HG3	16	0.18
(1,3644)	2:B:725:LYS:H	2:B:725:LYS:HG3	17	0.18
(1,3644)	2:B:725:LYS:H	2:B:725:LYS:HG3	19	0.18
(1,3644)	2:B:725:LYS:H	2:B:725:LYS:HG3	20	0.18
(1,341)	1:A:979:LEU:HA	1:A:981:THR:H	5	0.18
(1,341)	1:A:979:LEU:HA	1:A:981:THR:H	6	0.18
(1,341)	1:A:979:LEU:HA	1:A:981:THR:H	13	0.18
(1,341)	1:A:979:LEU:HA	1:A:981:THR:H	19	0.18
(1,3211)	2:B:704:ILE:HB	2:B:705:LEU:HB2	18	0.18
(1,3211)	2:B:704:ILE:HB	2:B:705:LEU:HB2	19	0.18
(1,3211)	2:B:704:ILE:HB	2:B:705:LEU:HB2	20	0.18
(1,2953)	2:B:693:ILE:H	2:B:693:ILE:HB	20	0.18
(1,2933)	2:B:692:ASP:HA	2:B:693:ILE:H	1	0.18
(1,2933)	2:B:692:ASP:HA	2:B:693:ILE:H	4	0.18
(1,2933)	2:B:692:ASP:HA	2:B:693:ILE:H	7	0.18
(1,2933)	2:B:692:ASP:HA	2:B:693:ILE:H	20	0.18
(1,2924)	2:B:691:PRO:HD3	2:B:692:ASP:H	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,289)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	3	0.18
(1,289)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	4	0.18
(1,289)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	5	0.18
(1,289)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	12	0.18
(1,289)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	19	0.18
(1,2833)	1:A:996:ASN:HA	1:A:997:ARG:H	1	0.18
(1,2812)	1:A:995:ARG:H	1:A:995:ARG:HB3	6	0.18
(1,2812)	1:A:995:ARG:H	1:A:995:ARG:HB3	11	0.18
(1,2808)	1:A:994:LYS:HB3	1:A:995:ARG:HG3	4	0.18
(1,2776)	1:A:993:PHE:H	1:A:994:LYS:HD3	1	0.18
(1,2755)	1:A:992:PHE:HB3	1:A:993:PHE:H	16	0.18
(1,273)	1:A:974:LEU:H	1:A:975:GLY:HA2	3	0.18
(1,273)	1:A:974:LEU:H	1:A:975:GLY:HA2	6	0.18
(1,273)	1:A:974:LEU:H	1:A:975:GLY:HA2	13	0.18
(1,273)	1:A:974:LEU:H	1:A:975:GLY:HA2	15	0.18
(1,2728)	1:A:990:VAL:HB	1:A:993:PHE:H	3	0.18
(1,2728)	1:A:990:VAL:HB	1:A:993:PHE:H	5	0.18
(1,2659)	1:A:989:LYS:H	1:A:989:LYS:HD3	18	0.18
(1,2640)	1:A:988:TRP:H	1:A:988:TRP:HB3	12	0.18
(1,2630)	1:A:987:MET:HG3	1:A:989:LYS:H	16	0.18
(1,2568)	1:A:985:LEU:HA	1:A:987:MET:H	4	0.18
(1,2568)	1:A:985:LEU:HA	1:A:987:MET:H	14	0.18
(1,2568)	1:A:985:LEU:HA	1:A:987:MET:H	17	0.18
(1,2543)	1:A:984:VAL:HA	1:A:988:TRP:HB3	3	0.18
(1,2533)	1:A:984:VAL:HA	1:A:987:MET:H	12	0.18
(1,2509)	1:A:983:LEU:HA	1:A:985:LEU:H	8	0.18
(1,2509)	1:A:983:LEU:HA	1:A:985:LEU:H	18	0.18
(1,2506)	1:A:983:LEU:H	1:A:985:LEU:H	8	0.18
(1,2506)	1:A:983:LEU:H	1:A:985:LEU:H	18	0.18
(1,2478)	1:A:982:ILE:HA	1:A:985:LEU:HB3	12	0.18
(1,2478)	1:A:982:ILE:HA	1:A:985:LEU:HB3	14	0.18
(1,2424)	1:A:979:LEU:HA	1:A:981:THR:H	5	0.18
(1,2424)	1:A:979:LEU:HA	1:A:981:THR:H	6	0.18
(1,2424)	1:A:979:LEU:HA	1:A:981:THR:H	13	0.18
(1,2424)	1:A:979:LEU:HA	1:A:981:THR:H	19	0.18
(1,2372)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	3	0.18
(1,2372)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	4	0.18
(1,2372)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	5	0.18
(1,2372)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	12	0.18
(1,2372)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	19	0.18
(1,2356)	1:A:974:LEU:H	1:A:975:GLY:HA2	3	0.18
(1,2356)	1:A:974:LEU:H	1:A:975:GLY:HA2	6	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2356)	1:A:974:LEU:H	1:A:975:GLY:HA2	13	0.18
(1,2356)	1:A:974:LEU:H	1:A:975:GLY:HA2	15	0.18
(1,2308)	1:A:971:VAL:H	1:A:973:VAL:H	1	0.18
(1,2308)	1:A:971:VAL:H	1:A:973:VAL:H	18	0.18
(1,2308)	1:A:971:VAL:H	1:A:973:VAL:H	19	0.18
(1,2258)	1:A:969:VAL:H	1:A:970:LEU:HB3	3	0.18
(1,2258)	1:A:969:VAL:H	1:A:970:LEU:HB3	6	0.18
(1,225)	1:A:971:VAL:H	1:A:973:VAL:H	1	0.18
(1,225)	1:A:971:VAL:H	1:A:973:VAL:H	18	0.18
(1,225)	1:A:971:VAL:H	1:A:973:VAL:H	19	0.18
(1,2215)	1:A:968:TRP:H	1:A:968:TRP:HB3	6	0.18
(1,2201)	1:A:967:TRP:HA	1:A:968:TRP:HB3	9	0.18
(1,2189)	1:A:967:TRP:H	1:A:967:TRP:HB3	5	0.18
(1,2091)	1:A:961:GLU:H	1:A:961:GLU:HB3	3	0.18
(1,2079)	1:A:988:TRP:HE1	2:B:719:ILE:HB	9	0.18
(1,2079)	1:A:988:TRP:HE1	2:B:719:ILE:HB	14	0.18
(1,2074)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	9	0.18
(1,2068)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	19	0.18
(1,2068)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	20	0.18
(1,2060)	1:A:984:VAL:H	2:B:712:LEU:HA	4	0.18
(1,2047)	1:A:979:LEU:H	2:B:704:ILE:HB	18	0.18
(1,2018)	1:A:973:VAL:H	2:B:700:VAL:HA	9	0.18
(1,1951)	2:B:755:THR:H	2:B:755:THR:HB	18	0.18
(1,1924)	2:B:750:ALA:H	2:B:751:THR:H	6	0.18
(1,1917)	2:B:749:GLU:H	2:B:749:GLU:HG3	1	0.18
(1,1890)	2:B:747:TYR:HB2	2:B:748:LYS:H	3	0.18
(1,1885)	2:B:747:TYR:H	2:B:747:TYR:HB3	16	0.18
(1,1830)	2:B:743:ASN:H	2:B:743:ASN:HD22	16	0.18
(1,1828)	2:B:743:ASN:HB3	2:B:743:ASN:H	2	0.18
(1,1826)	2:B:743:ASN:HB2	2:B:743:ASN:H	12	0.18
(1,1810)	2:B:741:THR:HA	2:B:742:ALA:H	16	0.18
(1,1805)	2:B:740:ASP:HA	2:B:741:THR:H	7	0.18
(1,1805)	2:B:740:ASP:HA	2:B:741:THR:H	14	0.18
(1,1799)	2:B:739:TRP:HB2	2:B:740:ASP:H	4	0.18
(1,1798)	2:B:739:TRP:HB3	2:B:740:ASP:H	4	0.18
(1,1798)	2:B:739:TRP:HB3	2:B:740:ASP:H	16	0.18
(1,1787)	2:B:738:LYS:HA	2:B:740:ASP:H	7	0.18
(1,1780)	2:B:738:LYS:HB3	2:B:739:TRP:H	8	0.18
(1,1780)	2:B:738:LYS:HB3	2:B:739:TRP:H	10	0.18
(1,1780)	2:B:738:LYS:HB3	2:B:739:TRP:H	12	0.18
(1,1769)	2:B:738:LYS:H	2:B:738:LYS:HG3	11	0.18
(1,1769)	2:B:738:LYS:H	2:B:738:LYS:HG3	15	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,175)	1:A:969:VAL:H	1:A:970:LEU:HB3	3	0.18
(1,175)	1:A:969:VAL:H	1:A:970:LEU:HB3	6	0.18
(1,1658)	2:B:730:PHE:HB3	2:B:731:GLU:HG3	9	0.18
(1,1563)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	17	0.18
(1,1561)	2:B:725:LYS:H	2:B:725:LYS:HG3	1	0.18
(1,1561)	2:B:725:LYS:H	2:B:725:LYS:HG3	11	0.18
(1,1561)	2:B:725:LYS:H	2:B:725:LYS:HG3	13	0.18
(1,1561)	2:B:725:LYS:H	2:B:725:LYS:HG3	15	0.18
(1,1561)	2:B:725:LYS:H	2:B:725:LYS:HG3	16	0.18
(1,1561)	2:B:725:LYS:H	2:B:725:LYS:HG3	17	0.18
(1,1561)	2:B:725:LYS:H	2:B:725:LYS:HG3	19	0.18
(1,1561)	2:B:725:LYS:H	2:B:725:LYS:HG3	20	0.18
(1,132)	1:A:968:TRP:H	1:A:968:TRP:HB3	6	0.18
(1,118)	1:A:967:TRP:HA	1:A:968:TRP:HB3	9	0.18
(1,1128)	2:B:704:ILE:HB	2:B:705:LEU:HB2	18	0.18
(1,1128)	2:B:704:ILE:HB	2:B:705:LEU:HB2	19	0.18
(1,1128)	2:B:704:ILE:HB	2:B:705:LEU:HB2	20	0.18
(1,106)	1:A:967:TRP:H	1:A:967:TRP:HB3	5	0.18
(3,270)	2:B:710:ALA:O	2:B:714:ILE:H	17	0.17
(3,111)	2:B:710:ALA:O	2:B:714:ILE:H	17	0.17
(1,870)	2:B:693:ILE:H	2:B:693:ILE:HB	4	0.17
(1,870)	2:B:693:ILE:H	2:B:693:ILE:HB	13	0.17
(1,851)	2:B:692:ASP:H	2:B:693:ILE:H	10	0.17
(1,850)	2:B:692:ASP:HA	2:B:693:ILE:H	5	0.17
(1,795)	1:A:1002:GLU:HA	1:A:1003:ASP:H	14	0.17
(1,761)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	14	0.17
(1,729)	1:A:995:ARG:H	1:A:995:ARG:HB3	8	0.17
(1,729)	1:A:995:ARG:H	1:A:995:ARG:HB3	18	0.17
(1,725)	1:A:994:LYS:HB3	1:A:995:ARG:HG3	3	0.17
(1,724)	1:A:994:LYS:HB2	1:A:995:ARG:HG3	10	0.17
(1,684)	1:A:993:PHE:HB3	1:A:993:PHE:H	4	0.17
(1,684)	1:A:993:PHE:HB3	1:A:993:PHE:H	9	0.17
(1,684)	1:A:993:PHE:HB3	1:A:993:PHE:H	14	0.17
(1,672)	1:A:992:PHE:HB3	1:A:993:PHE:H	2	0.17
(1,672)	1:A:992:PHE:HB3	1:A:993:PHE:H	5	0.17
(1,672)	1:A:992:PHE:HB3	1:A:993:PHE:H	14	0.17
(1,645)	1:A:990:VAL:HB	1:A:993:PHE:H	1	0.17
(1,645)	1:A:990:VAL:HB	1:A:993:PHE:H	4	0.17
(1,645)	1:A:990:VAL:HB	1:A:993:PHE:H	7	0.17
(1,645)	1:A:990:VAL:HB	1:A:993:PHE:H	18	0.17
(1,576)	1:A:989:LYS:H	1:A:989:LYS:HD3	2	0.17
(1,576)	1:A:989:LYS:H	1:A:989:LYS:HD3	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,557)	1:A:988:TRP:H	1:A:988:TRP:HB3	8	0.17
(1,548)	1:A:987:MET:HA	1:A:990:VAL:H	10	0.17
(1,548)	1:A:987:MET:HA	1:A:990:VAL:H	15	0.17
(1,547)	1:A:987:MET:HG3	1:A:989:LYS:H	8	0.17
(1,487)	1:A:985:LEU:H	1:A:987:MET:HG2	16	0.17
(1,485)	1:A:985:LEU:HA	1:A:987:MET:H	6	0.17
(1,485)	1:A:985:LEU:HA	1:A:987:MET:H	7	0.17
(1,485)	1:A:985:LEU:HA	1:A:987:MET:H	9	0.17
(1,485)	1:A:985:LEU:HA	1:A:987:MET:H	19	0.17
(1,485)	1:A:985:LEU:HA	1:A:987:MET:H	20	0.17
(1,426)	1:A:983:LEU:HA	1:A:985:LEU:H	19	0.17
(1,423)	1:A:983:LEU:H	1:A:985:LEU:H	13	0.17
(1,4162)	1:A:988:TRP:HE1	2:B:719:ILE:HB	10	0.17
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG21	13	0.17
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG22	13	0.17
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG23	13	0.17
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG21	16	0.17
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG22	16	0.17
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG23	16	0.17
(1,4143)	1:A:984:VAL:H	2:B:712:LEU:HA	11	0.17
(1,4101)	1:A:973:VAL:H	2:B:700:VAL:HA	1	0.17
(1,4032)	2:B:754:PHE:HB3	2:B:755:THR:H	10	0.17
(1,4000)	2:B:749:GLU:H	2:B:749:GLU:HG3	7	0.17
(1,3968)	2:B:747:TYR:H	2:B:747:TYR:HB3	8	0.17
(1,3968)	2:B:747:TYR:H	2:B:747:TYR:HB3	20	0.17
(1,3963)	2:B:746:LEU:HB2	2:B:747:TYR:H	15	0.17
(1,3954)	2:B:746:LEU:H	2:B:746:LEU:HB2	7	0.17
(1,3954)	2:B:746:LEU:H	2:B:746:LEU:HB2	15	0.17
(1,3954)	2:B:746:LEU:H	2:B:746:LEU:HB2	18	0.17
(1,3954)	2:B:746:LEU:H	2:B:746:LEU:HB2	19	0.17
(1,395)	1:A:982:ILE:HA	1:A:985:LEU:HB3	2	0.17
(1,3945)	2:B:745:PRO:HA	2:B:746:LEU:H	3	0.17
(1,393)	1:A:982:ILE:H	1:A:984:VAL:H	4	0.17
(1,3909)	2:B:743:ASN:HB2	2:B:743:ASN:H	15	0.17
(1,3904)	2:B:742:ALA:HB1	2:B:743:ASN:HD22	5	0.17
(1,3904)	2:B:742:ALA:HB2	2:B:743:ASN:HD22	5	0.17
(1,3904)	2:B:742:ALA:HB3	2:B:743:ASN:HD22	5	0.17
(1,3897)	2:B:741:THR:HA	2:B:744:ASN:H	20	0.17
(1,3882)	2:B:739:TRP:HB2	2:B:740:ASP:H	16	0.17
(1,3857)	2:B:738:LYS:HE3	2:B:738:LYS:HB3	12	0.17
(1,3801)	2:B:734:ARG:HD2	2:B:734:ARG:HB2	6	0.17
(1,3742)	2:B:730:PHE:HB3	2:B:731:GLU:HG2	5	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3718)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	4	0.17
(1,3646)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	9	0.17
(1,3646)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	16	0.17
(1,3644)	2:B:725:LYS:H	2:B:725:LYS:HG3	3	0.17
(1,3644)	2:B:725:LYS:H	2:B:725:LYS:HG3	5	0.17
(1,3644)	2:B:725:LYS:H	2:B:725:LYS:HG3	8	0.17
(1,3644)	2:B:725:LYS:H	2:B:725:LYS:HG3	9	0.17
(1,3644)	2:B:725:LYS:H	2:B:725:LYS:HG3	12	0.17
(1,3638)	2:B:724:ARG:HA	2:B:728:ALA:H	2	0.17
(1,3620)	2:B:724:ARG:HD3	2:B:724:ARG:HB3	18	0.17
(1,3579)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	1	0.17
(1,3579)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	2	0.17
(1,356)	1:A:980:LEU:HB3	1:A:981:THR:HA	11	0.17
(1,356)	1:A:980:LEU:HB3	1:A:981:THR:HA	12	0.17
(1,3495)	2:B:718:LEU:HB3	2:B:719:ILE:HG12	6	0.17
(1,341)	1:A:979:LEU:HA	1:A:981:THR:H	3	0.17
(1,341)	1:A:979:LEU:HA	1:A:981:THR:H	7	0.17
(1,341)	1:A:979:LEU:HA	1:A:981:THR:H	8	0.17
(1,3319)	2:B:709:LEU:H	2:B:711:ALA:H	9	0.17
(1,3211)	2:B:704:ILE:HB	2:B:705:LEU:HB2	9	0.17
(1,312)	1:A:977:LEU:HD11	1:A:977:LEU:HA	5	0.17
(1,312)	1:A:977:LEU:HD12	1:A:977:LEU:HA	5	0.17
(1,312)	1:A:977:LEU:HD13	1:A:977:LEU:HA	5	0.17
(1,2953)	2:B:693:ILE:H	2:B:693:ILE:HB	4	0.17
(1,2953)	2:B:693:ILE:H	2:B:693:ILE:HB	13	0.17
(1,2934)	2:B:692:ASP:H	2:B:693:ILE:H	10	0.17
(1,2933)	2:B:692:ASP:HA	2:B:693:ILE:H	5	0.17
(1,289)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	15	0.17
(1,289)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	18	0.17
(1,2878)	1:A:1002:GLU:HA	1:A:1003:ASP:H	14	0.17
(1,2844)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	14	0.17
(1,2812)	1:A:995:ARG:H	1:A:995:ARG:HB3	8	0.17
(1,2812)	1:A:995:ARG:H	1:A:995:ARG:HB3	18	0.17
(1,2808)	1:A:994:LYS:HB3	1:A:995:ARG:HG3	3	0.17
(1,2807)	1:A:994:LYS:HB2	1:A:995:ARG:HG3	10	0.17
(1,2767)	1:A:993:PHE:HB3	1:A:993:PHE:H	4	0.17
(1,2767)	1:A:993:PHE:HB3	1:A:993:PHE:H	9	0.17
(1,2767)	1:A:993:PHE:HB3	1:A:993:PHE:H	14	0.17
(1,2755)	1:A:992:PHE:HB3	1:A:993:PHE:H	2	0.17
(1,2755)	1:A:992:PHE:HB3	1:A:993:PHE:H	5	0.17
(1,2755)	1:A:992:PHE:HB3	1:A:993:PHE:H	14	0.17
(1,273)	1:A:974:LEU:H	1:A:975:GLY:HA2	8	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2728)	1:A:990:VAL:HB	1:A:993:PHE:H	1	0.17
(1,2728)	1:A:990:VAL:HB	1:A:993:PHE:H	4	0.17
(1,2728)	1:A:990:VAL:HB	1:A:993:PHE:H	7	0.17
(1,2728)	1:A:990:VAL:HB	1:A:993:PHE:H	18	0.17
(1,2659)	1:A:989:LYS:H	1:A:989:LYS:HD3	2	0.17
(1,2659)	1:A:989:LYS:H	1:A:989:LYS:HD3	13	0.17
(1,2640)	1:A:988:TRP:H	1:A:988:TRP:HB3	8	0.17
(1,2631)	1:A:987:MET:HA	1:A:990:VAL:H	10	0.17
(1,2631)	1:A:987:MET:HA	1:A:990:VAL:H	15	0.17
(1,2630)	1:A:987:MET:HG3	1:A:989:LYS:H	8	0.17
(1,2570)	1:A:985:LEU:H	1:A:987:MET:HG2	16	0.17
(1,2568)	1:A:985:LEU:HA	1:A:987:MET:H	6	0.17
(1,2568)	1:A:985:LEU:HA	1:A:987:MET:H	7	0.17
(1,2568)	1:A:985:LEU:HA	1:A:987:MET:H	9	0.17
(1,2568)	1:A:985:LEU:HA	1:A:987:MET:H	19	0.17
(1,2568)	1:A:985:LEU:HA	1:A:987:MET:H	20	0.17
(1,2509)	1:A:983:LEU:HA	1:A:985:LEU:H	19	0.17
(1,2506)	1:A:983:LEU:H	1:A:985:LEU:H	13	0.17
(1,2478)	1:A:982:ILE:HA	1:A:985:LEU:HB3	2	0.17
(1,2476)	1:A:982:ILE:H	1:A:984:VAL:H	4	0.17
(1,2439)	1:A:980:LEU:HB3	1:A:981:THR:HA	11	0.17
(1,2439)	1:A:980:LEU:HB3	1:A:981:THR:HA	12	0.17
(1,2424)	1:A:979:LEU:HA	1:A:981:THR:H	3	0.17
(1,2424)	1:A:979:LEU:HA	1:A:981:THR:H	7	0.17
(1,2424)	1:A:979:LEU:HA	1:A:981:THR:H	8	0.17
(1,2395)	1:A:977:LEU:HD11	1:A:977:LEU:HA	5	0.17
(1,2395)	1:A:977:LEU:HD12	1:A:977:LEU:HA	5	0.17
(1,2395)	1:A:977:LEU:HD13	1:A:977:LEU:HA	5	0.17
(1,2372)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	15	0.17
(1,2372)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	18	0.17
(1,2356)	1:A:974:LEU:H	1:A:975:GLY:HA2	8	0.17
(1,2308)	1:A:971:VAL:H	1:A:973:VAL:H	10	0.17
(1,2308)	1:A:971:VAL:H	1:A:973:VAL:H	17	0.17
(1,2291)	1:A:970:LEU:HB3	1:A:974:LEU:H	6	0.17
(1,225)	1:A:971:VAL:H	1:A:973:VAL:H	10	0.17
(1,225)	1:A:971:VAL:H	1:A:973:VAL:H	17	0.17
(1,2203)	1:A:967:TRP:HB3	1:A:968:TRP:HB3	7	0.17
(1,2097)	1:A:962:ARG:H	1:A:962:ARG:HB2	13	0.17
(1,208)	1:A:970:LEU:HB3	1:A:974:LEU:H	6	0.17
(1,2079)	1:A:988:TRP:HE1	2:B:719:ILE:HB	10	0.17
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG21	13	0.17
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG22	13	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG23	13	0.17
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG21	16	0.17
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG22	16	0.17
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG23	16	0.17
(1,2060)	1:A:984:VAL:H	2:B:712:LEU:HA	11	0.17
(1,2018)	1:A:973:VAL:H	2:B:700:VAL:HA	1	0.17
(1,1949)	2:B:754:PHE:HB3	2:B:755:THR:H	10	0.17
(1,1917)	2:B:749:GLU:H	2:B:749:GLU:HG3	7	0.17
(1,1885)	2:B:747:TYR:H	2:B:747:TYR:HB3	8	0.17
(1,1885)	2:B:747:TYR:H	2:B:747:TYR:HB3	20	0.17
(1,1880)	2:B:746:LEU:HB2	2:B:747:TYR:H	15	0.17
(1,1871)	2:B:746:LEU:H	2:B:746:LEU:HB2	7	0.17
(1,1871)	2:B:746:LEU:H	2:B:746:LEU:HB2	15	0.17
(1,1871)	2:B:746:LEU:H	2:B:746:LEU:HB2	18	0.17
(1,1871)	2:B:746:LEU:H	2:B:746:LEU:HB2	19	0.17
(1,1862)	2:B:745:PRO:HA	2:B:746:LEU:H	3	0.17
(1,1826)	2:B:743:ASN:HB2	2:B:743:ASN:H	15	0.17
(1,1821)	2:B:742:ALA:HB1	2:B:743:ASN:HD22	5	0.17
(1,1821)	2:B:742:ALA:HB2	2:B:743:ASN:HD22	5	0.17
(1,1821)	2:B:742:ALA:HB3	2:B:743:ASN:HD22	5	0.17
(1,1814)	2:B:741:THR:HA	2:B:744:ASN:H	20	0.17
(1,1799)	2:B:739:TRP:HB2	2:B:740:ASP:H	16	0.17
(1,1774)	2:B:738:LYS:HE3	2:B:738:LYS:HB3	12	0.17
(1,1718)	2:B:734:ARG:HD2	2:B:734:ARG:HB2	6	0.17
(1,1659)	2:B:730:PHE:HB3	2:B:731:GLU:HG2	5	0.17
(1,1635)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	4	0.17
(1,1563)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	9	0.17
(1,1563)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	16	0.17
(1,1561)	2:B:725:LYS:H	2:B:725:LYS:HG3	3	0.17
(1,1561)	2:B:725:LYS:H	2:B:725:LYS:HG3	5	0.17
(1,1561)	2:B:725:LYS:H	2:B:725:LYS:HG3	8	0.17
(1,1561)	2:B:725:LYS:H	2:B:725:LYS:HG3	9	0.17
(1,1561)	2:B:725:LYS:H	2:B:725:LYS:HG3	12	0.17
(1,1555)	2:B:724:ARG:HA	2:B:728:ALA:H	2	0.17
(1,1537)	2:B:724:ARG:HD3	2:B:724:ARG:HB3	18	0.17
(1,1496)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	1	0.17
(1,1496)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	2	0.17
(1,1412)	2:B:718:LEU:HB3	2:B:719:ILE:HG12	6	0.17
(1,14)	1:A:962:ARG:H	1:A:962:ARG:HB2	13	0.17
(1,1236)	2:B:709:LEU:H	2:B:711:ALA:H	9	0.17
(1,120)	1:A:967:TRP:HB3	1:A:968:TRP:HB3	7	0.17
(1,1128)	2:B:704:ILE:HB	2:B:705:LEU:HB2	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,43)	1:A:981:THR:O	1:A:984:VAL:H	13	0.16
(3,270)	2:B:710:ALA:O	2:B:714:ILE:H	12	0.16
(3,202)	1:A:981:THR:O	1:A:984:VAL:H	13	0.16
(3,111)	2:B:710:ALA:O	2:B:714:ILE:H	12	0.16
(1,870)	2:B:693:ILE:H	2:B:693:ILE:HB	5	0.16
(1,850)	2:B:692:ASP:HA	2:B:693:ILE:H	3	0.16
(1,850)	2:B:692:ASP:HA	2:B:693:ILE:H	11	0.16
(1,850)	2:B:692:ASP:HA	2:B:693:ILE:H	12	0.16
(1,850)	2:B:692:ASP:HA	2:B:693:ILE:H	16	0.16
(1,850)	2:B:692:ASP:HA	2:B:693:ILE:H	19	0.16
(1,8)	1:A:961:GLU:H	1:A:961:GLU:HB3	7	0.16
(1,8)	1:A:961:GLU:H	1:A:961:GLU:HB3	16	0.16
(1,790)	1:A:1001:GLU:H	1:A:1001:GLU:HB2	16	0.16
(1,762)	1:A:997:ARG:HA	1:A:999:PRO:HD2	4	0.16
(1,761)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	7	0.16
(1,761)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	8	0.16
(1,761)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	9	0.16
(1,761)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	20	0.16
(1,760)	1:A:997:ARG:HA	1:A:999:PRO:HD3	17	0.16
(1,753)	1:A:997:ARG:HD3	1:A:997:ARG:HA	12	0.16
(1,750)	1:A:996:ASN:HA	1:A:997:ARG:H	13	0.16
(1,750)	1:A:996:ASN:HA	1:A:997:ARG:H	16	0.16
(1,742)	1:A:996:ASN:H	1:A:996:ASN:HB2	6	0.16
(1,725)	1:A:994:LYS:HB3	1:A:995:ARG:HG3	1	0.16
(1,718)	1:A:994:LYS:HB2	1:A:995:ARG:H	12	0.16
(1,704)	1:A:994:LYS:H	1:A:994:LYS:HG3	2	0.16
(1,704)	1:A:994:LYS:H	1:A:994:LYS:HG3	9	0.16
(1,7)	1:A:960:GLU:HB2	1:A:961:GLU:H	8	0.16
(1,690)	1:A:993:PHE:HB2	1:A:994:LYS:H	4	0.16
(1,690)	1:A:993:PHE:HB2	1:A:994:LYS:H	17	0.16
(1,684)	1:A:993:PHE:HB3	1:A:993:PHE:H	13	0.16
(1,672)	1:A:992:PHE:HB3	1:A:993:PHE:H	3	0.16
(1,672)	1:A:992:PHE:HB3	1:A:993:PHE:H	4	0.16
(1,672)	1:A:992:PHE:HB3	1:A:993:PHE:H	20	0.16
(1,645)	1:A:990:VAL:HB	1:A:993:PHE:H	13	0.16
(1,645)	1:A:990:VAL:HB	1:A:993:PHE:H	19	0.16
(1,611)	1:A:989:LYS:HE3	1:A:993:PHE:HE1	18	0.16
(1,576)	1:A:989:LYS:H	1:A:989:LYS:HD3	1	0.16
(1,548)	1:A:987:MET:HA	1:A:990:VAL:H	2	0.16
(1,548)	1:A:987:MET:HA	1:A:990:VAL:H	4	0.16
(1,548)	1:A:987:MET:HA	1:A:990:VAL:H	18	0.16
(1,547)	1:A:987:MET:HG3	1:A:989:LYS:H	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,485)	1:A:985:LEU:HA	1:A:987:MET:H	5	0.16
(1,485)	1:A:985:LEU:HA	1:A:987:MET:H	15	0.16
(1,485)	1:A:985:LEU:HA	1:A:987:MET:H	16	0.16
(1,450)	1:A:984:VAL:HA	1:A:987:MET:H	9	0.16
(1,44)	1:A:964:ILE:H	1:A:965:PRO:HB2	11	0.16
(1,426)	1:A:983:LEU:HA	1:A:985:LEU:H	4	0.16
(1,426)	1:A:983:LEU:HA	1:A:985:LEU:H	12	0.16
(1,423)	1:A:983:LEU:H	1:A:985:LEU:H	3	0.16
(1,4151)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	17	0.16
(1,4111)	1:A:974:LEU:H	2:B:704:ILE:HG13	14	0.16
(1,4101)	1:A:973:VAL:H	2:B:700:VAL:HA	6	0.16
(1,4051)	2:B:757:ILE:H	2:B:757:ILE:HG12	10	0.16
(1,4051)	2:B:757:ILE:H	2:B:757:ILE:HG12	12	0.16
(1,4034)	2:B:755:THR:H	2:B:755:THR:HB	4	0.16
(1,4032)	2:B:754:PHE:HB3	2:B:755:THR:H	12	0.16
(1,4027)	2:B:753:THR:HA	2:B:754:PHE:H	11	0.16
(1,4000)	2:B:749:GLU:H	2:B:749:GLU:HG3	2	0.16
(1,3973)	2:B:747:TYR:HB2	2:B:748:LYS:H	16	0.16
(1,3968)	2:B:747:TYR:H	2:B:747:TYR:HB3	1	0.16
(1,3968)	2:B:747:TYR:H	2:B:747:TYR:HB3	19	0.16
(1,3954)	2:B:746:LEU:H	2:B:746:LEU:HB2	6	0.16
(1,395)	1:A:982:ILE:HA	1:A:985:LEU:HB3	4	0.16
(1,3945)	2:B:745:PRO:HA	2:B:746:LEU:H	10	0.16
(1,3918)	2:B:743:ASN:HA	2:B:744:ASN:H	9	0.16
(1,3918)	2:B:743:ASN:HA	2:B:744:ASN:H	12	0.16
(1,3911)	2:B:743:ASN:HB3	2:B:743:ASN:H	9	0.16
(1,3893)	2:B:741:THR:HA	2:B:742:ALA:H	11	0.16
(1,3893)	2:B:741:THR:HA	2:B:742:ALA:H	15	0.16
(1,3888)	2:B:740:ASP:HA	2:B:741:THR:H	8	0.16
(1,3888)	2:B:740:ASP:HA	2:B:741:THR:H	10	0.16
(1,3863)	2:B:738:LYS:HB3	2:B:739:TRP:H	14	0.16
(1,3863)	2:B:738:LYS:HB3	2:B:739:TRP:H	17	0.16
(1,3860)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	17	0.16
(1,3836)	2:B:736:ARG:HG2	2:B:739:TRP:H	15	0.16
(1,3801)	2:B:734:ARG:HD2	2:B:734:ARG:HB2	3	0.16
(1,3718)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	16	0.16
(1,3706)	2:B:728:ALA:H	2:B:730:PHE:H	5	0.16
(1,3646)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	3	0.16
(1,3646)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	12	0.16
(1,3644)	2:B:725:LYS:H	2:B:725:LYS:HG3	2	0.16
(1,3644)	2:B:725:LYS:H	2:B:725:LYS:HG3	6	0.16
(1,3644)	2:B:725:LYS:H	2:B:725:LYS:HG3	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3644)	2:B:725:LYS:H	2:B:725:LYS:HG3	18	0.16
(1,3638)	2:B:724:ARG:HA	2:B:728:ALA:H	8	0.16
(1,3638)	2:B:724:ARG:HA	2:B:728:ALA:H	11	0.16
(1,3638)	2:B:724:ARG:HA	2:B:728:ALA:H	20	0.16
(1,3579)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	7	0.16
(1,3579)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	12	0.16
(1,3579)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	19	0.16
(1,356)	1:A:980:LEU:HB3	1:A:981:THR:HA	18	0.16
(1,3508)	2:B:718:LEU:HD21	2:B:721:ILE:HB	2	0.16
(1,3508)	2:B:718:LEU:HD22	2:B:721:ILE:HB	2	0.16
(1,3508)	2:B:718:LEU:HD23	2:B:721:ILE:HB	2	0.16
(1,3495)	2:B:718:LEU:HB3	2:B:719:ILE:HG12	10	0.16
(1,3470)	2:B:717:LEU:H	2:B:719:ILE:H	2	0.16
(1,342)	1:A:979:LEU:HA	1:A:982:ILE:HB	16	0.16
(1,341)	1:A:979:LEU:HA	1:A:981:THR:H	1	0.16
(1,341)	1:A:979:LEU:HA	1:A:981:THR:H	2	0.16
(1,341)	1:A:979:LEU:HA	1:A:981:THR:H	4	0.16
(1,341)	1:A:979:LEU:HA	1:A:981:THR:H	10	0.16
(1,341)	1:A:979:LEU:HA	1:A:981:THR:H	15	0.16
(1,3319)	2:B:709:LEU:H	2:B:711:ALA:H	2	0.16
(1,3319)	2:B:709:LEU:H	2:B:711:ALA:H	11	0.16
(1,3318)	2:B:709:LEU:HB3	2:B:710:ALA:HA	19	0.16
(1,3211)	2:B:704:ILE:HB	2:B:705:LEU:HB2	6	0.16
(1,3211)	2:B:704:ILE:HB	2:B:705:LEU:HB2	11	0.16
(1,2953)	2:B:693:ILE:H	2:B:693:ILE:HB	5	0.16
(1,2933)	2:B:692:ASP:HA	2:B:693:ILE:H	3	0.16
(1,2933)	2:B:692:ASP:HA	2:B:693:ILE:H	11	0.16
(1,2933)	2:B:692:ASP:HA	2:B:693:ILE:H	12	0.16
(1,2933)	2:B:692:ASP:HA	2:B:693:ILE:H	16	0.16
(1,2933)	2:B:692:ASP:HA	2:B:693:ILE:H	19	0.16
(1,289)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	2	0.16
(1,289)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	6	0.16
(1,2873)	1:A:1001:GLU:H	1:A:1001:GLU:HB2	16	0.16
(1,2845)	1:A:997:ARG:HA	1:A:999:PRO:HD2	4	0.16
(1,2844)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	7	0.16
(1,2844)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	8	0.16
(1,2844)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	9	0.16
(1,2844)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	20	0.16
(1,2843)	1:A:997:ARG:HA	1:A:999:PRO:HD3	17	0.16
(1,2836)	1:A:997:ARG:HD3	1:A:997:ARG:HA	12	0.16
(1,2833)	1:A:996:ASN:HA	1:A:997:ARG:H	13	0.16
(1,2833)	1:A:996:ASN:HA	1:A:997:ARG:H	16	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2825)	1:A:996:ASN:H	1:A:996:ASN:HB2	6	0.16
(1,2808)	1:A:994:LYS:HB3	1:A:995:ARG:HG3	1	0.16
(1,2801)	1:A:994:LYS:HB2	1:A:995:ARG:H	12	0.16
(1,28)	1:A:964:ILE:H	1:A:964:ILE:HB	4	0.16
(1,2787)	1:A:994:LYS:H	1:A:994:LYS:HG3	2	0.16
(1,2787)	1:A:994:LYS:H	1:A:994:LYS:HG3	9	0.16
(1,2773)	1:A:993:PHE:HB2	1:A:994:LYS:H	4	0.16
(1,2773)	1:A:993:PHE:HB2	1:A:994:LYS:H	17	0.16
(1,2767)	1:A:993:PHE:HB3	1:A:993:PHE:H	13	0.16
(1,2755)	1:A:992:PHE:HB3	1:A:993:PHE:H	3	0.16
(1,2755)	1:A:992:PHE:HB3	1:A:993:PHE:H	4	0.16
(1,2755)	1:A:992:PHE:HB3	1:A:993:PHE:H	20	0.16
(1,273)	1:A:974:LEU:H	1:A:975:GLY:HA2	16	0.16
(1,273)	1:A:974:LEU:H	1:A:975:GLY:HA2	17	0.16
(1,2728)	1:A:990:VAL:HB	1:A:993:PHE:H	13	0.16
(1,2728)	1:A:990:VAL:HB	1:A:993:PHE:H	19	0.16
(1,2694)	1:A:989:LYS:HE3	1:A:993:PHE:HE1	18	0.16
(1,2659)	1:A:989:LYS:H	1:A:989:LYS:HD3	1	0.16
(1,2631)	1:A:987:MET:HA	1:A:990:VAL:H	2	0.16
(1,2631)	1:A:987:MET:HA	1:A:990:VAL:H	4	0.16
(1,2631)	1:A:987:MET:HA	1:A:990:VAL:H	18	0.16
(1,2630)	1:A:987:MET:HG3	1:A:989:LYS:H	18	0.16
(1,2568)	1:A:985:LEU:HA	1:A:987:MET:H	5	0.16
(1,2568)	1:A:985:LEU:HA	1:A:987:MET:H	15	0.16
(1,2568)	1:A:985:LEU:HA	1:A:987:MET:H	16	0.16
(1,2533)	1:A:984:VAL:HA	1:A:987:MET:H	9	0.16
(1,2509)	1:A:983:LEU:HA	1:A:985:LEU:H	4	0.16
(1,2509)	1:A:983:LEU:HA	1:A:985:LEU:H	12	0.16
(1,2506)	1:A:983:LEU:H	1:A:985:LEU:H	3	0.16
(1,2478)	1:A:982:ILE:HA	1:A:985:LEU:HB3	4	0.16
(1,2439)	1:A:980:LEU:HB3	1:A:981:THR:HA	18	0.16
(1,243)	1:A:972:GLY:H	1:A:976:GLY:H	17	0.16
(1,2425)	1:A:979:LEU:HA	1:A:982:ILE:HB	16	0.16
(1,2424)	1:A:979:LEU:HA	1:A:981:THR:H	1	0.16
(1,2424)	1:A:979:LEU:HA	1:A:981:THR:H	2	0.16
(1,2424)	1:A:979:LEU:HA	1:A:981:THR:H	4	0.16
(1,2424)	1:A:979:LEU:HA	1:A:981:THR:H	10	0.16
(1,2424)	1:A:979:LEU:HA	1:A:981:THR:H	15	0.16
(1,2372)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	2	0.16
(1,2372)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	6	0.16
(1,2356)	1:A:974:LEU:H	1:A:975:GLY:HA2	16	0.16
(1,2356)	1:A:974:LEU:H	1:A:975:GLY:HA2	17	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2326)	1:A:972:GLY:H	1:A:976:GLY:H	17	0.16
(1,2308)	1:A:971:VAL:H	1:A:973:VAL:H	12	0.16
(1,2291)	1:A:970:LEU:HB3	1:A:974:LEU:H	14	0.16
(1,2266)	1:A:969:VAL:H	1:A:972:GLY:HA3	18	0.16
(1,2258)	1:A:969:VAL:H	1:A:970:LEU:HB3	5	0.16
(1,2258)	1:A:969:VAL:H	1:A:970:LEU:HB3	17	0.16
(1,225)	1:A:971:VAL:H	1:A:973:VAL:H	12	0.16
(1,2238)	1:A:968:TRP:HA	1:A:971:VAL:H	4	0.16
(1,2238)	1:A:968:TRP:HA	1:A:971:VAL:H	11	0.16
(1,2238)	1:A:968:TRP:HA	1:A:971:VAL:H	17	0.16
(1,2215)	1:A:968:TRP:H	1:A:968:TRP:HB3	7	0.16
(1,2201)	1:A:967:TRP:HA	1:A:968:TRP:HB3	3	0.16
(1,2201)	1:A:967:TRP:HA	1:A:968:TRP:HB3	4	0.16
(1,2201)	1:A:967:TRP:HA	1:A:968:TRP:HB3	5	0.16
(1,2201)	1:A:967:TRP:HA	1:A:968:TRP:HB3	8	0.16
(1,2127)	1:A:964:ILE:H	1:A:965:PRO:HB2	11	0.16
(1,2111)	1:A:964:ILE:H	1:A:964:ILE:HB	4	0.16
(1,2097)	1:A:962:ARG:H	1:A:962:ARG:HB2	6	0.16
(1,2091)	1:A:961:GLU:H	1:A:961:GLU:HB3	7	0.16
(1,2091)	1:A:961:GLU:H	1:A:961:GLU:HB3	16	0.16
(1,2090)	1:A:960:GLU:HB2	1:A:961:GLU:H	8	0.16
(1,208)	1:A:970:LEU:HB3	1:A:974:LEU:H	14	0.16
(1,2068)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	17	0.16
(1,2028)	1:A:974:LEU:H	2:B:704:ILE:HG13	14	0.16
(1,2018)	1:A:973:VAL:H	2:B:700:VAL:HA	6	0.16
(1,1968)	2:B:757:ILE:H	2:B:757:ILE:HG12	10	0.16
(1,1968)	2:B:757:ILE:H	2:B:757:ILE:HG12	12	0.16
(1,1951)	2:B:755:THR:H	2:B:755:THR:HB	4	0.16
(1,1949)	2:B:754:PHE:HB3	2:B:755:THR:H	12	0.16
(1,1944)	2:B:753:THR:HA	2:B:754:PHE:H	11	0.16
(1,1917)	2:B:749:GLU:H	2:B:749:GLU:HG3	2	0.16
(1,1890)	2:B:747:TYR:HB2	2:B:748:LYS:H	16	0.16
(1,1885)	2:B:747:TYR:H	2:B:747:TYR:HB3	1	0.16
(1,1885)	2:B:747:TYR:H	2:B:747:TYR:HB3	19	0.16
(1,1871)	2:B:746:LEU:H	2:B:746:LEU:HB2	6	0.16
(1,1862)	2:B:745:PRO:HA	2:B:746:LEU:H	10	0.16
(1,1835)	2:B:743:ASN:HA	2:B:744:ASN:H	9	0.16
(1,1835)	2:B:743:ASN:HA	2:B:744:ASN:H	12	0.16
(1,183)	1:A:969:VAL:H	1:A:972:GLY:HA3	18	0.16
(1,1828)	2:B:743:ASN:HB3	2:B:743:ASN:H	9	0.16
(1,1810)	2:B:741:THR:HA	2:B:742:ALA:H	11	0.16
(1,1810)	2:B:741:THR:HA	2:B:742:ALA:H	15	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1805)	2:B:740:ASP:HA	2:B:741:THR:H	8	0.16
(1,1805)	2:B:740:ASP:HA	2:B:741:THR:H	10	0.16
(1,1780)	2:B:738:LYS:HB3	2:B:739:TRP:H	14	0.16
(1,1780)	2:B:738:LYS:HB3	2:B:739:TRP:H	17	0.16
(1,1777)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	17	0.16
(1,1753)	2:B:736:ARG:HG2	2:B:739:TRP:H	15	0.16
(1,175)	1:A:969:VAL:H	1:A:970:LEU:HB3	5	0.16
(1,175)	1:A:969:VAL:H	1:A:970:LEU:HB3	17	0.16
(1,1718)	2:B:734:ARG:HD2	2:B:734:ARG:HB2	3	0.16
(1,1635)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	16	0.16
(1,1623)	2:B:728:ALA:H	2:B:730:PHE:H	5	0.16
(1,1563)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	3	0.16
(1,1563)	2:B:725:LYS:HE3	2:B:725:LYS:HB3	12	0.16
(1,1561)	2:B:725:LYS:H	2:B:725:LYS:HG3	2	0.16
(1,1561)	2:B:725:LYS:H	2:B:725:LYS:HG3	6	0.16
(1,1561)	2:B:725:LYS:H	2:B:725:LYS:HG3	14	0.16
(1,1561)	2:B:725:LYS:H	2:B:725:LYS:HG3	18	0.16
(1,1555)	2:B:724:ARG:HA	2:B:728:ALA:H	8	0.16
(1,1555)	2:B:724:ARG:HA	2:B:728:ALA:H	11	0.16
(1,1555)	2:B:724:ARG:HA	2:B:728:ALA:H	20	0.16
(1,155)	1:A:968:TRP:HA	1:A:971:VAL:H	4	0.16
(1,155)	1:A:968:TRP:HA	1:A:971:VAL:H	11	0.16
(1,155)	1:A:968:TRP:HA	1:A:971:VAL:H	17	0.16
(1,1496)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	7	0.16
(1,1496)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	12	0.16
(1,1496)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	19	0.16
(1,1425)	2:B:718:LEU:HD21	2:B:721:ILE:HB	2	0.16
(1,1425)	2:B:718:LEU:HD22	2:B:721:ILE:HB	2	0.16
(1,1425)	2:B:718:LEU:HD23	2:B:721:ILE:HB	2	0.16
(1,1412)	2:B:718:LEU:HB3	2:B:719:ILE:HG12	10	0.16
(1,14)	1:A:962:ARG:H	1:A:962:ARG:HB2	6	0.16
(1,1387)	2:B:717:LEU:H	2:B:719:ILE:H	2	0.16
(1,132)	1:A:968:TRP:H	1:A:968:TRP:HB3	7	0.16
(1,1236)	2:B:709:LEU:H	2:B:711:ALA:H	2	0.16
(1,1236)	2:B:709:LEU:H	2:B:711:ALA:H	11	0.16
(1,1235)	2:B:709:LEU:HB3	2:B:710:ALA:HA	19	0.16
(1,118)	1:A:967:TRP:HA	1:A:968:TRP:HB3	3	0.16
(1,118)	1:A:967:TRP:HA	1:A:968:TRP:HB3	4	0.16
(1,118)	1:A:967:TRP:HA	1:A:968:TRP:HB3	5	0.16
(1,118)	1:A:967:TRP:HA	1:A:968:TRP:HB3	8	0.16
(1,1128)	2:B:704:ILE:HB	2:B:705:LEU:HB2	6	0.16
(1,1128)	2:B:704:ILE:HB	2:B:705:LEU:HB2	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,52)	1:A:984:VAL:O	1:A:987:MET:H	16	0.15
(3,270)	2:B:710:ALA:O	2:B:714:ILE:H	1	0.15
(3,211)	1:A:984:VAL:O	1:A:987:MET:H	16	0.15
(3,111)	2:B:710:ALA:O	2:B:714:ILE:H	1	0.15
(1,976)	2:B:697:LEU:HB3	2:B:699:SER:H	5	0.15
(1,850)	2:B:692:ASP:HA	2:B:693:ILE:H	10	0.15
(1,813)	1:A:1006:GLU:H	1:A:1006:GLU:HB2	13	0.15
(1,8)	1:A:961:GLU:H	1:A:961:GLU:HB3	9	0.15
(1,798)	1:A:1003:ASP:H	1:A:1003:ASP:HB2	13	0.15
(1,750)	1:A:996:ASN:HA	1:A:997:ARG:H	7	0.15
(1,750)	1:A:996:ASN:HA	1:A:997:ARG:H	17	0.15
(1,742)	1:A:996:ASN:H	1:A:996:ASN:HB2	3	0.15
(1,725)	1:A:994:LYS:HB3	1:A:995:ARG:HG3	7	0.15
(1,7)	1:A:960:GLU:HB2	1:A:961:GLU:H	4	0.15
(1,7)	1:A:960:GLU:HB2	1:A:961:GLU:H	13	0.15
(1,690)	1:A:993:PHE:HB2	1:A:994:LYS:H	12	0.15
(1,690)	1:A:993:PHE:HB2	1:A:994:LYS:H	16	0.15
(1,684)	1:A:993:PHE:HB3	1:A:993:PHE:H	12	0.15
(1,684)	1:A:993:PHE:HB3	1:A:993:PHE:H	20	0.15
(1,672)	1:A:992:PHE:HB3	1:A:993:PHE:H	17	0.15
(1,645)	1:A:990:VAL:HB	1:A:993:PHE:H	6	0.15
(1,645)	1:A:990:VAL:HB	1:A:993:PHE:H	12	0.15
(1,576)	1:A:989:LYS:H	1:A:989:LYS:HD3	3	0.15
(1,576)	1:A:989:LYS:H	1:A:989:LYS:HD3	12	0.15
(1,548)	1:A:987:MET:HA	1:A:990:VAL:H	14	0.15
(1,533)	1:A:987:MET:H	1:A:987:MET:HG2	18	0.15
(1,485)	1:A:985:LEU:HA	1:A:987:MET:H	2	0.15
(1,485)	1:A:985:LEU:HA	1:A:987:MET:H	8	0.15
(1,485)	1:A:985:LEU:HA	1:A:987:MET:H	10	0.15
(1,485)	1:A:985:LEU:HA	1:A:987:MET:H	18	0.15
(1,450)	1:A:984:VAL:HA	1:A:987:MET:H	10	0.15
(1,437)	1:A:984:VAL:H	1:A:984:VAL:HG11	1	0.15
(1,437)	1:A:984:VAL:H	1:A:984:VAL:HG12	1	0.15
(1,437)	1:A:984:VAL:H	1:A:984:VAL:HG13	1	0.15
(1,437)	1:A:984:VAL:H	1:A:984:VAL:HG11	7	0.15
(1,437)	1:A:984:VAL:H	1:A:984:VAL:HG12	7	0.15
(1,437)	1:A:984:VAL:H	1:A:984:VAL:HG13	7	0.15
(1,426)	1:A:983:LEU:HA	1:A:985:LEU:H	1	0.15
(1,426)	1:A:983:LEU:HA	1:A:985:LEU:H	9	0.15
(1,4162)	1:A:988:TRP:HE1	2:B:719:ILE:HB	3	0.15
(1,4162)	1:A:988:TRP:HE1	2:B:719:ILE:HB	8	0.15
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG21	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG22	9	0.15
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG23	9	0.15
(1,4157)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	5	0.15
(1,4151)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	2	0.15
(1,4151)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	18	0.15
(1,4143)	1:A:984:VAL:H	2:B:712:LEU:HA	13	0.15
(1,4132)	1:A:979:LEU:HD21	2:B:708:GLY:H	6	0.15
(1,4132)	1:A:979:LEU:HD22	2:B:708:GLY:H	6	0.15
(1,4132)	1:A:979:LEU:HD23	2:B:708:GLY:H	6	0.15
(1,412)	1:A:983:LEU:HD11	1:A:983:LEU:H	1	0.15
(1,412)	1:A:983:LEU:HD12	1:A:983:LEU:H	1	0.15
(1,412)	1:A:983:LEU:HD13	1:A:983:LEU:H	1	0.15
(1,4111)	1:A:974:LEU:H	2:B:704:ILE:HG13	9	0.15
(1,4101)	1:A:973:VAL:H	2:B:700:VAL:HA	18	0.15
(1,4053)	2:B:757:ILE:H	2:B:757:ILE:HG13	2	0.15
(1,4051)	2:B:757:ILE:H	2:B:757:ILE:HG12	1	0.15
(1,4051)	2:B:757:ILE:H	2:B:757:ILE:HG12	11	0.15
(1,4032)	2:B:754:PHE:HB3	2:B:755:THR:H	19	0.15
(1,4027)	2:B:753:THR:HA	2:B:754:PHE:H	12	0.15
(1,4007)	2:B:750:ALA:H	2:B:751:THR:H	19	0.15
(1,4000)	2:B:749:GLU:H	2:B:749:GLU:HG3	13	0.15
(1,4000)	2:B:749:GLU:H	2:B:749:GLU:HG3	18	0.15
(1,4000)	2:B:749:GLU:H	2:B:749:GLU:HG3	19	0.15
(1,3968)	2:B:747:TYR:H	2:B:747:TYR:HB3	12	0.15
(1,3968)	2:B:747:TYR:H	2:B:747:TYR:HB3	18	0.15
(1,3954)	2:B:746:LEU:H	2:B:746:LEU:HB2	17	0.15
(1,395)	1:A:982:ILE:HA	1:A:985:LEU:HB3	7	0.15
(1,3911)	2:B:743:ASN:HB3	2:B:743:ASN:H	5	0.15
(1,3904)	2:B:742:ALA:HB1	2:B:743:ASN:HD22	9	0.15
(1,3904)	2:B:742:ALA:HB2	2:B:743:ASN:HD22	9	0.15
(1,3904)	2:B:742:ALA:HB3	2:B:743:ASN:HD22	9	0.15
(1,3888)	2:B:740:ASP:HA	2:B:741:THR:H	3	0.15
(1,3888)	2:B:740:ASP:HA	2:B:741:THR:H	15	0.15
(1,3888)	2:B:740:ASP:HA	2:B:741:THR:H	17	0.15
(1,3881)	2:B:739:TRP:HB3	2:B:740:ASP:H	1	0.15
(1,3863)	2:B:738:LYS:HB3	2:B:739:TRP:H	4	0.15
(1,3863)	2:B:738:LYS:HB3	2:B:739:TRP:H	13	0.15
(1,3863)	2:B:738:LYS:HB3	2:B:739:TRP:H	20	0.15
(1,3860)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	5	0.15
(1,3860)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	10	0.15
(1,3746)	2:B:730:PHE:HE1	2:B:734:ARG:HG3	19	0.15
(1,3718)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3638)	2:B:724:ARG:HA	2:B:728:ALA:H	7	0.15
(1,3638)	2:B:724:ARG:HA	2:B:728:ALA:H	10	0.15
(1,3620)	2:B:724:ARG:HD3	2:B:724:ARG:HB3	15	0.15
(1,3617)	2:B:724:ARG:H	2:B:724:ARG:HB3	1	0.15
(1,3617)	2:B:724:ARG:H	2:B:724:ARG:HB3	19	0.15
(1,3579)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	3	0.15
(1,356)	1:A:980:LEU:HB3	1:A:981:THR:HA	2	0.15
(1,356)	1:A:980:LEU:HB3	1:A:981:THR:HA	4	0.15
(1,356)	1:A:980:LEU:HB3	1:A:981:THR:HA	9	0.15
(1,356)	1:A:980:LEU:HB3	1:A:981:THR:HA	10	0.15
(1,356)	1:A:980:LEU:HB3	1:A:981:THR:HA	19	0.15
(1,356)	1:A:980:LEU:HB3	1:A:981:THR:HA	20	0.15
(1,3507)	2:B:718:LEU:HD11	2:B:721:ILE:HB	13	0.15
(1,3507)	2:B:718:LEU:HD12	2:B:721:ILE:HB	13	0.15
(1,3507)	2:B:718:LEU:HD13	2:B:721:ILE:HB	13	0.15
(1,3470)	2:B:717:LEU:H	2:B:719:ILE:H	5	0.15
(1,3470)	2:B:717:LEU:H	2:B:719:ILE:H	6	0.15
(1,3470)	2:B:717:LEU:H	2:B:719:ILE:H	10	0.15
(1,341)	1:A:979:LEU:HA	1:A:981:THR:H	11	0.15
(1,3319)	2:B:709:LEU:H	2:B:711:ALA:H	5	0.15
(1,3319)	2:B:709:LEU:H	2:B:711:ALA:H	7	0.15
(1,3319)	2:B:709:LEU:H	2:B:711:ALA:H	8	0.15
(1,3211)	2:B:704:ILE:HB	2:B:705:LEU:HB2	14	0.15
(1,3126)	2:B:700:VAL:HB	2:B:701:MET:HG2	8	0.15
(1,3059)	2:B:697:LEU:HB3	2:B:699:SER:H	5	0.15
(1,2933)	2:B:692:ASP:HA	2:B:693:ILE:H	10	0.15
(1,2896)	1:A:1006:GLU:H	1:A:1006:GLU:HB2	13	0.15
(1,289)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	10	0.15
(1,289)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	17	0.15
(1,289)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	20	0.15
(1,2881)	1:A:1003:ASP:H	1:A:1003:ASP:HB2	13	0.15
(1,2833)	1:A:996:ASN:HA	1:A:997:ARG:H	7	0.15
(1,2833)	1:A:996:ASN:HA	1:A:997:ARG:H	17	0.15
(1,2825)	1:A:996:ASN:H	1:A:996:ASN:HB2	3	0.15
(1,2808)	1:A:994:LYS:HB3	1:A:995:ARG:HG3	7	0.15
(1,2773)	1:A:993:PHE:HB2	1:A:994:LYS:H	12	0.15
(1,2773)	1:A:993:PHE:HB2	1:A:994:LYS:H	16	0.15
(1,2767)	1:A:993:PHE:HB3	1:A:993:PHE:H	12	0.15
(1,2767)	1:A:993:PHE:HB3	1:A:993:PHE:H	20	0.15
(1,2755)	1:A:992:PHE:HB3	1:A:993:PHE:H	17	0.15
(1,273)	1:A:974:LEU:H	1:A:975:GLY:HA2	9	0.15
(1,2728)	1:A:990:VAL:HB	1:A:993:PHE:H	6	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2728)	1:A:990:VAL:HB	1:A:993:PHE:H	12	0.15
(1,2659)	1:A:989:LYS:H	1:A:989:LYS:HD3	3	0.15
(1,2659)	1:A:989:LYS:H	1:A:989:LYS:HD3	12	0.15
(1,2631)	1:A:987:MET:HA	1:A:990:VAL:H	14	0.15
(1,2616)	1:A:987:MET:H	1:A:987:MET:HG2	18	0.15
(1,2568)	1:A:985:LEU:HA	1:A:987:MET:H	2	0.15
(1,2568)	1:A:985:LEU:HA	1:A:987:MET:H	8	0.15
(1,2568)	1:A:985:LEU:HA	1:A:987:MET:H	10	0.15
(1,2568)	1:A:985:LEU:HA	1:A:987:MET:H	18	0.15
(1,2533)	1:A:984:VAL:HA	1:A:987:MET:H	10	0.15
(1,2520)	1:A:984:VAL:H	1:A:984:VAL:HG11	1	0.15
(1,2520)	1:A:984:VAL:H	1:A:984:VAL:HG12	1	0.15
(1,2520)	1:A:984:VAL:H	1:A:984:VAL:HG13	1	0.15
(1,2520)	1:A:984:VAL:H	1:A:984:VAL:HG11	7	0.15
(1,2520)	1:A:984:VAL:H	1:A:984:VAL:HG12	7	0.15
(1,2520)	1:A:984:VAL:H	1:A:984:VAL:HG13	7	0.15
(1,2509)	1:A:983:LEU:HA	1:A:985:LEU:H	1	0.15
(1,2509)	1:A:983:LEU:HA	1:A:985:LEU:H	9	0.15
(1,2495)	1:A:983:LEU:HD11	1:A:983:LEU:H	1	0.15
(1,2495)	1:A:983:LEU:HD12	1:A:983:LEU:H	1	0.15
(1,2495)	1:A:983:LEU:HD13	1:A:983:LEU:H	1	0.15
(1,2478)	1:A:982:ILE:HA	1:A:985:LEU:HB3	7	0.15
(1,2439)	1:A:980:LEU:HB3	1:A:981:THR:HA	2	0.15
(1,2439)	1:A:980:LEU:HB3	1:A:981:THR:HA	4	0.15
(1,2439)	1:A:980:LEU:HB3	1:A:981:THR:HA	9	0.15
(1,2439)	1:A:980:LEU:HB3	1:A:981:THR:HA	10	0.15
(1,2439)	1:A:980:LEU:HB3	1:A:981:THR:HA	19	0.15
(1,2439)	1:A:980:LEU:HB3	1:A:981:THR:HA	20	0.15
(1,2424)	1:A:979:LEU:HA	1:A:981:THR:H	11	0.15
(1,2372)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	10	0.15
(1,2372)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	17	0.15
(1,2372)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	20	0.15
(1,2356)	1:A:974:LEU:H	1:A:975:GLY:HA2	9	0.15
(1,2313)	1:A:971:VAL:HA	1:A:974:LEU:HB3	1	0.15
(1,2308)	1:A:971:VAL:H	1:A:973:VAL:H	2	0.15
(1,2308)	1:A:971:VAL:H	1:A:973:VAL:H	4	0.15
(1,2308)	1:A:971:VAL:H	1:A:973:VAL:H	5	0.15
(1,2308)	1:A:971:VAL:H	1:A:973:VAL:H	13	0.15
(1,2308)	1:A:971:VAL:H	1:A:973:VAL:H	15	0.15
(1,230)	1:A:971:VAL:HA	1:A:974:LEU:HB3	1	0.15
(1,2291)	1:A:970:LEU:HB3	1:A:974:LEU:H	10	0.15
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD21	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD22	11	0.15
(1,2273)	1:A:970:LEU:H	1:A:970:LEU:HD23	11	0.15
(1,2266)	1:A:969:VAL:H	1:A:972:GLY:HA3	9	0.15
(1,2258)	1:A:969:VAL:H	1:A:970:LEU:HB3	2	0.15
(1,2258)	1:A:969:VAL:H	1:A:970:LEU:HB3	15	0.15
(1,225)	1:A:971:VAL:H	1:A:973:VAL:H	2	0.15
(1,225)	1:A:971:VAL:H	1:A:973:VAL:H	4	0.15
(1,225)	1:A:971:VAL:H	1:A:973:VAL:H	5	0.15
(1,225)	1:A:971:VAL:H	1:A:973:VAL:H	13	0.15
(1,225)	1:A:971:VAL:H	1:A:973:VAL:H	15	0.15
(1,2238)	1:A:968:TRP:HA	1:A:971:VAL:H	15	0.15
(1,2208)	1:A:967:TRP:H	1:A:970:LEU:H	2	0.15
(1,2208)	1:A:967:TRP:H	1:A:970:LEU:H	6	0.15
(1,2187)	1:A:966:ILE:HA	1:A:970:LEU:H	8	0.15
(1,2091)	1:A:961:GLU:H	1:A:961:GLU:HB3	9	0.15
(1,2090)	1:A:960:GLU:HB2	1:A:961:GLU:H	4	0.15
(1,2090)	1:A:960:GLU:HB2	1:A:961:GLU:H	13	0.15
(1,208)	1:A:970:LEU:HB3	1:A:974:LEU:H	10	0.15
(1,2079)	1:A:988:TRP:HE1	2:B:719:ILE:HB	3	0.15
(1,2079)	1:A:988:TRP:HE1	2:B:719:ILE:HB	8	0.15
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG21	9	0.15
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG22	9	0.15
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG23	9	0.15
(1,2074)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	5	0.15
(1,2068)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	2	0.15
(1,2068)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	18	0.15
(1,2060)	1:A:984:VAL:H	2:B:712:LEU:HA	13	0.15
(1,2049)	1:A:979:LEU:HD21	2:B:708:GLY:H	6	0.15
(1,2049)	1:A:979:LEU:HD22	2:B:708:GLY:H	6	0.15
(1,2049)	1:A:979:LEU:HD23	2:B:708:GLY:H	6	0.15
(1,2028)	1:A:974:LEU:H	2:B:704:ILE:HG13	9	0.15
(1,2018)	1:A:973:VAL:H	2:B:700:VAL:HA	18	0.15
(1,1970)	2:B:757:ILE:H	2:B:757:ILE:HG13	2	0.15
(1,1968)	2:B:757:ILE:H	2:B:757:ILE:HG12	1	0.15
(1,1968)	2:B:757:ILE:H	2:B:757:ILE:HG12	11	0.15
(1,1949)	2:B:754:PHE:HB3	2:B:755:THR:H	19	0.15
(1,1944)	2:B:753:THR:HA	2:B:754:PHE:H	12	0.15
(1,1924)	2:B:750:ALA:H	2:B:751:THR:H	19	0.15
(1,1917)	2:B:749:GLU:H	2:B:749:GLU:HG3	13	0.15
(1,1917)	2:B:749:GLU:H	2:B:749:GLU:HG3	18	0.15
(1,1917)	2:B:749:GLU:H	2:B:749:GLU:HG3	19	0.15
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD21	11	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD22	11	0.15
(1,190)	1:A:970:LEU:H	1:A:970:LEU:HD23	11	0.15
(1,1885)	2:B:747:TYR:H	2:B:747:TYR:HB3	12	0.15
(1,1885)	2:B:747:TYR:H	2:B:747:TYR:HB3	18	0.15
(1,1871)	2:B:746:LEU:H	2:B:746:LEU:HB2	17	0.15
(1,183)	1:A:969:VAL:H	1:A:972:GLY:HA3	9	0.15
(1,1828)	2:B:743:ASN:HB3	2:B:743:ASN:H	5	0.15
(1,1821)	2:B:742:ALA:HB1	2:B:743:ASN:HD22	9	0.15
(1,1821)	2:B:742:ALA:HB2	2:B:743:ASN:HD22	9	0.15
(1,1821)	2:B:742:ALA:HB3	2:B:743:ASN:HD22	9	0.15
(1,1805)	2:B:740:ASP:HA	2:B:741:THR:H	3	0.15
(1,1805)	2:B:740:ASP:HA	2:B:741:THR:H	15	0.15
(1,1805)	2:B:740:ASP:HA	2:B:741:THR:H	17	0.15
(1,1798)	2:B:739:TRP:HB3	2:B:740:ASP:H	1	0.15
(1,1780)	2:B:738:LYS:HB3	2:B:739:TRP:H	4	0.15
(1,1780)	2:B:738:LYS:HB3	2:B:739:TRP:H	13	0.15
(1,1780)	2:B:738:LYS:HB3	2:B:739:TRP:H	20	0.15
(1,1777)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	5	0.15
(1,1777)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	10	0.15
(1,175)	1:A:969:VAL:H	1:A:970:LEU:HB3	2	0.15
(1,175)	1:A:969:VAL:H	1:A:970:LEU:HB3	15	0.15
(1,1663)	2:B:730:PHE:HE1	2:B:734:ARG:HG3	19	0.15
(1,1635)	2:B:729:LYS:HE3	2:B:729:LYS:HB3	7	0.15
(1,1555)	2:B:724:ARG:HA	2:B:728:ALA:H	7	0.15
(1,1555)	2:B:724:ARG:HA	2:B:728:ALA:H	10	0.15
(1,155)	1:A:968:TRP:HA	1:A:971:VAL:H	15	0.15
(1,1537)	2:B:724:ARG:HD3	2:B:724:ARG:HB3	15	0.15
(1,1534)	2:B:724:ARG:H	2:B:724:ARG:HB3	1	0.15
(1,1534)	2:B:724:ARG:H	2:B:724:ARG:HB3	19	0.15
(1,1496)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	3	0.15
(1,1424)	2:B:718:LEU:HD11	2:B:721:ILE:HB	13	0.15
(1,1424)	2:B:718:LEU:HD12	2:B:721:ILE:HB	13	0.15
(1,1424)	2:B:718:LEU:HD13	2:B:721:ILE:HB	13	0.15
(1,1387)	2:B:717:LEU:H	2:B:719:ILE:H	5	0.15
(1,1387)	2:B:717:LEU:H	2:B:719:ILE:H	6	0.15
(1,1387)	2:B:717:LEU:H	2:B:719:ILE:H	10	0.15
(1,125)	1:A:967:TRP:H	1:A:970:LEU:H	2	0.15
(1,125)	1:A:967:TRP:H	1:A:970:LEU:H	6	0.15
(1,1236)	2:B:709:LEU:H	2:B:711:ALA:H	5	0.15
(1,1236)	2:B:709:LEU:H	2:B:711:ALA:H	7	0.15
(1,1236)	2:B:709:LEU:H	2:B:711:ALA:H	8	0.15
(1,1128)	2:B:704:ILE:HB	2:B:705:LEU:HB2	14	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1043)	2:B:700:VAL:HB	2:B:701:MET:HG2	8	0.15
(1,104)	1:A:966:ILE:HA	1:A:970:LEU:H	8	0.15
(3,81)	2:B:700:VAL:O	2:B:704:ILE:H	1	0.14
(3,43)	1:A:981:THR:O	1:A:984:VAL:H	1	0.14
(3,43)	1:A:981:THR:O	1:A:984:VAL:H	3	0.14
(3,43)	1:A:981:THR:O	1:A:984:VAL:H	17	0.14
(3,270)	2:B:710:ALA:O	2:B:714:ILE:H	10	0.14
(3,270)	2:B:710:ALA:O	2:B:714:ILE:H	20	0.14
(3,240)	2:B:700:VAL:O	2:B:704:ILE:H	1	0.14
(3,24)	1:A:974:LEU:O	1:A:978:LEU:H	19	0.14
(3,202)	1:A:981:THR:O	1:A:984:VAL:H	1	0.14
(3,202)	1:A:981:THR:O	1:A:984:VAL:H	3	0.14
(3,202)	1:A:981:THR:O	1:A:984:VAL:H	17	0.14
(3,183)	1:A:974:LEU:O	1:A:978:LEU:H	19	0.14
(3,111)	2:B:710:ALA:O	2:B:714:ILE:H	10	0.14
(3,111)	2:B:710:ALA:O	2:B:714:ILE:H	20	0.14
(1,99)	1:A:966:ILE:HA	1:A:969:VAL:H	14	0.14
(1,870)	2:B:693:ILE:H	2:B:693:ILE:HB	2	0.14
(1,851)	2:B:692:ASP:H	2:B:693:ILE:H	11	0.14
(1,848)	2:B:692:ASP:H	2:B:692:ASP:HB3	15	0.14
(1,811)	1:A:1006:GLU:H	1:A:1006:GLU:HB3	4	0.14
(1,807)	1:A:1005:GLU:H	1:A:1005:GLU:HB3	13	0.14
(1,803)	1:A:1004:ASP:HA	1:A:1005:GLU:H	13	0.14
(1,803)	1:A:1004:ASP:HA	1:A:1005:GLU:H	15	0.14
(1,791)	1:A:1002:GLU:H	1:A:1002:GLU:HB3	11	0.14
(1,790)	1:A:1001:GLU:H	1:A:1001:GLU:HB2	5	0.14
(1,750)	1:A:996:ASN:HA	1:A:997:ARG:H	2	0.14
(1,742)	1:A:996:ASN:H	1:A:996:ASN:HB2	2	0.14
(1,742)	1:A:996:ASN:H	1:A:996:ASN:HB2	7	0.14
(1,742)	1:A:996:ASN:H	1:A:996:ASN:HB2	9	0.14
(1,742)	1:A:996:ASN:H	1:A:996:ASN:HB2	12	0.14
(1,725)	1:A:994:LYS:HB3	1:A:995:ARG:HG3	15	0.14
(1,725)	1:A:994:LYS:HB3	1:A:995:ARG:HG3	16	0.14
(1,724)	1:A:994:LYS:HB2	1:A:995:ARG:HG3	1	0.14
(1,724)	1:A:994:LYS:HB2	1:A:995:ARG:HG3	16	0.14
(1,704)	1:A:994:LYS:H	1:A:994:LYS:HG3	7	0.14
(1,704)	1:A:994:LYS:H	1:A:994:LYS:HG3	15	0.14
(1,7)	1:A:960:GLU:HB2	1:A:961:GLU:H	6	0.14
(1,693)	1:A:993:PHE:H	1:A:994:LYS:HD3	9	0.14
(1,672)	1:A:992:PHE:HB3	1:A:993:PHE:H	7	0.14
(1,645)	1:A:990:VAL:HB	1:A:993:PHE:H	2	0.14
(1,576)	1:A:989:LYS:H	1:A:989:LYS:HD3	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,557)	1:A:988:TRP:H	1:A:988:TRP:HB3	7	0.14
(1,557)	1:A:988:TRP:H	1:A:988:TRP:HB3	14	0.14
(1,557)	1:A:988:TRP:H	1:A:988:TRP:HB3	15	0.14
(1,548)	1:A:987:MET:HA	1:A:990:VAL:H	6	0.14
(1,548)	1:A:987:MET:HA	1:A:990:VAL:H	9	0.14
(1,487)	1:A:985:LEU:H	1:A:987:MET:HG2	18	0.14
(1,46)	1:A:964:ILE:HB	1:A:965:PRO:HD2	2	0.14
(1,46)	1:A:964:ILE:HB	1:A:965:PRO:HD2	6	0.14
(1,426)	1:A:983:LEU:HA	1:A:985:LEU:H	6	0.14
(1,426)	1:A:983:LEU:HA	1:A:985:LEU:H	16	0.14
(1,423)	1:A:983:LEU:H	1:A:985:LEU:H	16	0.14
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG21	4	0.14
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG22	4	0.14
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG23	4	0.14
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG21	7	0.14
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG22	7	0.14
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG23	7	0.14
(1,4157)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	8	0.14
(1,4157)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	15	0.14
(1,4155)	1:A:988:TRP:H	2:B:715:TRP:HB3	16	0.14
(1,4151)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	11	0.14
(1,4143)	1:A:984:VAL:H	2:B:712:LEU:HA	12	0.14
(1,4111)	1:A:974:LEU:H	2:B:704:ILE:HG13	18	0.14
(1,4101)	1:A:973:VAL:H	2:B:700:VAL:HA	4	0.14
(1,4093)	1:A:969:VAL:HA	2:B:700:VAL:H	16	0.14
(1,4085)	1:A:968:TRP:HE1	2:B:693:ILE:HB	12	0.14
(1,408)	1:A:983:LEU:H	1:A:983:LEU:HB3	9	0.14
(1,4040)	2:B:756:ASN:H	2:B:756:ASN:HB2	12	0.14
(1,4027)	2:B:753:THR:HA	2:B:754:PHE:H	5	0.14
(1,4000)	2:B:749:GLU:H	2:B:749:GLU:HG3	5	0.14
(1,4000)	2:B:749:GLU:H	2:B:749:GLU:HG3	12	0.14
(1,3918)	2:B:743:ASN:HA	2:B:744:ASN:H	14	0.14
(1,3888)	2:B:740:ASP:HA	2:B:741:THR:H	18	0.14
(1,3881)	2:B:739:TRP:HB3	2:B:740:ASP:H	5	0.14
(1,3869)	2:B:738:LYS:H	2:B:740:ASP:H	7	0.14
(1,3863)	2:B:738:LYS:HB3	2:B:739:TRP:H	5	0.14
(1,3863)	2:B:738:LYS:HB3	2:B:739:TRP:H	6	0.14
(1,3863)	2:B:738:LYS:HB3	2:B:739:TRP:H	7	0.14
(1,3863)	2:B:738:LYS:HB3	2:B:739:TRP:H	16	0.14
(1,3863)	2:B:738:LYS:HB3	2:B:739:TRP:H	19	0.14
(1,3860)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	2	0.14
(1,3850)	2:B:738:LYS:HA	2:B:738:LYS:HD3	1	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3850)	2:B:738:LYS:HA	2:B:738:LYS:HD3	3	0.14
(1,3850)	2:B:738:LYS:HA	2:B:738:LYS:HD3	4	0.14
(1,3850)	2:B:738:LYS:HA	2:B:738:LYS:HD3	8	0.14
(1,3850)	2:B:738:LYS:HA	2:B:738:LYS:HD3	9	0.14
(1,3850)	2:B:738:LYS:HA	2:B:738:LYS:HD3	16	0.14
(1,3706)	2:B:728:ALA:H	2:B:730:PHE:H	7	0.14
(1,3664)	2:B:725:LYS:HA	2:B:728:ALA:H	15	0.14
(1,3644)	2:B:725:LYS:H	2:B:725:LYS:HG3	7	0.14
(1,3644)	2:B:725:LYS:H	2:B:725:LYS:HG3	10	0.14
(1,3638)	2:B:724:ARG:HA	2:B:728:ALA:H	14	0.14
(1,3620)	2:B:724:ARG:HD3	2:B:724:ARG:HB3	5	0.14
(1,3617)	2:B:724:ARG:H	2:B:724:ARG:HB3	4	0.14
(1,3617)	2:B:724:ARG:H	2:B:724:ARG:HB3	5	0.14
(1,3617)	2:B:724:ARG:H	2:B:724:ARG:HB3	7	0.14
(1,3617)	2:B:724:ARG:H	2:B:724:ARG:HB3	8	0.14
(1,3617)	2:B:724:ARG:H	2:B:724:ARG:HB3	11	0.14
(1,3617)	2:B:724:ARG:H	2:B:724:ARG:HB3	13	0.14
(1,3617)	2:B:724:ARG:H	2:B:724:ARG:HB3	15	0.14
(1,360)	1:A:980:LEU:HA	1:A:983:LEU:HB3	17	0.14
(1,3579)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	13	0.14
(1,356)	1:A:980:LEU:HB3	1:A:981:THR:HA	1	0.14
(1,356)	1:A:980:LEU:HB3	1:A:981:THR:HA	3	0.14
(1,356)	1:A:980:LEU:HB3	1:A:981:THR:HA	6	0.14
(1,356)	1:A:980:LEU:HB3	1:A:981:THR:HA	7	0.14
(1,356)	1:A:980:LEU:HB3	1:A:981:THR:HA	15	0.14
(1,3553)	2:B:720:THR:HG21	2:B:724:ARG:HD3	17	0.14
(1,3553)	2:B:720:THR:HG22	2:B:724:ARG:HD3	17	0.14
(1,3553)	2:B:720:THR:HG23	2:B:724:ARG:HD3	17	0.14
(1,341)	1:A:979:LEU:HA	1:A:981:THR:H	9	0.14
(1,341)	1:A:979:LEU:HA	1:A:981:THR:H	18	0.14
(1,3319)	2:B:709:LEU:H	2:B:711:ALA:H	4	0.14
(1,3319)	2:B:709:LEU:H	2:B:711:ALA:H	15	0.14
(1,3319)	2:B:709:LEU:H	2:B:711:ALA:H	18	0.14
(1,331)	1:A:978:LEU:HA	1:A:981:THR:H	1	0.14
(1,331)	1:A:978:LEU:HA	1:A:981:THR:H	7	0.14
(1,331)	1:A:978:LEU:HA	1:A:981:THR:H	10	0.14
(1,331)	1:A:978:LEU:HA	1:A:981:THR:H	11	0.14
(1,3211)	2:B:704:ILE:HB	2:B:705:LEU:HB2	17	0.14
(1,321)	1:A:977:LEU:HB2	1:A:981:THR:H	2	0.14
(1,321)	1:A:977:LEU:HB2	1:A:981:THR:H	19	0.14
(1,3185)	2:B:703:ALA:HA	2:B:706:LEU:HB3	16	0.14
(1,2953)	2:B:693:ILE:H	2:B:693:ILE:HB	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2934)	2:B:692:ASP:H	2:B:693:ILE:H	11	0.14
(1,2931)	2:B:692:ASP:H	2:B:692:ASP:HB3	15	0.14
(1,2894)	1:A:1006:GLU:H	1:A:1006:GLU:HB3	4	0.14
(1,2890)	1:A:1005:GLU:H	1:A:1005:GLU:HB3	13	0.14
(1,289)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	11	0.14
(1,2886)	1:A:1004:ASP:HA	1:A:1005:GLU:H	13	0.14
(1,2886)	1:A:1004:ASP:HA	1:A:1005:GLU:H	15	0.14
(1,2874)	1:A:1002:GLU:H	1:A:1002:GLU:HB3	11	0.14
(1,2873)	1:A:1001:GLU:H	1:A:1001:GLU:HB2	5	0.14
(1,2833)	1:A:996:ASN:HA	1:A:997:ARG:H	2	0.14
(1,2825)	1:A:996:ASN:H	1:A:996:ASN:HB2	2	0.14
(1,2825)	1:A:996:ASN:H	1:A:996:ASN:HB2	7	0.14
(1,2825)	1:A:996:ASN:H	1:A:996:ASN:HB2	9	0.14
(1,2825)	1:A:996:ASN:H	1:A:996:ASN:HB2	12	0.14
(1,2808)	1:A:994:LYS:HB3	1:A:995:ARG:HG3	15	0.14
(1,2808)	1:A:994:LYS:HB3	1:A:995:ARG:HG3	16	0.14
(1,2807)	1:A:994:LYS:HB2	1:A:995:ARG:HG3	1	0.14
(1,2807)	1:A:994:LYS:HB2	1:A:995:ARG:HG3	16	0.14
(1,2787)	1:A:994:LYS:H	1:A:994:LYS:HG3	7	0.14
(1,2787)	1:A:994:LYS:H	1:A:994:LYS:HG3	15	0.14
(1,2776)	1:A:993:PHE:H	1:A:994:LYS:HD3	9	0.14
(1,2755)	1:A:992:PHE:HB3	1:A:993:PHE:H	7	0.14
(1,275)	1:A:974:LEU:HB2	1:A:975:GLY:H	13	0.14
(1,273)	1:A:974:LEU:H	1:A:975:GLY:HA2	4	0.14
(1,273)	1:A:974:LEU:H	1:A:975:GLY:HA2	11	0.14
(1,273)	1:A:974:LEU:H	1:A:975:GLY:HA2	18	0.14
(1,2728)	1:A:990:VAL:HB	1:A:993:PHE:H	2	0.14
(1,2659)	1:A:989:LYS:H	1:A:989:LYS:HD3	10	0.14
(1,2640)	1:A:988:TRP:H	1:A:988:TRP:HB3	7	0.14
(1,2640)	1:A:988:TRP:H	1:A:988:TRP:HB3	14	0.14
(1,2640)	1:A:988:TRP:H	1:A:988:TRP:HB3	15	0.14
(1,2631)	1:A:987:MET:HA	1:A:990:VAL:H	6	0.14
(1,2631)	1:A:987:MET:HA	1:A:990:VAL:H	9	0.14
(1,2570)	1:A:985:LEU:H	1:A:987:MET:HG2	18	0.14
(1,2509)	1:A:983:LEU:HA	1:A:985:LEU:H	6	0.14
(1,2509)	1:A:983:LEU:HA	1:A:985:LEU:H	16	0.14
(1,2506)	1:A:983:LEU:H	1:A:985:LEU:H	16	0.14
(1,2491)	1:A:983:LEU:H	1:A:983:LEU:HB3	9	0.14
(1,2443)	1:A:980:LEU:HA	1:A:983:LEU:HB3	17	0.14
(1,2439)	1:A:980:LEU:HB3	1:A:981:THR:HA	1	0.14
(1,2439)	1:A:980:LEU:HB3	1:A:981:THR:HA	3	0.14
(1,2439)	1:A:980:LEU:HB3	1:A:981:THR:HA	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2439)	1:A:980:LEU:HB3	1:A:981:THR:HA	7	0.14
(1,2439)	1:A:980:LEU:HB3	1:A:981:THR:HA	15	0.14
(1,2424)	1:A:979:LEU:HA	1:A:981:THR:H	9	0.14
(1,2424)	1:A:979:LEU:HA	1:A:981:THR:H	18	0.14
(1,2414)	1:A:978:LEU:HA	1:A:981:THR:H	1	0.14
(1,2414)	1:A:978:LEU:HA	1:A:981:THR:H	7	0.14
(1,2414)	1:A:978:LEU:HA	1:A:981:THR:H	10	0.14
(1,2414)	1:A:978:LEU:HA	1:A:981:THR:H	11	0.14
(1,2404)	1:A:977:LEU:HB2	1:A:981:THR:H	2	0.14
(1,2404)	1:A:977:LEU:HB2	1:A:981:THR:H	19	0.14
(1,2372)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	11	0.14
(1,2358)	1:A:974:LEU:HB2	1:A:975:GLY:H	13	0.14
(1,2356)	1:A:974:LEU:H	1:A:975:GLY:HA2	4	0.14
(1,2356)	1:A:974:LEU:H	1:A:975:GLY:HA2	11	0.14
(1,2356)	1:A:974:LEU:H	1:A:975:GLY:HA2	18	0.14
(1,2313)	1:A:971:VAL:HA	1:A:974:LEU:HB3	12	0.14
(1,230)	1:A:971:VAL:HA	1:A:974:LEU:HB3	12	0.14
(1,2291)	1:A:970:LEU:HB3	1:A:974:LEU:H	2	0.14
(1,2291)	1:A:970:LEU:HB3	1:A:974:LEU:H	8	0.14
(1,2238)	1:A:968:TRP:HA	1:A:971:VAL:H	12	0.14
(1,2215)	1:A:968:TRP:H	1:A:968:TRP:HB3	20	0.14
(1,2201)	1:A:967:TRP:HA	1:A:968:TRP:HB3	11	0.14
(1,2187)	1:A:966:ILE:HA	1:A:970:LEU:H	4	0.14
(1,2187)	1:A:966:ILE:HA	1:A:970:LEU:H	5	0.14
(1,2187)	1:A:966:ILE:HA	1:A:970:LEU:H	11	0.14
(1,2182)	1:A:966:ILE:HA	1:A:969:VAL:H	14	0.14
(1,2129)	1:A:964:ILE:HB	1:A:965:PRO:HD2	2	0.14
(1,2129)	1:A:964:ILE:HB	1:A:965:PRO:HD2	6	0.14
(1,2097)	1:A:962:ARG:H	1:A:962:ARG:HB2	4	0.14
(1,2090)	1:A:960:GLU:HB2	1:A:961:GLU:H	6	0.14
(1,208)	1:A:970:LEU:HB3	1:A:974:LEU:H	2	0.14
(1,208)	1:A:970:LEU:HB3	1:A:974:LEU:H	8	0.14
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG21	4	0.14
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG22	4	0.14
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG23	4	0.14
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG21	7	0.14
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG22	7	0.14
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG23	7	0.14
(1,2074)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	8	0.14
(1,2074)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	15	0.14
(1,2072)	1:A:988:TRP:H	2:B:715:TRP:HB3	16	0.14
(1,2068)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2060)	1:A:984:VAL:H	2:B:712:LEU:HA	12	0.14
(1,2028)	1:A:974:LEU:H	2:B:704:ILE:HG13	18	0.14
(1,2018)	1:A:973:VAL:H	2:B:700:VAL:HA	4	0.14
(1,2010)	1:A:969:VAL:HA	2:B:700:VAL:H	16	0.14
(1,2002)	1:A:968:TRP:HE1	2:B:693:ILE:HB	12	0.14
(1,1957)	2:B:756:ASN:H	2:B:756:ASN:HB2	12	0.14
(1,1944)	2:B:753:THR:HA	2:B:754:PHE:H	5	0.14
(1,1917)	2:B:749:GLU:H	2:B:749:GLU:HG3	5	0.14
(1,1917)	2:B:749:GLU:H	2:B:749:GLU:HG3	12	0.14
(1,1835)	2:B:743:ASN:HA	2:B:744:ASN:H	14	0.14
(1,1805)	2:B:740:ASP:HA	2:B:741:THR:H	18	0.14
(1,1798)	2:B:739:TRP:HB3	2:B:740:ASP:H	5	0.14
(1,1786)	2:B:738:LYS:H	2:B:740:ASP:H	7	0.14
(1,1780)	2:B:738:LYS:HB3	2:B:739:TRP:H	5	0.14
(1,1780)	2:B:738:LYS:HB3	2:B:739:TRP:H	6	0.14
(1,1780)	2:B:738:LYS:HB3	2:B:739:TRP:H	7	0.14
(1,1780)	2:B:738:LYS:HB3	2:B:739:TRP:H	16	0.14
(1,1780)	2:B:738:LYS:HB3	2:B:739:TRP:H	19	0.14
(1,1777)	2:B:738:LYS:HB3	2:B:738:LYS:HD3	2	0.14
(1,1767)	2:B:738:LYS:HA	2:B:738:LYS:HD3	1	0.14
(1,1767)	2:B:738:LYS:HA	2:B:738:LYS:HD3	3	0.14
(1,1767)	2:B:738:LYS:HA	2:B:738:LYS:HD3	4	0.14
(1,1767)	2:B:738:LYS:HA	2:B:738:LYS:HD3	8	0.14
(1,1767)	2:B:738:LYS:HA	2:B:738:LYS:HD3	9	0.14
(1,1767)	2:B:738:LYS:HA	2:B:738:LYS:HD3	16	0.14
(1,1623)	2:B:728:ALA:H	2:B:730:PHE:H	7	0.14
(1,1581)	2:B:725:LYS:HA	2:B:728:ALA:H	15	0.14
(1,1561)	2:B:725:LYS:H	2:B:725:LYS:HG3	7	0.14
(1,1561)	2:B:725:LYS:H	2:B:725:LYS:HG3	10	0.14
(1,1555)	2:B:724:ARG:HA	2:B:728:ALA:H	14	0.14
(1,155)	1:A:968:TRP:HA	1:A:971:VAL:H	12	0.14
(1,1537)	2:B:724:ARG:HD3	2:B:724:ARG:HB3	5	0.14
(1,1534)	2:B:724:ARG:H	2:B:724:ARG:HB3	4	0.14
(1,1534)	2:B:724:ARG:H	2:B:724:ARG:HB3	5	0.14
(1,1534)	2:B:724:ARG:H	2:B:724:ARG:HB3	7	0.14
(1,1534)	2:B:724:ARG:H	2:B:724:ARG:HB3	8	0.14
(1,1534)	2:B:724:ARG:H	2:B:724:ARG:HB3	11	0.14
(1,1534)	2:B:724:ARG:H	2:B:724:ARG:HB3	13	0.14
(1,1534)	2:B:724:ARG:H	2:B:724:ARG:HB3	15	0.14
(1,1496)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	13	0.14
(1,1470)	2:B:720:THR:HG21	2:B:724:ARG:HD3	17	0.14
(1,1470)	2:B:720:THR:HG22	2:B:724:ARG:HD3	17	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1470)	2:B:720:THR:HG23	2:B:724:ARG:HD3	17	0.14
(1,14)	1:A:962:ARG:H	1:A:962:ARG:HB2	4	0.14
(1,132)	1:A:968:TRP:H	1:A:968:TRP:HB3	20	0.14
(1,1236)	2:B:709:LEU:H	2:B:711:ALA:H	4	0.14
(1,1236)	2:B:709:LEU:H	2:B:711:ALA:H	15	0.14
(1,1236)	2:B:709:LEU:H	2:B:711:ALA:H	18	0.14
(1,118)	1:A:967:TRP:HA	1:A:968:TRP:HB3	11	0.14
(1,1128)	2:B:704:ILE:HB	2:B:705:LEU:HB2	17	0.14
(1,1102)	2:B:703:ALA:HA	2:B:706:LEU:HB3	16	0.14
(1,104)	1:A:966:ILE:HA	1:A:970:LEU:H	4	0.14
(1,104)	1:A:966:ILE:HA	1:A:970:LEU:H	5	0.14
(1,104)	1:A:966:ILE:HA	1:A:970:LEU:H	11	0.14
(3,52)	1:A:984:VAL:O	1:A:987:MET:H	8	0.13
(3,43)	1:A:981:THR:O	1:A:984:VAL:H	15	0.13
(3,43)	1:A:981:THR:O	1:A:984:VAL:H	16	0.13
(3,24)	1:A:974:LEU:O	1:A:978:LEU:H	6	0.13
(3,24)	1:A:974:LEU:O	1:A:978:LEU:H	10	0.13
(3,211)	1:A:984:VAL:O	1:A:987:MET:H	8	0.13
(3,202)	1:A:981:THR:O	1:A:984:VAL:H	15	0.13
(3,202)	1:A:981:THR:O	1:A:984:VAL:H	16	0.13
(3,183)	1:A:974:LEU:O	1:A:978:LEU:H	6	0.13
(3,183)	1:A:974:LEU:O	1:A:978:LEU:H	10	0.13
(1,99)	1:A:966:ILE:HA	1:A:969:VAL:H	12	0.13
(1,965)	2:B:697:LEU:H	2:B:697:LEU:HB3	7	0.13
(1,870)	2:B:693:ILE:H	2:B:693:ILE:HB	3	0.13
(1,870)	2:B:693:ILE:H	2:B:693:ILE:HB	10	0.13
(1,864)	2:B:692:ASP:H	2:B:696:VAL:H	17	0.13
(1,851)	2:B:692:ASP:H	2:B:693:ILE:H	5	0.13
(1,851)	2:B:692:ASP:H	2:B:693:ILE:H	12	0.13
(1,851)	2:B:692:ASP:H	2:B:693:ILE:H	16	0.13
(1,850)	2:B:692:ASP:HA	2:B:693:ILE:H	14	0.13
(1,821)	2:B:689:LYS:H	2:B:689:LYS:HD2	8	0.13
(1,807)	1:A:1005:GLU:H	1:A:1005:GLU:HB3	9	0.13
(1,801)	1:A:1004:ASP:H	1:A:1004:ASP:HB3	17	0.13
(1,791)	1:A:1002:GLU:H	1:A:1002:GLU:HB3	9	0.13
(1,791)	1:A:1002:GLU:H	1:A:1002:GLU:HB3	18	0.13
(1,761)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	2	0.13
(1,761)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	15	0.13
(1,740)	1:A:995:ARG:H	1:A:996:ASN:H	6	0.13
(1,725)	1:A:994:LYS:HB3	1:A:995:ARG:HG3	10	0.13
(1,724)	1:A:994:LYS:HB2	1:A:995:ARG:HG3	4	0.13
(1,724)	1:A:994:LYS:HB2	1:A:995:ARG:HG3	5	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,718)	1:A:994:LYS:HB2	1:A:995:ARG:H	9	0.13
(1,701)	1:A:993:PHE:HA	1:A:996:ASN:H	9	0.13
(1,7)	1:A:960:GLU:HB2	1:A:961:GLU:H	2	0.13
(1,7)	1:A:960:GLU:HB2	1:A:961:GLU:H	5	0.13
(1,693)	1:A:993:PHE:H	1:A:994:LYS:HD3	19	0.13
(1,690)	1:A:993:PHE:HB2	1:A:994:LYS:H	10	0.13
(1,690)	1:A:993:PHE:HB2	1:A:994:LYS:H	11	0.13
(1,672)	1:A:992:PHE:HB3	1:A:993:PHE:H	9	0.13
(1,672)	1:A:992:PHE:HB3	1:A:993:PHE:H	15	0.13
(1,645)	1:A:990:VAL:HB	1:A:993:PHE:H	17	0.13
(1,638)	1:A:990:VAL:H	1:A:992:PHE:H	9	0.13
(1,557)	1:A:988:TRP:H	1:A:988:TRP:HB3	5	0.13
(1,557)	1:A:988:TRP:H	1:A:988:TRP:HB3	10	0.13
(1,557)	1:A:988:TRP:H	1:A:988:TRP:HB3	19	0.13
(1,548)	1:A:987:MET:HA	1:A:990:VAL:H	7	0.13
(1,548)	1:A:987:MET:HA	1:A:990:VAL:H	13	0.13
(1,548)	1:A:987:MET:HA	1:A:990:VAL:H	20	0.13
(1,532)	1:A:987:MET:H	1:A:987:MET:HG3	1	0.13
(1,437)	1:A:984:VAL:H	1:A:984:VAL:HG11	4	0.13
(1,437)	1:A:984:VAL:H	1:A:984:VAL:HG12	4	0.13
(1,437)	1:A:984:VAL:H	1:A:984:VAL:HG13	4	0.13
(1,437)	1:A:984:VAL:H	1:A:984:VAL:HG11	17	0.13
(1,437)	1:A:984:VAL:H	1:A:984:VAL:HG12	17	0.13
(1,437)	1:A:984:VAL:H	1:A:984:VAL:HG13	17	0.13
(1,432)	1:A:983:LEU:HB2	1:A:987:MET:H	13	0.13
(1,426)	1:A:983:LEU:HA	1:A:985:LEU:H	2	0.13
(1,426)	1:A:983:LEU:HA	1:A:985:LEU:H	10	0.13
(1,426)	1:A:983:LEU:HA	1:A:985:LEU:H	11	0.13
(1,4163)	1:A:988:TRP:HE1	2:B:719:ILE:HG21	12	0.13
(1,4163)	1:A:988:TRP:HE1	2:B:719:ILE:HG22	12	0.13
(1,4163)	1:A:988:TRP:HE1	2:B:719:ILE:HG23	12	0.13
(1,4162)	1:A:988:TRP:HE1	2:B:719:ILE:HB	12	0.13
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG21	2	0.13
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG22	2	0.13
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG23	2	0.13
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG21	6	0.13
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG22	6	0.13
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG23	6	0.13
(1,4157)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	4	0.13
(1,4157)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	10	0.13
(1,4157)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	17	0.13
(1,4156)	1:A:988:TRP:HE1	2:B:715:TRP:HD1	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4131)	1:A:979:LEU:H	2:B:707:ILE:HB	16	0.13
(1,4121)	1:A:976:GLY:H	2:B:707:ILE:HB	11	0.13
(1,4111)	1:A:974:LEU:H	2:B:704:ILE:HG13	16	0.13
(1,4101)	1:A:973:VAL:H	2:B:700:VAL:HA	5	0.13
(1,4101)	1:A:973:VAL:H	2:B:700:VAL:HA	13	0.13
(1,4101)	1:A:973:VAL:H	2:B:700:VAL:HA	15	0.13
(1,4101)	1:A:973:VAL:H	2:B:700:VAL:HA	17	0.13
(1,4040)	2:B:756:ASN:H	2:B:756:ASN:HB2	10	0.13
(1,4033)	2:B:754:PHE:HA	2:B:755:THR:H	1	0.13
(1,4032)	2:B:754:PHE:HB3	2:B:755:THR:H	7	0.13
(1,4032)	2:B:754:PHE:HB3	2:B:755:THR:H	8	0.13
(1,4032)	2:B:754:PHE:HB3	2:B:755:THR:H	13	0.13
(1,4032)	2:B:754:PHE:HB3	2:B:755:THR:H	16	0.13
(1,4028)	2:B:754:PHE:H	2:B:754:PHE:HB2	8	0.13
(1,4027)	2:B:753:THR:HA	2:B:754:PHE:H	8	0.13
(1,4014)	2:B:751:THR:HA	2:B:752:SER:H	4	0.13
(1,4010)	2:B:751:THR:H	2:B:751:THR:HG21	10	0.13
(1,4010)	2:B:751:THR:H	2:B:751:THR:HG22	10	0.13
(1,4010)	2:B:751:THR:H	2:B:751:THR:HG23	10	0.13
(1,3968)	2:B:747:TYR:H	2:B:747:TYR:HB3	3	0.13
(1,3963)	2:B:746:LEU:HB2	2:B:747:TYR:H	6	0.13
(1,3954)	2:B:746:LEU:H	2:B:746:LEU:HB2	1	0.13
(1,3954)	2:B:746:LEU:H	2:B:746:LEU:HB2	2	0.13
(1,395)	1:A:982:ILE:HA	1:A:985:LEU:HB3	5	0.13
(1,3921)	2:B:744:ASN:H	2:B:744:ASN:HB2	9	0.13
(1,3903)	2:B:742:ALA:HB1	2:B:743:ASN:H	15	0.13
(1,3903)	2:B:742:ALA:HB2	2:B:743:ASN:H	15	0.13
(1,3903)	2:B:742:ALA:HB3	2:B:743:ASN:H	15	0.13
(1,3894)	2:B:741:THR:HB	2:B:742:ALA:H	19	0.13
(1,3881)	2:B:739:TRP:HB3	2:B:740:ASP:H	2	0.13
(1,3881)	2:B:739:TRP:HB3	2:B:740:ASP:H	3	0.13
(1,3881)	2:B:739:TRP:HB3	2:B:740:ASP:H	17	0.13
(1,3869)	2:B:738:LYS:H	2:B:740:ASP:H	9	0.13
(1,3863)	2:B:738:LYS:HB3	2:B:739:TRP:H	3	0.13
(1,3850)	2:B:738:LYS:HA	2:B:738:LYS:HD3	6	0.13
(1,3850)	2:B:738:LYS:HA	2:B:738:LYS:HD3	13	0.13
(1,3850)	2:B:738:LYS:HA	2:B:738:LYS:HD3	18	0.13
(1,3850)	2:B:738:LYS:HA	2:B:738:LYS:HD3	20	0.13
(1,3668)	2:B:725:LYS:HG3	2:B:729:LYS:HE3	6	0.13
(1,3664)	2:B:725:LYS:HA	2:B:728:ALA:H	1	0.13
(1,3664)	2:B:725:LYS:HA	2:B:728:ALA:H	5	0.13
(1,3638)	2:B:724:ARG:HA	2:B:728:ALA:H	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3638)	2:B:724:ARG:HA	2:B:728:ALA:H	6	0.13
(1,3638)	2:B:724:ARG:HA	2:B:728:ALA:H	9	0.13
(1,3638)	2:B:724:ARG:HA	2:B:728:ALA:H	13	0.13
(1,3638)	2:B:724:ARG:HA	2:B:728:ALA:H	15	0.13
(1,3638)	2:B:724:ARG:HA	2:B:728:ALA:H	17	0.13
(1,3638)	2:B:724:ARG:HA	2:B:728:ALA:H	18	0.13
(1,3638)	2:B:724:ARG:HA	2:B:728:ALA:H	19	0.13
(1,3620)	2:B:724:ARG:HD3	2:B:724:ARG:HB3	1	0.13
(1,3617)	2:B:724:ARG:H	2:B:724:ARG:HB3	2	0.13
(1,3617)	2:B:724:ARG:H	2:B:724:ARG:HB3	14	0.13
(1,3617)	2:B:724:ARG:H	2:B:724:ARG:HB3	18	0.13
(1,3617)	2:B:724:ARG:H	2:B:724:ARG:HB3	20	0.13
(1,3579)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	4	0.13
(1,3579)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	5	0.13
(1,3579)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	15	0.13
(1,3579)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	18	0.13
(1,356)	1:A:980:LEU:HB3	1:A:981:THR:HA	5	0.13
(1,356)	1:A:980:LEU:HB3	1:A:981:THR:HA	13	0.13
(1,3553)	2:B:720:THR:HG21	2:B:724:ARG:HD3	19	0.13
(1,3553)	2:B:720:THR:HG22	2:B:724:ARG:HD3	19	0.13
(1,3553)	2:B:720:THR:HG23	2:B:724:ARG:HD3	19	0.13
(1,3495)	2:B:718:LEU:HB3	2:B:719:ILE:HG12	15	0.13
(1,3470)	2:B:717:LEU:H	2:B:719:ILE:H	7	0.13
(1,3470)	2:B:717:LEU:H	2:B:719:ILE:H	16	0.13
(1,342)	1:A:979:LEU:HA	1:A:982:ILE:HB	14	0.13
(1,3356)	2:B:712:LEU:HB3	2:B:713:LEU:HB2	5	0.13
(1,3356)	2:B:712:LEU:HB3	2:B:713:LEU:HB2	15	0.13
(1,3321)	2:B:709:LEU:HA	2:B:712:LEU:HB2	4	0.13
(1,3319)	2:B:709:LEU:H	2:B:711:ALA:H	3	0.13
(1,331)	1:A:978:LEU:HA	1:A:981:THR:H	2	0.13
(1,331)	1:A:978:LEU:HA	1:A:981:THR:H	8	0.13
(1,331)	1:A:978:LEU:HA	1:A:981:THR:H	9	0.13
(1,331)	1:A:978:LEU:HA	1:A:981:THR:H	14	0.13
(1,331)	1:A:978:LEU:HA	1:A:981:THR:H	19	0.13
(1,331)	1:A:978:LEU:HA	1:A:981:THR:H	20	0.13
(1,321)	1:A:977:LEU:HB2	1:A:981:THR:H	17	0.13
(1,3185)	2:B:703:ALA:HA	2:B:706:LEU:HB3	7	0.13
(1,3185)	2:B:703:ALA:HA	2:B:706:LEU:HB3	9	0.13
(1,3185)	2:B:703:ALA:HA	2:B:706:LEU:HB3	12	0.13
(1,3148)	2:B:701:MET:HG3	2:B:704:ILE:HG13	6	0.13
(1,313)	1:A:977:LEU:HB2	1:A:978:LEU:H	5	0.13
(1,3048)	2:B:697:LEU:H	2:B:697:LEU:HB3	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2953)	2:B:693:ILE:H	2:B:693:ILE:HB	3	0.13
(1,2953)	2:B:693:ILE:H	2:B:693:ILE:HB	10	0.13
(1,2947)	2:B:692:ASP:H	2:B:696:VAL:H	17	0.13
(1,2934)	2:B:692:ASP:H	2:B:693:ILE:H	5	0.13
(1,2934)	2:B:692:ASP:H	2:B:693:ILE:H	12	0.13
(1,2934)	2:B:692:ASP:H	2:B:693:ILE:H	16	0.13
(1,2933)	2:B:692:ASP:HA	2:B:693:ILE:H	14	0.13
(1,2904)	2:B:689:LYS:H	2:B:689:LYS:HD2	8	0.13
(1,2890)	1:A:1005:GLU:H	1:A:1005:GLU:HB3	9	0.13
(1,289)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	16	0.13
(1,2884)	1:A:1004:ASP:H	1:A:1004:ASP:HB3	17	0.13
(1,2874)	1:A:1002:GLU:H	1:A:1002:GLU:HB3	9	0.13
(1,2874)	1:A:1002:GLU:H	1:A:1002:GLU:HB3	18	0.13
(1,2844)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	2	0.13
(1,2844)	1:A:997:ARG:HD3	1:A:999:PRO:HG3	15	0.13
(1,2823)	1:A:995:ARG:H	1:A:996:ASN:H	6	0.13
(1,2808)	1:A:994:LYS:HB3	1:A:995:ARG:HG3	10	0.13
(1,2807)	1:A:994:LYS:HB2	1:A:995:ARG:HG3	4	0.13
(1,2807)	1:A:994:LYS:HB2	1:A:995:ARG:HG3	5	0.13
(1,2801)	1:A:994:LYS:HB2	1:A:995:ARG:H	9	0.13
(1,2784)	1:A:993:PHE:HA	1:A:996:ASN:H	9	0.13
(1,2776)	1:A:993:PHE:H	1:A:994:LYS:HD3	19	0.13
(1,2773)	1:A:993:PHE:HB2	1:A:994:LYS:H	10	0.13
(1,2773)	1:A:993:PHE:HB2	1:A:994:LYS:H	11	0.13
(1,2755)	1:A:992:PHE:HB3	1:A:993:PHE:H	9	0.13
(1,2755)	1:A:992:PHE:HB3	1:A:993:PHE:H	15	0.13
(1,273)	1:A:974:LEU:H	1:A:975:GLY:HA2	5	0.13
(1,2728)	1:A:990:VAL:HB	1:A:993:PHE:H	17	0.13
(1,2721)	1:A:990:VAL:H	1:A:992:PHE:H	9	0.13
(1,2640)	1:A:988:TRP:H	1:A:988:TRP:HB3	5	0.13
(1,2640)	1:A:988:TRP:H	1:A:988:TRP:HB3	10	0.13
(1,2640)	1:A:988:TRP:H	1:A:988:TRP:HB3	19	0.13
(1,2631)	1:A:987:MET:HA	1:A:990:VAL:H	7	0.13
(1,2631)	1:A:987:MET:HA	1:A:990:VAL:H	13	0.13
(1,2631)	1:A:987:MET:HA	1:A:990:VAL:H	20	0.13
(1,2615)	1:A:987:MET:H	1:A:987:MET:HG3	1	0.13
(1,2520)	1:A:984:VAL:H	1:A:984:VAL:HG11	4	0.13
(1,2520)	1:A:984:VAL:H	1:A:984:VAL:HG12	4	0.13
(1,2520)	1:A:984:VAL:H	1:A:984:VAL:HG13	4	0.13
(1,2520)	1:A:984:VAL:H	1:A:984:VAL:HG11	17	0.13
(1,2520)	1:A:984:VAL:H	1:A:984:VAL:HG12	17	0.13
(1,2520)	1:A:984:VAL:H	1:A:984:VAL:HG13	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2515)	1:A:983:LEU:HB2	1:A:987:MET:H	13	0.13
(1,2509)	1:A:983:LEU:HA	1:A:985:LEU:H	2	0.13
(1,2509)	1:A:983:LEU:HA	1:A:985:LEU:H	10	0.13
(1,2509)	1:A:983:LEU:HA	1:A:985:LEU:H	11	0.13
(1,2478)	1:A:982:ILE:HA	1:A:985:LEU:HB3	5	0.13
(1,2439)	1:A:980:LEU:HB3	1:A:981:THR:HA	5	0.13
(1,2439)	1:A:980:LEU:HB3	1:A:981:THR:HA	13	0.13
(1,243)	1:A:972:GLY:H	1:A:976:GLY:H	8	0.13
(1,2425)	1:A:979:LEU:HA	1:A:982:ILE:HB	14	0.13
(1,2414)	1:A:978:LEU:HA	1:A:981:THR:H	2	0.13
(1,2414)	1:A:978:LEU:HA	1:A:981:THR:H	8	0.13
(1,2414)	1:A:978:LEU:HA	1:A:981:THR:H	9	0.13
(1,2414)	1:A:978:LEU:HA	1:A:981:THR:H	14	0.13
(1,2414)	1:A:978:LEU:HA	1:A:981:THR:H	19	0.13
(1,2414)	1:A:978:LEU:HA	1:A:981:THR:H	20	0.13
(1,2404)	1:A:977:LEU:HB2	1:A:981:THR:H	17	0.13
(1,2396)	1:A:977:LEU:HB2	1:A:978:LEU:H	5	0.13
(1,2372)	1:A:975:GLY:HA3	1:A:978:LEU:HB3	16	0.13
(1,2356)	1:A:974:LEU:H	1:A:975:GLY:HA2	5	0.13
(1,2326)	1:A:972:GLY:H	1:A:976:GLY:H	8	0.13
(1,2313)	1:A:971:VAL:HA	1:A:974:LEU:HB3	19	0.13
(1,2308)	1:A:971:VAL:H	1:A:973:VAL:H	3	0.13
(1,2308)	1:A:971:VAL:H	1:A:973:VAL:H	6	0.13
(1,230)	1:A:971:VAL:HA	1:A:974:LEU:HB3	19	0.13
(1,2291)	1:A:970:LEU:HB3	1:A:974:LEU:H	7	0.13
(1,2291)	1:A:970:LEU:HB3	1:A:974:LEU:H	19	0.13
(1,225)	1:A:971:VAL:H	1:A:973:VAL:H	3	0.13
(1,225)	1:A:971:VAL:H	1:A:973:VAL:H	6	0.13
(1,2215)	1:A:968:TRP:H	1:A:968:TRP:HB3	2	0.13
(1,2203)	1:A:967:TRP:HB3	1:A:968:TRP:HB3	20	0.13
(1,2189)	1:A:967:TRP:H	1:A:967:TRP:HB3	9	0.13
(1,2189)	1:A:967:TRP:H	1:A:967:TRP:HB3	11	0.13
(1,2189)	1:A:967:TRP:H	1:A:967:TRP:HB3	13	0.13
(1,2187)	1:A:966:ILE:HA	1:A:970:LEU:H	9	0.13
(1,2182)	1:A:966:ILE:HA	1:A:969:VAL:H	12	0.13
(1,2090)	1:A:960:GLU:HB2	1:A:961:GLU:H	2	0.13
(1,2090)	1:A:960:GLU:HB2	1:A:961:GLU:H	5	0.13
(1,2080)	1:A:988:TRP:HE1	2:B:719:ILE:HG21	12	0.13
(1,2080)	1:A:988:TRP:HE1	2:B:719:ILE:HG22	12	0.13
(1,2080)	1:A:988:TRP:HE1	2:B:719:ILE:HG23	12	0.13
(1,208)	1:A:970:LEU:HB3	1:A:974:LEU:H	7	0.13
(1,208)	1:A:970:LEU:HB3	1:A:974:LEU:H	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2079)	1:A:988:TRP:HE1	2:B:719:ILE:HB	12	0.13
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG21	2	0.13
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG22	2	0.13
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG23	2	0.13
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG21	6	0.13
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG22	6	0.13
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG23	6	0.13
(1,2074)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	4	0.13
(1,2074)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	10	0.13
(1,2074)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	17	0.13
(1,2073)	1:A:988:TRP:HE1	2:B:715:TRP:HD1	8	0.13
(1,2048)	1:A:979:LEU:H	2:B:707:ILE:HB	16	0.13
(1,2038)	1:A:976:GLY:H	2:B:707:ILE:HB	11	0.13
(1,2028)	1:A:974:LEU:H	2:B:704:ILE:HG13	16	0.13
(1,2018)	1:A:973:VAL:H	2:B:700:VAL:HA	5	0.13
(1,2018)	1:A:973:VAL:H	2:B:700:VAL:HA	13	0.13
(1,2018)	1:A:973:VAL:H	2:B:700:VAL:HA	15	0.13
(1,2018)	1:A:973:VAL:H	2:B:700:VAL:HA	17	0.13
(1,1957)	2:B:756:ASN:H	2:B:756:ASN:HB2	10	0.13
(1,1950)	2:B:754:PHE:HA	2:B:755:THR:H	1	0.13
(1,1949)	2:B:754:PHE:HB3	2:B:755:THR:H	7	0.13
(1,1949)	2:B:754:PHE:HB3	2:B:755:THR:H	8	0.13
(1,1949)	2:B:754:PHE:HB3	2:B:755:THR:H	13	0.13
(1,1949)	2:B:754:PHE:HB3	2:B:755:THR:H	16	0.13
(1,1945)	2:B:754:PHE:H	2:B:754:PHE:HB2	8	0.13
(1,1944)	2:B:753:THR:HA	2:B:754:PHE:H	8	0.13
(1,1931)	2:B:751:THR:HA	2:B:752:SER:H	4	0.13
(1,1927)	2:B:751:THR:H	2:B:751:THR:HG21	10	0.13
(1,1927)	2:B:751:THR:H	2:B:751:THR:HG22	10	0.13
(1,1927)	2:B:751:THR:H	2:B:751:THR:HG23	10	0.13
(1,1885)	2:B:747:TYR:H	2:B:747:TYR:HB3	3	0.13
(1,1880)	2:B:746:LEU:HB2	2:B:747:TYR:H	6	0.13
(1,1871)	2:B:746:LEU:H	2:B:746:LEU:HB2	1	0.13
(1,1871)	2:B:746:LEU:H	2:B:746:LEU:HB2	2	0.13
(1,1838)	2:B:744:ASN:H	2:B:744:ASN:HB2	9	0.13
(1,1820)	2:B:742:ALA:HB1	2:B:743:ASN:H	15	0.13
(1,1820)	2:B:742:ALA:HB2	2:B:743:ASN:H	15	0.13
(1,1820)	2:B:742:ALA:HB3	2:B:743:ASN:H	15	0.13
(1,1811)	2:B:741:THR:HB	2:B:742:ALA:H	19	0.13
(1,1798)	2:B:739:TRP:HB3	2:B:740:ASP:H	2	0.13
(1,1798)	2:B:739:TRP:HB3	2:B:740:ASP:H	3	0.13
(1,1798)	2:B:739:TRP:HB3	2:B:740:ASP:H	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1786)	2:B:738:LYS:H	2:B:740:ASP:H	9	0.13
(1,1780)	2:B:738:LYS:HB3	2:B:739:TRP:H	3	0.13
(1,1767)	2:B:738:LYS:HA	2:B:738:LYS:HD3	6	0.13
(1,1767)	2:B:738:LYS:HA	2:B:738:LYS:HD3	13	0.13
(1,1767)	2:B:738:LYS:HA	2:B:738:LYS:HD3	18	0.13
(1,1767)	2:B:738:LYS:HA	2:B:738:LYS:HD3	20	0.13
(1,1585)	2:B:725:LYS:HG3	2:B:729:LYS:HE3	6	0.13
(1,1581)	2:B:725:LYS:HA	2:B:728:ALA:H	1	0.13
(1,1581)	2:B:725:LYS:HA	2:B:728:ALA:H	5	0.13
(1,1555)	2:B:724:ARG:HA	2:B:728:ALA:H	1	0.13
(1,1555)	2:B:724:ARG:HA	2:B:728:ALA:H	6	0.13
(1,1555)	2:B:724:ARG:HA	2:B:728:ALA:H	9	0.13
(1,1555)	2:B:724:ARG:HA	2:B:728:ALA:H	13	0.13
(1,1555)	2:B:724:ARG:HA	2:B:728:ALA:H	15	0.13
(1,1555)	2:B:724:ARG:HA	2:B:728:ALA:H	17	0.13
(1,1555)	2:B:724:ARG:HA	2:B:728:ALA:H	18	0.13
(1,1555)	2:B:724:ARG:HA	2:B:728:ALA:H	19	0.13
(1,1537)	2:B:724:ARG:HD3	2:B:724:ARG:HB3	1	0.13
(1,1534)	2:B:724:ARG:H	2:B:724:ARG:HB3	2	0.13
(1,1534)	2:B:724:ARG:H	2:B:724:ARG:HB3	14	0.13
(1,1534)	2:B:724:ARG:H	2:B:724:ARG:HB3	18	0.13
(1,1534)	2:B:724:ARG:H	2:B:724:ARG:HB3	20	0.13
(1,1496)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	4	0.13
(1,1496)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	5	0.13
(1,1496)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	15	0.13
(1,1496)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	18	0.13
(1,1470)	2:B:720:THR:HG21	2:B:724:ARG:HD3	19	0.13
(1,1470)	2:B:720:THR:HG22	2:B:724:ARG:HD3	19	0.13
(1,1470)	2:B:720:THR:HG23	2:B:724:ARG:HD3	19	0.13
(1,1412)	2:B:718:LEU:HB3	2:B:719:ILE:HG12	15	0.13
(1,1387)	2:B:717:LEU:H	2:B:719:ILE:H	7	0.13
(1,1387)	2:B:717:LEU:H	2:B:719:ILE:H	16	0.13
(1,132)	1:A:968:TRP:H	1:A:968:TRP:HB3	2	0.13
(1,1273)	2:B:712:LEU:HB3	2:B:713:LEU:HB2	5	0.13
(1,1273)	2:B:712:LEU:HB3	2:B:713:LEU:HB2	15	0.13
(1,1238)	2:B:709:LEU:HA	2:B:712:LEU:HB2	4	0.13
(1,1236)	2:B:709:LEU:H	2:B:711:ALA:H	3	0.13
(1,120)	1:A:967:TRP:HB3	1:A:968:TRP:HB3	20	0.13
(1,1102)	2:B:703:ALA:HA	2:B:706:LEU:HB3	7	0.13
(1,1102)	2:B:703:ALA:HA	2:B:706:LEU:HB3	9	0.13
(1,1102)	2:B:703:ALA:HA	2:B:706:LEU:HB3	12	0.13
(1,1065)	2:B:701:MET:HG3	2:B:704:ILE:HG13	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,106)	1:A:967:TRP:H	1:A:967:TRP:HB3	9	0.13
(1,106)	1:A:967:TRP:H	1:A:967:TRP:HB3	11	0.13
(1,106)	1:A:967:TRP:H	1:A:967:TRP:HB3	13	0.13
(1,104)	1:A:966:ILE:HA	1:A:970:LEU:H	9	0.13
(3,81)	2:B:700:VAL:O	2:B:704:ILE:H	20	0.12
(3,43)	1:A:981:THR:O	1:A:984:VAL:H	5	0.12
(3,43)	1:A:981:THR:O	1:A:984:VAL:H	7	0.12
(3,43)	1:A:981:THR:O	1:A:984:VAL:H	8	0.12
(3,43)	1:A:981:THR:O	1:A:984:VAL:H	12	0.12
(3,43)	1:A:981:THR:O	1:A:984:VAL:H	18	0.12
(3,43)	1:A:981:THR:O	1:A:984:VAL:H	20	0.12
(3,270)	2:B:710:ALA:O	2:B:714:ILE:H	4	0.12
(3,270)	2:B:710:ALA:O	2:B:714:ILE:H	11	0.12
(3,270)	2:B:710:ALA:O	2:B:714:ILE:H	13	0.12
(3,270)	2:B:710:ALA:O	2:B:714:ILE:H	19	0.12
(3,240)	2:B:700:VAL:O	2:B:704:ILE:H	20	0.12
(3,24)	1:A:974:LEU:O	1:A:978:LEU:H	5	0.12
(3,202)	1:A:981:THR:O	1:A:984:VAL:H	5	0.12
(3,202)	1:A:981:THR:O	1:A:984:VAL:H	7	0.12
(3,202)	1:A:981:THR:O	1:A:984:VAL:H	8	0.12
(3,202)	1:A:981:THR:O	1:A:984:VAL:H	12	0.12
(3,202)	1:A:981:THR:O	1:A:984:VAL:H	18	0.12
(3,202)	1:A:981:THR:O	1:A:984:VAL:H	20	0.12
(3,183)	1:A:974:LEU:O	1:A:978:LEU:H	5	0.12
(3,111)	2:B:710:ALA:O	2:B:714:ILE:H	4	0.12
(3,111)	2:B:710:ALA:O	2:B:714:ILE:H	11	0.12
(3,111)	2:B:710:ALA:O	2:B:714:ILE:H	13	0.12
(3,111)	2:B:710:ALA:O	2:B:714:ILE:H	19	0.12
(1,950)	2:B:696:VAL:H	2:B:696:VAL:HB	5	0.12
(1,950)	2:B:696:VAL:H	2:B:696:VAL:HB	17	0.12
(1,870)	2:B:693:ILE:H	2:B:693:ILE:HB	12	0.12
(1,870)	2:B:693:ILE:H	2:B:693:ILE:HB	16	0.12
(1,864)	2:B:692:ASP:H	2:B:696:VAL:H	1	0.12
(1,850)	2:B:692:ASP:HA	2:B:693:ILE:H	9	0.12
(1,848)	2:B:692:ASP:H	2:B:692:ASP:HB3	14	0.12
(1,848)	2:B:692:ASP:H	2:B:692:ASP:HB3	16	0.12
(1,820)	2:B:689:LYS:H	2:B:689:LYS:HB2	7	0.12
(1,811)	1:A:1006:GLU:H	1:A:1006:GLU:HB3	1	0.12
(1,811)	1:A:1006:GLU:H	1:A:1006:GLU:HB3	16	0.12
(1,807)	1:A:1005:GLU:H	1:A:1005:GLU:HB3	2	0.12
(1,802)	1:A:1004:ASP:H	1:A:1004:ASP:HB2	13	0.12
(1,8)	1:A:961:GLU:H	1:A:961:GLU:HB3	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,8)	1:A:961:GLU:H	1:A:961:GLU:HB3	18	0.12
(1,778)	1:A:1000:LEU:H	1:A:1000:LEU:HB3	15	0.12
(1,774)	1:A:999:PRO:HB2	1:A:1000:LEU:H	6	0.12
(1,760)	1:A:997:ARG:HA	1:A:999:PRO:HD3	13	0.12
(1,751)	1:A:996:ASN:H	1:A:997:ARG:H	17	0.12
(1,729)	1:A:995:ARG:H	1:A:995:ARG:HB3	12	0.12
(1,729)	1:A:995:ARG:H	1:A:995:ARG:HB3	13	0.12
(1,725)	1:A:994:LYS:HB3	1:A:995:ARG:HG3	2	0.12
(1,725)	1:A:994:LYS:HB3	1:A:995:ARG:HG3	14	0.12
(1,724)	1:A:994:LYS:HB2	1:A:995:ARG:HG3	14	0.12
(1,718)	1:A:994:LYS:HB2	1:A:995:ARG:H	11	0.12
(1,707)	1:A:994:LYS:HE3	1:A:994:LYS:HG3	19	0.12
(1,704)	1:A:994:LYS:H	1:A:994:LYS:HG3	4	0.12
(1,704)	1:A:994:LYS:H	1:A:994:LYS:HG3	10	0.12
(1,704)	1:A:994:LYS:H	1:A:994:LYS:HG3	16	0.12
(1,7)	1:A:960:GLU:HB2	1:A:961:GLU:H	7	0.12
(1,7)	1:A:960:GLU:HB2	1:A:961:GLU:H	10	0.12
(1,7)	1:A:960:GLU:HB2	1:A:961:GLU:H	14	0.12
(1,7)	1:A:960:GLU:HB2	1:A:961:GLU:H	17	0.12
(1,697)	1:A:993:PHE:H	1:A:995:ARG:H	12	0.12
(1,690)	1:A:993:PHE:HB2	1:A:994:LYS:H	7	0.12
(1,690)	1:A:993:PHE:HB2	1:A:994:LYS:H	8	0.12
(1,672)	1:A:992:PHE:HB3	1:A:993:PHE:H	13	0.12
(1,638)	1:A:990:VAL:H	1:A:992:PHE:H	1	0.12
(1,63)	1:A:965:PRO:HG3	1:A:967:TRP:HB2	2	0.12
(1,63)	1:A:965:PRO:HG3	1:A:967:TRP:HB2	6	0.12
(1,611)	1:A:989:LYS:HE3	1:A:993:PHE:HE1	11	0.12
(1,557)	1:A:988:TRP:H	1:A:988:TRP:HB3	2	0.12
(1,557)	1:A:988:TRP:H	1:A:988:TRP:HB3	6	0.12
(1,557)	1:A:988:TRP:H	1:A:988:TRP:HB3	13	0.12
(1,451)	1:A:984:VAL:H	1:A:987:MET:H	1	0.12
(1,437)	1:A:984:VAL:H	1:A:984:VAL:HG11	20	0.12
(1,437)	1:A:984:VAL:H	1:A:984:VAL:HG12	20	0.12
(1,437)	1:A:984:VAL:H	1:A:984:VAL:HG13	20	0.12
(1,4163)	1:A:988:TRP:HE1	2:B:719:ILE:HG21	11	0.12
(1,4163)	1:A:988:TRP:HE1	2:B:719:ILE:HG22	11	0.12
(1,4163)	1:A:988:TRP:HE1	2:B:719:ILE:HG23	11	0.12
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG21	19	0.12
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG22	19	0.12
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG23	19	0.12
(1,4157)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	1	0.12
(1,4157)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4157)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	11	0.12
(1,4157)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	20	0.12
(1,4156)	1:A:988:TRP:HE1	2:B:715:TRP:HD1	1	0.12
(1,4156)	1:A:988:TRP:HE1	2:B:715:TRP:HD1	2	0.12
(1,4151)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	15	0.12
(1,4118)	1:A:976:GLY:H	2:B:704:ILE:HB	6	0.12
(1,4111)	1:A:974:LEU:H	2:B:704:ILE:HG13	11	0.12
(1,4101)	1:A:973:VAL:H	2:B:700:VAL:HA	8	0.12
(1,4101)	1:A:973:VAL:H	2:B:700:VAL:HA	12	0.12
(1,4093)	1:A:969:VAL:HA	2:B:700:VAL:H	7	0.12
(1,408)	1:A:983:LEU:H	1:A:983:LEU:HB3	14	0.12
(1,4073)	2:B:759:TYR:HA	2:B:760:ARG:H	9	0.12
(1,4051)	2:B:757:ILE:H	2:B:757:ILE:HG12	13	0.12
(1,4038)	2:B:755:THR:H	2:B:756:ASN:H	11	0.12
(1,4032)	2:B:754:PHE:HB3	2:B:755:THR:H	14	0.12
(1,4027)	2:B:753:THR:HA	2:B:754:PHE:H	1	0.12
(1,4027)	2:B:753:THR:HA	2:B:754:PHE:H	2	0.12
(1,4027)	2:B:753:THR:HA	2:B:754:PHE:H	6	0.12
(1,4027)	2:B:753:THR:HA	2:B:754:PHE:H	9	0.12
(1,3968)	2:B:747:TYR:H	2:B:747:TYR:HB3	7	0.12
(1,3968)	2:B:747:TYR:H	2:B:747:TYR:HB3	9	0.12
(1,3968)	2:B:747:TYR:H	2:B:747:TYR:HB3	17	0.12
(1,3954)	2:B:746:LEU:H	2:B:746:LEU:HB2	4	0.12
(1,3954)	2:B:746:LEU:H	2:B:746:LEU:HB2	10	0.12
(1,3954)	2:B:746:LEU:H	2:B:746:LEU:HB2	14	0.12
(1,3954)	2:B:746:LEU:H	2:B:746:LEU:HB2	16	0.12
(1,395)	1:A:982:ILE:HA	1:A:985:LEU:HB3	9	0.12
(1,395)	1:A:982:ILE:HA	1:A:985:LEU:HB3	20	0.12
(1,3944)	2:B:745:PRO:HD2	2:B:746:LEU:H	16	0.12
(1,3921)	2:B:744:ASN:H	2:B:744:ASN:HB2	1	0.12
(1,3921)	2:B:744:ASN:H	2:B:744:ASN:HB2	4	0.12
(1,3921)	2:B:744:ASN:H	2:B:744:ASN:HB2	11	0.12
(1,3911)	2:B:743:ASN:HB3	2:B:743:ASN:H	19	0.12
(1,3904)	2:B:742:ALA:HB1	2:B:743:ASN:HD22	16	0.12
(1,3904)	2:B:742:ALA:HB2	2:B:743:ASN:HD22	16	0.12
(1,3904)	2:B:742:ALA:HB3	2:B:743:ASN:HD22	16	0.12
(1,3894)	2:B:741:THR:HB	2:B:742:ALA:H	6	0.12
(1,3888)	2:B:740:ASP:HA	2:B:741:THR:H	5	0.12
(1,3888)	2:B:740:ASP:HA	2:B:741:THR:H	6	0.12
(1,3881)	2:B:739:TRP:HB3	2:B:740:ASP:H	6	0.12
(1,3881)	2:B:739:TRP:HB3	2:B:740:ASP:H	11	0.12
(1,3881)	2:B:739:TRP:HB3	2:B:740:ASP:H	12	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3881)	2:B:739:TRP:HB3	2:B:740:ASP:H	13	0.12
(1,3881)	2:B:739:TRP:HB3	2:B:740:ASP:H	14	0.12
(1,3881)	2:B:739:TRP:HB3	2:B:740:ASP:H	18	0.12
(1,3869)	2:B:738:LYS:H	2:B:740:ASP:H	16	0.12
(1,3869)	2:B:738:LYS:H	2:B:740:ASP:H	18	0.12
(1,3850)	2:B:738:LYS:HA	2:B:738:LYS:HD3	11	0.12
(1,3850)	2:B:738:LYS:HA	2:B:738:LYS:HD3	14	0.12
(1,3850)	2:B:738:LYS:HA	2:B:738:LYS:HD3	19	0.12
(1,3822)	2:B:736:ARG:H	2:B:736:ARG:HB3	5	0.12
(1,3744)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	11	0.12
(1,3741)	2:B:730:PHE:HB3	2:B:731:GLU:HG3	7	0.12
(1,3708)	2:B:728:ALA:HB1	2:B:731:GLU:HG2	7	0.12
(1,3708)	2:B:728:ALA:HB2	2:B:731:GLU:HG2	7	0.12
(1,3708)	2:B:728:ALA:HB3	2:B:731:GLU:HG2	7	0.12
(1,3706)	2:B:728:ALA:H	2:B:730:PHE:H	1	0.12
(1,3706)	2:B:728:ALA:H	2:B:730:PHE:H	3	0.12
(1,3706)	2:B:728:ALA:H	2:B:730:PHE:H	4	0.12
(1,3706)	2:B:728:ALA:H	2:B:730:PHE:H	8	0.12
(1,3706)	2:B:728:ALA:H	2:B:730:PHE:H	9	0.12
(1,3706)	2:B:728:ALA:H	2:B:730:PHE:H	10	0.12
(1,3706)	2:B:728:ALA:H	2:B:730:PHE:H	11	0.12
(1,3706)	2:B:728:ALA:H	2:B:730:PHE:H	18	0.12
(1,3666)	2:B:725:LYS:HA	2:B:729:LYS:HE3	4	0.12
(1,3664)	2:B:725:LYS:HA	2:B:728:ALA:H	3	0.12
(1,3664)	2:B:725:LYS:HA	2:B:728:ALA:H	6	0.12
(1,3664)	2:B:725:LYS:HA	2:B:728:ALA:H	14	0.12
(1,3648)	2:B:725:LYS:HE3	2:B:725:LYS:HG3	20	0.12
(1,3638)	2:B:724:ARG:HA	2:B:728:ALA:H	3	0.12
(1,3617)	2:B:724:ARG:H	2:B:724:ARG:HB3	6	0.12
(1,3617)	2:B:724:ARG:H	2:B:724:ARG:HB3	10	0.12
(1,3617)	2:B:724:ARG:H	2:B:724:ARG:HB3	12	0.12
(1,3617)	2:B:724:ARG:H	2:B:724:ARG:HB3	16	0.12
(1,3470)	2:B:717:LEU:H	2:B:719:ILE:H	8	0.12
(1,3470)	2:B:717:LEU:H	2:B:719:ILE:H	11	0.12
(1,3470)	2:B:717:LEU:H	2:B:719:ILE:H	20	0.12
(1,3319)	2:B:709:LEU:H	2:B:711:ALA:H	1	0.12
(1,3319)	2:B:709:LEU:H	2:B:711:ALA:H	14	0.12
(1,3318)	2:B:709:LEU:HB3	2:B:710:ALA:HA	20	0.12
(1,331)	1:A:978:LEU:HA	1:A:981:THR:H	13	0.12
(1,331)	1:A:978:LEU:HA	1:A:981:THR:H	17	0.12
(1,321)	1:A:977:LEU:HB2	1:A:981:THR:H	8	0.12
(1,321)	1:A:977:LEU:HB2	1:A:981:THR:H	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,321)	1:A:977:LEU:HB2	1:A:981:THR:H	13	0.12
(1,3185)	2:B:703:ALA:HA	2:B:706:LEU:HB3	11	0.12
(1,3185)	2:B:703:ALA:HA	2:B:706:LEU:HB3	20	0.12
(1,3033)	2:B:696:VAL:H	2:B:696:VAL:HB	5	0.12
(1,3033)	2:B:696:VAL:H	2:B:696:VAL:HB	17	0.12
(1,2953)	2:B:693:ILE:H	2:B:693:ILE:HB	12	0.12
(1,2953)	2:B:693:ILE:H	2:B:693:ILE:HB	16	0.12
(1,2947)	2:B:692:ASP:H	2:B:696:VAL:H	1	0.12
(1,2933)	2:B:692:ASP:HA	2:B:693:ILE:H	9	0.12
(1,2931)	2:B:692:ASP:H	2:B:692:ASP:HB3	14	0.12
(1,2931)	2:B:692:ASP:H	2:B:692:ASP:HB3	16	0.12
(1,2903)	2:B:689:LYS:H	2:B:689:LYS:HB2	7	0.12
(1,2894)	1:A:1006:GLU:H	1:A:1006:GLU:HB3	1	0.12
(1,2894)	1:A:1006:GLU:H	1:A:1006:GLU:HB3	16	0.12
(1,2890)	1:A:1005:GLU:H	1:A:1005:GLU:HB3	2	0.12
(1,2885)	1:A:1004:ASP:H	1:A:1004:ASP:HB2	13	0.12
(1,2861)	1:A:1000:LEU:H	1:A:1000:LEU:HB3	15	0.12
(1,2857)	1:A:999:PRO:HB2	1:A:1000:LEU:H	6	0.12
(1,2843)	1:A:997:ARG:HA	1:A:999:PRO:HD3	13	0.12
(1,2834)	1:A:996:ASN:H	1:A:997:ARG:H	17	0.12
(1,2812)	1:A:995:ARG:H	1:A:995:ARG:HB3	12	0.12
(1,2812)	1:A:995:ARG:H	1:A:995:ARG:HB3	13	0.12
(1,2808)	1:A:994:LYS:HB3	1:A:995:ARG:HG3	2	0.12
(1,2808)	1:A:994:LYS:HB3	1:A:995:ARG:HG3	14	0.12
(1,2807)	1:A:994:LYS:HB2	1:A:995:ARG:HG3	14	0.12
(1,2801)	1:A:994:LYS:HB2	1:A:995:ARG:H	11	0.12
(1,2790)	1:A:994:LYS:HE3	1:A:994:LYS:HG3	19	0.12
(1,2787)	1:A:994:LYS:H	1:A:994:LYS:HG3	4	0.12
(1,2787)	1:A:994:LYS:H	1:A:994:LYS:HG3	10	0.12
(1,2787)	1:A:994:LYS:H	1:A:994:LYS:HG3	16	0.12
(1,2780)	1:A:993:PHE:H	1:A:995:ARG:H	12	0.12
(1,2773)	1:A:993:PHE:HB2	1:A:994:LYS:H	7	0.12
(1,2773)	1:A:993:PHE:HB2	1:A:994:LYS:H	8	0.12
(1,2755)	1:A:992:PHE:HB3	1:A:993:PHE:H	13	0.12
(1,275)	1:A:974:LEU:HB2	1:A:975:GLY:H	5	0.12
(1,275)	1:A:974:LEU:HB2	1:A:975:GLY:H	10	0.12
(1,2721)	1:A:990:VAL:H	1:A:992:PHE:H	1	0.12
(1,2694)	1:A:989:LYS:HE3	1:A:993:PHE:HE1	11	0.12
(1,2640)	1:A:988:TRP:H	1:A:988:TRP:HB3	2	0.12
(1,2640)	1:A:988:TRP:H	1:A:988:TRP:HB3	6	0.12
(1,2640)	1:A:988:TRP:H	1:A:988:TRP:HB3	13	0.12
(1,2534)	1:A:984:VAL:H	1:A:987:MET:H	1	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2520)	1:A:984:VAL:H	1:A:984:VAL:HG11	20	0.12
(1,2520)	1:A:984:VAL:H	1:A:984:VAL:HG12	20	0.12
(1,2520)	1:A:984:VAL:H	1:A:984:VAL:HG13	20	0.12
(1,2491)	1:A:983:LEU:H	1:A:983:LEU:HB3	14	0.12
(1,2478)	1:A:982:ILE:HA	1:A:985:LEU:HB3	9	0.12
(1,2478)	1:A:982:ILE:HA	1:A:985:LEU:HB3	20	0.12
(1,2414)	1:A:978:LEU:HA	1:A:981:THR:H	13	0.12
(1,2414)	1:A:978:LEU:HA	1:A:981:THR:H	17	0.12
(1,2404)	1:A:977:LEU:HB2	1:A:981:THR:H	8	0.12
(1,2404)	1:A:977:LEU:HB2	1:A:981:THR:H	9	0.12
(1,2404)	1:A:977:LEU:HB2	1:A:981:THR:H	13	0.12
(1,2358)	1:A:974:LEU:HB2	1:A:975:GLY:H	5	0.12
(1,2358)	1:A:974:LEU:HB2	1:A:975:GLY:H	10	0.12
(1,2313)	1:A:971:VAL:HA	1:A:974:LEU:HB3	3	0.12
(1,2313)	1:A:971:VAL:HA	1:A:974:LEU:HB3	5	0.12
(1,230)	1:A:971:VAL:HA	1:A:974:LEU:HB3	3	0.12
(1,230)	1:A:971:VAL:HA	1:A:974:LEU:HB3	5	0.12
(1,2291)	1:A:970:LEU:HB3	1:A:974:LEU:H	16	0.12
(1,2272)	1:A:970:LEU:H	1:A:970:LEU:HB3	20	0.12
(1,2266)	1:A:969:VAL:H	1:A:972:GLY:HA3	12	0.12
(1,2266)	1:A:969:VAL:H	1:A:972:GLY:HA3	13	0.12
(1,2266)	1:A:969:VAL:H	1:A:972:GLY:HA3	14	0.12
(1,2258)	1:A:969:VAL:H	1:A:970:LEU:HB3	7	0.12
(1,2238)	1:A:968:TRP:HA	1:A:971:VAL:H	3	0.12
(1,2238)	1:A:968:TRP:HA	1:A:971:VAL:H	7	0.12
(1,2238)	1:A:968:TRP:HA	1:A:971:VAL:H	8	0.12
(1,2215)	1:A:968:TRP:H	1:A:968:TRP:HB3	1	0.12
(1,2203)	1:A:967:TRP:HB3	1:A:968:TRP:HB3	4	0.12
(1,2203)	1:A:967:TRP:HB3	1:A:968:TRP:HB3	10	0.12
(1,2203)	1:A:967:TRP:HB3	1:A:968:TRP:HB3	15	0.12
(1,2189)	1:A:967:TRP:H	1:A:967:TRP:HB3	10	0.12
(1,2189)	1:A:967:TRP:H	1:A:967:TRP:HB3	16	0.12
(1,2187)	1:A:966:ILE:HA	1:A:970:LEU:H	3	0.12
(1,2146)	1:A:965:PRO:HG3	1:A:967:TRP:HB2	2	0.12
(1,2146)	1:A:965:PRO:HG3	1:A:967:TRP:HB2	6	0.12
(1,2091)	1:A:961:GLU:H	1:A:961:GLU:HB3	15	0.12
(1,2091)	1:A:961:GLU:H	1:A:961:GLU:HB3	18	0.12
(1,2090)	1:A:960:GLU:HB2	1:A:961:GLU:H	7	0.12
(1,2090)	1:A:960:GLU:HB2	1:A:961:GLU:H	10	0.12
(1,2090)	1:A:960:GLU:HB2	1:A:961:GLU:H	14	0.12
(1,2090)	1:A:960:GLU:HB2	1:A:961:GLU:H	17	0.12
(1,2080)	1:A:988:TRP:HE1	2:B:719:ILE:HG21	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2080)	1:A:988:TRP:HE1	2:B:719:ILE:HG22	11	0.12
(1,2080)	1:A:988:TRP:HE1	2:B:719:ILE:HG23	11	0.12
(1,208)	1:A:970:LEU:HB3	1:A:974:LEU:H	16	0.12
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG21	19	0.12
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG22	19	0.12
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG23	19	0.12
(1,2074)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	1	0.12
(1,2074)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	6	0.12
(1,2074)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	11	0.12
(1,2074)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	20	0.12
(1,2073)	1:A:988:TRP:HE1	2:B:715:TRP:HD1	1	0.12
(1,2073)	1:A:988:TRP:HE1	2:B:715:TRP:HD1	2	0.12
(1,2068)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	15	0.12
(1,2035)	1:A:976:GLY:H	2:B:704:ILE:HB	6	0.12
(1,2028)	1:A:974:LEU:H	2:B:704:ILE:HG13	11	0.12
(1,2018)	1:A:973:VAL:H	2:B:700:VAL:HA	8	0.12
(1,2018)	1:A:973:VAL:H	2:B:700:VAL:HA	12	0.12
(1,2010)	1:A:969:VAL:HA	2:B:700:VAL:H	7	0.12
(1,1990)	2:B:759:TYR:HA	2:B:760:ARG:H	9	0.12
(1,1968)	2:B:757:ILE:H	2:B:757:ILE:HG12	13	0.12
(1,1955)	2:B:755:THR:H	2:B:756:ASN:H	11	0.12
(1,1949)	2:B:754:PHE:HB3	2:B:755:THR:H	14	0.12
(1,1944)	2:B:753:THR:HA	2:B:754:PHE:H	1	0.12
(1,1944)	2:B:753:THR:HA	2:B:754:PHE:H	2	0.12
(1,1944)	2:B:753:THR:HA	2:B:754:PHE:H	6	0.12
(1,1944)	2:B:753:THR:HA	2:B:754:PHE:H	9	0.12
(1,189)	1:A:970:LEU:H	1:A:970:LEU:HB3	20	0.12
(1,1885)	2:B:747:TYR:H	2:B:747:TYR:HB3	7	0.12
(1,1885)	2:B:747:TYR:H	2:B:747:TYR:HB3	9	0.12
(1,1885)	2:B:747:TYR:H	2:B:747:TYR:HB3	17	0.12
(1,1871)	2:B:746:LEU:H	2:B:746:LEU:HB2	4	0.12
(1,1871)	2:B:746:LEU:H	2:B:746:LEU:HB2	10	0.12
(1,1871)	2:B:746:LEU:H	2:B:746:LEU:HB2	14	0.12
(1,1871)	2:B:746:LEU:H	2:B:746:LEU:HB2	16	0.12
(1,1861)	2:B:745:PRO:HD2	2:B:746:LEU:H	16	0.12
(1,1838)	2:B:744:ASN:H	2:B:744:ASN:HB2	1	0.12
(1,1838)	2:B:744:ASN:H	2:B:744:ASN:HB2	4	0.12
(1,1838)	2:B:744:ASN:H	2:B:744:ASN:HB2	11	0.12
(1,183)	1:A:969:VAL:H	1:A:972:GLY:HA3	12	0.12
(1,183)	1:A:969:VAL:H	1:A:972:GLY:HA3	13	0.12
(1,183)	1:A:969:VAL:H	1:A:972:GLY:HA3	14	0.12
(1,1828)	2:B:743:ASN:HB3	2:B:743:ASN:H	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1821)	2:B:742:ALA:HB1	2:B:743:ASN:HD22	16	0.12
(1,1821)	2:B:742:ALA:HB2	2:B:743:ASN:HD22	16	0.12
(1,1821)	2:B:742:ALA:HB3	2:B:743:ASN:HD22	16	0.12
(1,1811)	2:B:741:THR:HB	2:B:742:ALA:H	6	0.12
(1,1805)	2:B:740:ASP:HA	2:B:741:THR:H	5	0.12
(1,1805)	2:B:740:ASP:HA	2:B:741:THR:H	6	0.12
(1,1798)	2:B:739:TRP:HB3	2:B:740:ASP:H	6	0.12
(1,1798)	2:B:739:TRP:HB3	2:B:740:ASP:H	11	0.12
(1,1798)	2:B:739:TRP:HB3	2:B:740:ASP:H	12	0.12
(1,1798)	2:B:739:TRP:HB3	2:B:740:ASP:H	13	0.12
(1,1798)	2:B:739:TRP:HB3	2:B:740:ASP:H	14	0.12
(1,1798)	2:B:739:TRP:HB3	2:B:740:ASP:H	18	0.12
(1,1786)	2:B:738:LYS:H	2:B:740:ASP:H	16	0.12
(1,1786)	2:B:738:LYS:H	2:B:740:ASP:H	18	0.12
(1,1767)	2:B:738:LYS:HA	2:B:738:LYS:HD3	11	0.12
(1,1767)	2:B:738:LYS:HA	2:B:738:LYS:HD3	14	0.12
(1,1767)	2:B:738:LYS:HA	2:B:738:LYS:HD3	19	0.12
(1,175)	1:A:969:VAL:H	1:A:970:LEU:HB3	7	0.12
(1,1739)	2:B:736:ARG:H	2:B:736:ARG:HB3	5	0.12
(1,1661)	2:B:730:PHE:HE1	2:B:734:ARG:HD3	11	0.12
(1,1658)	2:B:730:PHE:HB3	2:B:731:GLU:HG3	7	0.12
(1,1625)	2:B:728:ALA:HB1	2:B:731:GLU:HG2	7	0.12
(1,1625)	2:B:728:ALA:HB2	2:B:731:GLU:HG2	7	0.12
(1,1625)	2:B:728:ALA:HB3	2:B:731:GLU:HG2	7	0.12
(1,1623)	2:B:728:ALA:H	2:B:730:PHE:H	1	0.12
(1,1623)	2:B:728:ALA:H	2:B:730:PHE:H	3	0.12
(1,1623)	2:B:728:ALA:H	2:B:730:PHE:H	4	0.12
(1,1623)	2:B:728:ALA:H	2:B:730:PHE:H	8	0.12
(1,1623)	2:B:728:ALA:H	2:B:730:PHE:H	9	0.12
(1,1623)	2:B:728:ALA:H	2:B:730:PHE:H	10	0.12
(1,1623)	2:B:728:ALA:H	2:B:730:PHE:H	11	0.12
(1,1623)	2:B:728:ALA:H	2:B:730:PHE:H	18	0.12
(1,1583)	2:B:725:LYS:HA	2:B:729:LYS:HE3	4	0.12
(1,1581)	2:B:725:LYS:HA	2:B:728:ALA:H	3	0.12
(1,1581)	2:B:725:LYS:HA	2:B:728:ALA:H	6	0.12
(1,1581)	2:B:725:LYS:HA	2:B:728:ALA:H	14	0.12
(1,1565)	2:B:725:LYS:HE3	2:B:725:LYS:HG3	20	0.12
(1,1555)	2:B:724:ARG:HA	2:B:728:ALA:H	3	0.12
(1,155)	1:A:968:TRP:HA	1:A:971:VAL:H	3	0.12
(1,155)	1:A:968:TRP:HA	1:A:971:VAL:H	7	0.12
(1,155)	1:A:968:TRP:HA	1:A:971:VAL:H	8	0.12
(1,1534)	2:B:724:ARG:H	2:B:724:ARG:HB3	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1534)	2:B:724:ARG:H	2:B:724:ARG:HB3	10	0.12
(1,1534)	2:B:724:ARG:H	2:B:724:ARG:HB3	12	0.12
(1,1534)	2:B:724:ARG:H	2:B:724:ARG:HB3	16	0.12
(1,1387)	2:B:717:LEU:H	2:B:719:ILE:H	8	0.12
(1,1387)	2:B:717:LEU:H	2:B:719:ILE:H	11	0.12
(1,1387)	2:B:717:LEU:H	2:B:719:ILE:H	20	0.12
(1,132)	1:A:968:TRP:H	1:A:968:TRP:HB3	1	0.12
(1,1236)	2:B:709:LEU:H	2:B:711:ALA:H	1	0.12
(1,1236)	2:B:709:LEU:H	2:B:711:ALA:H	14	0.12
(1,1235)	2:B:709:LEU:HB3	2:B:710:ALA:HA	20	0.12
(1,120)	1:A:967:TRP:HB3	1:A:968:TRP:HB3	4	0.12
(1,120)	1:A:967:TRP:HB3	1:A:968:TRP:HB3	10	0.12
(1,120)	1:A:967:TRP:HB3	1:A:968:TRP:HB3	15	0.12
(1,1102)	2:B:703:ALA:HA	2:B:706:LEU:HB3	11	0.12
(1,1102)	2:B:703:ALA:HA	2:B:706:LEU:HB3	20	0.12
(1,106)	1:A:967:TRP:H	1:A:967:TRP:HB3	10	0.12
(1,106)	1:A:967:TRP:H	1:A:967:TRP:HB3	16	0.12
(1,104)	1:A:966:ILE:HA	1:A:970:LEU:H	3	0.12
(3,66)	2:B:695:VAL:O	2:B:699:SER:H	17	0.11
(3,52)	1:A:984:VAL:O	1:A:987:MET:H	18	0.11
(3,43)	1:A:981:THR:O	1:A:984:VAL:H	10	0.11
(3,43)	1:A:981:THR:O	1:A:984:VAL:H	14	0.11
(3,288)	2:B:716:LYS:O	2:B:720:THR:H	3	0.11
(3,270)	2:B:710:ALA:O	2:B:714:ILE:H	18	0.11
(3,24)	1:A:974:LEU:O	1:A:978:LEU:H	2	0.11
(3,24)	1:A:974:LEU:O	1:A:978:LEU:H	15	0.11
(3,225)	2:B:695:VAL:O	2:B:699:SER:H	17	0.11
(3,211)	1:A:984:VAL:O	1:A:987:MET:H	18	0.11
(3,202)	1:A:981:THR:O	1:A:984:VAL:H	10	0.11
(3,202)	1:A:981:THR:O	1:A:984:VAL:H	14	0.11
(3,183)	1:A:974:LEU:O	1:A:978:LEU:H	2	0.11
(3,183)	1:A:974:LEU:O	1:A:978:LEU:H	15	0.11
(3,129)	2:B:716:LYS:O	2:B:720:THR:H	3	0.11
(3,111)	2:B:710:ALA:O	2:B:714:ILE:H	18	0.11
(1,990)	2:B:698:LEU:H	2:B:698:LEU:HB3	15	0.11
(1,99)	1:A:966:ILE:HA	1:A:969:VAL:H	10	0.11
(1,99)	1:A:966:ILE:HA	1:A:969:VAL:H	15	0.11
(1,976)	2:B:697:LEU:HB3	2:B:699:SER:H	1	0.11
(1,950)	2:B:696:VAL:H	2:B:696:VAL:HB	4	0.11
(1,950)	2:B:696:VAL:H	2:B:696:VAL:HB	6	0.11
(1,950)	2:B:696:VAL:H	2:B:696:VAL:HB	7	0.11
(1,950)	2:B:696:VAL:H	2:B:696:VAL:HB	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,950)	2:B:696:VAL:H	2:B:696:VAL:HB	12	0.11
(1,950)	2:B:696:VAL:H	2:B:696:VAL:HB	13	0.11
(1,950)	2:B:696:VAL:H	2:B:696:VAL:HB	18	0.11
(1,950)	2:B:696:VAL:H	2:B:696:VAL:HB	19	0.11
(1,90)	1:A:966:ILE:HB	1:A:967:TRP:H	8	0.11
(1,851)	2:B:692:ASP:H	2:B:693:ILE:H	14	0.11
(1,850)	2:B:692:ASP:HA	2:B:693:ILE:H	2	0.11
(1,850)	2:B:692:ASP:HA	2:B:693:ILE:H	18	0.11
(1,849)	2:B:692:ASP:HB3	2:B:693:ILE:H	18	0.11
(1,84)	1:A:966:ILE:H	1:A:966:ILE:HD11	15	0.11
(1,84)	1:A:966:ILE:H	1:A:966:ILE:HD12	15	0.11
(1,84)	1:A:966:ILE:H	1:A:966:ILE:HD13	15	0.11
(1,811)	1:A:1006:GLU:H	1:A:1006:GLU:HB3	8	0.11
(1,811)	1:A:1006:GLU:H	1:A:1006:GLU:HB3	14	0.11
(1,807)	1:A:1005:GLU:H	1:A:1005:GLU:HB3	18	0.11
(1,803)	1:A:1004:ASP:HA	1:A:1005:GLU:H	17	0.11
(1,802)	1:A:1004:ASP:H	1:A:1004:ASP:HB2	7	0.11
(1,802)	1:A:1004:ASP:H	1:A:1004:ASP:HB2	16	0.11
(1,801)	1:A:1004:ASP:H	1:A:1004:ASP:HB3	19	0.11
(1,8)	1:A:961:GLU:H	1:A:961:GLU:HB3	1	0.11
(1,8)	1:A:961:GLU:H	1:A:961:GLU:HB3	10	0.11
(1,8)	1:A:961:GLU:H	1:A:961:GLU:HB3	13	0.11
(1,8)	1:A:961:GLU:H	1:A:961:GLU:HB3	19	0.11
(1,791)	1:A:1002:GLU:H	1:A:1002:GLU:HB3	4	0.11
(1,791)	1:A:1002:GLU:H	1:A:1002:GLU:HB3	5	0.11
(1,791)	1:A:1002:GLU:H	1:A:1002:GLU:HB3	15	0.11
(1,791)	1:A:1002:GLU:H	1:A:1002:GLU:HB3	16	0.11
(1,790)	1:A:1001:GLU:H	1:A:1001:GLU:HB2	9	0.11
(1,750)	1:A:996:ASN:HA	1:A:997:ARG:H	6	0.11
(1,738)	1:A:995:ARG:HA	1:A:996:ASN:H	9	0.11
(1,729)	1:A:995:ARG:H	1:A:995:ARG:HB3	3	0.11
(1,729)	1:A:995:ARG:H	1:A:995:ARG:HB3	9	0.11
(1,725)	1:A:994:LYS:HB3	1:A:995:ARG:HG3	12	0.11
(1,725)	1:A:994:LYS:HB3	1:A:995:ARG:HG3	19	0.11
(1,704)	1:A:994:LYS:H	1:A:994:LYS:HG3	1	0.11
(1,701)	1:A:993:PHE:HA	1:A:996:ASN:H	15	0.11
(1,7)	1:A:960:GLU:HB2	1:A:961:GLU:H	11	0.11
(1,7)	1:A:960:GLU:HB2	1:A:961:GLU:H	20	0.11
(1,697)	1:A:993:PHE:H	1:A:995:ARG:H	18	0.11
(1,693)	1:A:993:PHE:H	1:A:994:LYS:HD3	2	0.11
(1,690)	1:A:993:PHE:HB2	1:A:994:LYS:H	2	0.11
(1,690)	1:A:993:PHE:HB2	1:A:994:LYS:H	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,690)	1:A:993:PHE:HB2	1:A:994:LYS:H	18	0.11
(1,690)	1:A:993:PHE:HB2	1:A:994:LYS:H	19	0.11
(1,684)	1:A:993:PHE:HB3	1:A:993:PHE:H	3	0.11
(1,684)	1:A:993:PHE:HB3	1:A:993:PHE:H	19	0.11
(1,672)	1:A:992:PHE:HB3	1:A:993:PHE:H	6	0.11
(1,647)	1:A:991:GLY:H	1:A:992:PHE:H	3	0.11
(1,647)	1:A:991:GLY:H	1:A:992:PHE:H	12	0.11
(1,647)	1:A:991:GLY:H	1:A:992:PHE:H	19	0.11
(1,638)	1:A:990:VAL:H	1:A:992:PHE:H	7	0.11
(1,611)	1:A:989:LYS:HE3	1:A:993:PHE:HE1	9	0.11
(1,576)	1:A:989:LYS:H	1:A:989:LYS:HD3	4	0.11
(1,576)	1:A:989:LYS:H	1:A:989:LYS:HD3	16	0.11
(1,557)	1:A:988:TRP:H	1:A:988:TRP:HB3	1	0.11
(1,557)	1:A:988:TRP:H	1:A:988:TRP:HB3	4	0.11
(1,557)	1:A:988:TRP:H	1:A:988:TRP:HB3	9	0.11
(1,548)	1:A:987:MET:HA	1:A:990:VAL:H	3	0.11
(1,548)	1:A:987:MET:HA	1:A:990:VAL:H	5	0.11
(1,548)	1:A:987:MET:HA	1:A:990:VAL:H	12	0.11
(1,548)	1:A:987:MET:HA	1:A:990:VAL:H	17	0.11
(1,548)	1:A:987:MET:HA	1:A:990:VAL:H	19	0.11
(1,546)	1:A:987:MET:HA	1:A:989:LYS:H	15	0.11
(1,488)	1:A:985:LEU:H	1:A:987:MET:HG3	10	0.11
(1,451)	1:A:984:VAL:H	1:A:987:MET:H	12	0.11
(1,437)	1:A:984:VAL:H	1:A:984:VAL:HG11	2	0.11
(1,437)	1:A:984:VAL:H	1:A:984:VAL:HG12	2	0.11
(1,437)	1:A:984:VAL:H	1:A:984:VAL:HG13	2	0.11
(1,432)	1:A:983:LEU:HB2	1:A:987:MET:H	1	0.11
(1,432)	1:A:983:LEU:HB2	1:A:987:MET:H	3	0.11
(1,432)	1:A:983:LEU:HB2	1:A:987:MET:H	9	0.11
(1,432)	1:A:983:LEU:HB2	1:A:987:MET:H	12	0.11
(1,432)	1:A:983:LEU:HB2	1:A:987:MET:H	17	0.11
(1,4162)	1:A:988:TRP:HE1	2:B:719:ILE:HB	11	0.11
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG21	8	0.11
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG22	8	0.11
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG23	8	0.11
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG21	10	0.11
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG22	10	0.11
(1,4160)	1:A:988:TRP:H	2:B:719:ILE:HG23	10	0.11
(1,4157)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	2	0.11
(1,4156)	1:A:988:TRP:HE1	2:B:715:TRP:HD1	9	0.11
(1,4156)	1:A:988:TRP:HE1	2:B:715:TRP:HD1	10	0.11
(1,4151)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4101)	1:A:973:VAL:H	2:B:700:VAL:HA	2	0.11
(1,4101)	1:A:973:VAL:H	2:B:700:VAL:HA	10	0.11
(1,4093)	1:A:969:VAL:HA	2:B:700:VAL:H	12	0.11
(1,4093)	1:A:969:VAL:HA	2:B:700:VAL:H	20	0.11
(1,4085)	1:A:968:TRP:HE1	2:B:693:ILE:HB	5	0.11
(1,408)	1:A:983:LEU:H	1:A:983:LEU:HB3	2	0.11
(1,408)	1:A:983:LEU:H	1:A:983:LEU:HB3	12	0.11
(1,4079)	2:B:760:ARG:HD3	2:B:760:ARG:HB2	1	0.11
(1,4070)	2:B:759:TYR:H	2:B:759:TYR:HB2	20	0.11
(1,4066)	2:B:758:THR:HB	2:B:759:TYR:H	11	0.11
(1,4049)	2:B:756:ASN:H	2:B:757:ILE:HD11	3	0.11
(1,4049)	2:B:756:ASN:H	2:B:757:ILE:HD12	3	0.11
(1,4049)	2:B:756:ASN:H	2:B:757:ILE:HD13	3	0.11
(1,4049)	2:B:756:ASN:H	2:B:757:ILE:HD11	4	0.11
(1,4049)	2:B:756:ASN:H	2:B:757:ILE:HD12	4	0.11
(1,4049)	2:B:756:ASN:H	2:B:757:ILE:HD13	4	0.11
(1,4040)	2:B:756:ASN:H	2:B:756:ASN:HB2	19	0.11
(1,4034)	2:B:755:THR:H	2:B:755:THR:HB	19	0.11
(1,4032)	2:B:754:PHE:HB3	2:B:755:THR:H	6	0.11
(1,4032)	2:B:754:PHE:HB3	2:B:755:THR:H	15	0.11
(1,4032)	2:B:754:PHE:HB3	2:B:755:THR:H	20	0.11
(1,4027)	2:B:753:THR:HA	2:B:754:PHE:H	7	0.11
(1,4027)	2:B:753:THR:HA	2:B:754:PHE:H	10	0.11
(1,4027)	2:B:753:THR:HA	2:B:754:PHE:H	19	0.11
(1,4013)	2:B:751:THR:H	2:B:752:SER:H	20	0.11
(1,4000)	2:B:749:GLU:H	2:B:749:GLU:HG3	8	0.11
(1,4000)	2:B:749:GLU:H	2:B:749:GLU:HG3	11	0.11
(1,3968)	2:B:747:TYR:H	2:B:747:TYR:HB3	2	0.11
(1,3968)	2:B:747:TYR:H	2:B:747:TYR:HB3	14	0.11
(1,3954)	2:B:746:LEU:H	2:B:746:LEU:HB2	12	0.11
(1,395)	1:A:982:ILE:HA	1:A:985:LEU:HB3	6	0.11
(1,395)	1:A:982:ILE:HA	1:A:985:LEU:HB3	15	0.11
(1,395)	1:A:982:ILE:HA	1:A:985:LEU:HB3	16	0.11
(1,3935)	2:B:744:ASN:HA	2:B:747:TYR:H	16	0.11
(1,3921)	2:B:744:ASN:H	2:B:744:ASN:HB2	2	0.11
(1,3921)	2:B:744:ASN:H	2:B:744:ASN:HB2	8	0.11
(1,3897)	2:B:741:THR:HA	2:B:744:ASN:H	2	0.11
(1,3897)	2:B:741:THR:HA	2:B:744:ASN:H	5	0.11
(1,3897)	2:B:741:THR:HA	2:B:744:ASN:H	14	0.11
(1,3897)	2:B:741:THR:HA	2:B:744:ASN:H	15	0.11
(1,3894)	2:B:741:THR:HB	2:B:742:ALA:H	1	0.11
(1,3888)	2:B:740:ASP:HA	2:B:741:THR:H	16	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3887)	2:B:740:ASP:HB3	2:B:741:THR:H	1	0.11
(1,3881)	2:B:739:TRP:HB3	2:B:740:ASP:H	8	0.11
(1,3881)	2:B:739:TRP:HB3	2:B:740:ASP:H	9	0.11
(1,3881)	2:B:739:TRP:HB3	2:B:740:ASP:H	10	0.11
(1,3881)	2:B:739:TRP:HB3	2:B:740:ASP:H	19	0.11
(1,3881)	2:B:739:TRP:HB3	2:B:740:ASP:H	20	0.11
(1,3872)	2:B:738:LYS:HA	2:B:741:THR:H	19	0.11
(1,3869)	2:B:738:LYS:H	2:B:740:ASP:H	13	0.11
(1,3857)	2:B:738:LYS:HE3	2:B:738:LYS:HB3	2	0.11
(1,3857)	2:B:738:LYS:HE3	2:B:738:LYS:HB3	5	0.11
(1,3822)	2:B:736:ARG:H	2:B:736:ARG:HB3	11	0.11
(1,3745)	2:B:730:PHE:HE1	2:B:734:ARG:HD2	13	0.11
(1,3745)	2:B:730:PHE:HE1	2:B:734:ARG:HD2	15	0.11
(1,3745)	2:B:730:PHE:HE1	2:B:734:ARG:HD2	19	0.11
(1,3742)	2:B:730:PHE:HB3	2:B:731:GLU:HG2	19	0.11
(1,3706)	2:B:728:ALA:H	2:B:730:PHE:H	13	0.11
(1,3706)	2:B:728:ALA:H	2:B:730:PHE:H	14	0.11
(1,3706)	2:B:728:ALA:H	2:B:730:PHE:H	15	0.11
(1,3706)	2:B:728:ALA:H	2:B:730:PHE:H	17	0.11
(1,3664)	2:B:725:LYS:HA	2:B:728:ALA:H	2	0.11
(1,3664)	2:B:725:LYS:HA	2:B:728:ALA:H	11	0.11
(1,3664)	2:B:725:LYS:HA	2:B:728:ALA:H	12	0.11
(1,3655)	2:B:725:LYS:HD3	2:B:725:LYS:HB3	1	0.11
(1,3655)	2:B:725:LYS:HD3	2:B:725:LYS:HB3	2	0.11
(1,3655)	2:B:725:LYS:HD3	2:B:725:LYS:HB3	5	0.11
(1,3655)	2:B:725:LYS:HD3	2:B:725:LYS:HB3	6	0.11
(1,3655)	2:B:725:LYS:HD3	2:B:725:LYS:HB3	8	0.11
(1,3655)	2:B:725:LYS:HD3	2:B:725:LYS:HB3	9	0.11
(1,3655)	2:B:725:LYS:HD3	2:B:725:LYS:HB3	10	0.11
(1,3655)	2:B:725:LYS:HD3	2:B:725:LYS:HB3	13	0.11
(1,3655)	2:B:725:LYS:HD3	2:B:725:LYS:HB3	14	0.11
(1,3655)	2:B:725:LYS:HD3	2:B:725:LYS:HB3	15	0.11
(1,3648)	2:B:725:LYS:HE3	2:B:725:LYS:HG3	13	0.11
(1,3648)	2:B:725:LYS:HE3	2:B:725:LYS:HG3	18	0.11
(1,3638)	2:B:724:ARG:HA	2:B:728:ALA:H	4	0.11
(1,3638)	2:B:724:ARG:HA	2:B:728:ALA:H	5	0.11
(1,3638)	2:B:724:ARG:HA	2:B:728:ALA:H	12	0.11
(1,3620)	2:B:724:ARG:HD3	2:B:724:ARG:HB3	13	0.11
(1,3617)	2:B:724:ARG:H	2:B:724:ARG:HB3	3	0.11
(1,3617)	2:B:724:ARG:H	2:B:724:ARG:HB3	9	0.11
(1,3617)	2:B:724:ARG:H	2:B:724:ARG:HB3	17	0.11
(1,3579)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3553)	2:B:720:THR:HG21	2:B:724:ARG:HD3	4	0.11
(1,3553)	2:B:720:THR:HG22	2:B:724:ARG:HD3	4	0.11
(1,3553)	2:B:720:THR:HG23	2:B:724:ARG:HD3	4	0.11
(1,3553)	2:B:720:THR:HG21	2:B:724:ARG:HD3	8	0.11
(1,3553)	2:B:720:THR:HG22	2:B:724:ARG:HD3	8	0.11
(1,3553)	2:B:720:THR:HG23	2:B:724:ARG:HD3	8	0.11
(1,3553)	2:B:720:THR:HG21	2:B:724:ARG:HD3	18	0.11
(1,3553)	2:B:720:THR:HG22	2:B:724:ARG:HD3	18	0.11
(1,3553)	2:B:720:THR:HG23	2:B:724:ARG:HD3	18	0.11
(1,3508)	2:B:718:LEU:HD21	2:B:721:ILE:HB	19	0.11
(1,3508)	2:B:718:LEU:HD22	2:B:721:ILE:HB	19	0.11
(1,3508)	2:B:718:LEU:HD23	2:B:721:ILE:HB	19	0.11
(1,3495)	2:B:718:LEU:HB3	2:B:719:ILE:HG12	9	0.11
(1,3495)	2:B:718:LEU:HB3	2:B:719:ILE:HG12	16	0.11
(1,3470)	2:B:717:LEU:H	2:B:719:ILE:H	9	0.11
(1,3470)	2:B:717:LEU:H	2:B:719:ILE:H	12	0.11
(1,3470)	2:B:717:LEU:H	2:B:719:ILE:H	13	0.11
(1,3470)	2:B:717:LEU:H	2:B:719:ILE:H	19	0.11
(1,3356)	2:B:712:LEU:HB3	2:B:713:LEU:HB2	20	0.11
(1,321)	1:A:977:LEU:HB2	1:A:981:THR:H	7	0.11
(1,3185)	2:B:703:ALA:HA	2:B:706:LEU:HB3	1	0.11
(1,3185)	2:B:703:ALA:HA	2:B:706:LEU:HB3	2	0.11
(1,3185)	2:B:703:ALA:HA	2:B:706:LEU:HB3	5	0.11
(1,3185)	2:B:703:ALA:HA	2:B:706:LEU:HB3	6	0.11
(1,3185)	2:B:703:ALA:HA	2:B:706:LEU:HB3	8	0.11
(1,3185)	2:B:703:ALA:HA	2:B:706:LEU:HB3	10	0.11
(1,3185)	2:B:703:ALA:HA	2:B:706:LEU:HB3	13	0.11
(1,3185)	2:B:703:ALA:HA	2:B:706:LEU:HB3	19	0.11
(1,3148)	2:B:701:MET:HG3	2:B:704:ILE:HG13	2	0.11
(1,3073)	2:B:698:LEU:H	2:B:698:LEU:HB3	15	0.11
(1,3059)	2:B:697:LEU:HB3	2:B:699:SER:H	1	0.11
(1,3033)	2:B:696:VAL:H	2:B:696:VAL:HB	4	0.11
(1,3033)	2:B:696:VAL:H	2:B:696:VAL:HB	6	0.11
(1,3033)	2:B:696:VAL:H	2:B:696:VAL:HB	7	0.11
(1,3033)	2:B:696:VAL:H	2:B:696:VAL:HB	10	0.11
(1,3033)	2:B:696:VAL:H	2:B:696:VAL:HB	12	0.11
(1,3033)	2:B:696:VAL:H	2:B:696:VAL:HB	13	0.11
(1,3033)	2:B:696:VAL:H	2:B:696:VAL:HB	18	0.11
(1,3033)	2:B:696:VAL:H	2:B:696:VAL:HB	19	0.11
(1,2934)	2:B:692:ASP:H	2:B:693:ILE:H	14	0.11
(1,2933)	2:B:692:ASP:HA	2:B:693:ILE:H	2	0.11
(1,2933)	2:B:692:ASP:HA	2:B:693:ILE:H	18	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2932)	2:B:692:ASP:HB3	2:B:693:ILE:H	18	0.11
(1,2894)	1:A:1006:GLU:H	1:A:1006:GLU:HB3	8	0.11
(1,2894)	1:A:1006:GLU:H	1:A:1006:GLU:HB3	14	0.11
(1,2890)	1:A:1005:GLU:H	1:A:1005:GLU:HB3	18	0.11
(1,2886)	1:A:1004:ASP:HA	1:A:1005:GLU:H	17	0.11
(1,2885)	1:A:1004:ASP:H	1:A:1004:ASP:HB2	7	0.11
(1,2885)	1:A:1004:ASP:H	1:A:1004:ASP:HB2	16	0.11
(1,2884)	1:A:1004:ASP:H	1:A:1004:ASP:HB3	19	0.11
(1,2874)	1:A:1002:GLU:H	1:A:1002:GLU:HB3	4	0.11
(1,2874)	1:A:1002:GLU:H	1:A:1002:GLU:HB3	5	0.11
(1,2874)	1:A:1002:GLU:H	1:A:1002:GLU:HB3	15	0.11
(1,2874)	1:A:1002:GLU:H	1:A:1002:GLU:HB3	16	0.11
(1,2873)	1:A:1001:GLU:H	1:A:1001:GLU:HB2	9	0.11
(1,2833)	1:A:996:ASN:HA	1:A:997:ARG:H	6	0.11
(1,2821)	1:A:995:ARG:HA	1:A:996:ASN:H	9	0.11
(1,2812)	1:A:995:ARG:H	1:A:995:ARG:HB3	3	0.11
(1,2812)	1:A:995:ARG:H	1:A:995:ARG:HB3	9	0.11
(1,2808)	1:A:994:LYS:HB3	1:A:995:ARG:HG3	12	0.11
(1,2808)	1:A:994:LYS:HB3	1:A:995:ARG:HG3	19	0.11
(1,2787)	1:A:994:LYS:H	1:A:994:LYS:HG3	1	0.11
(1,2784)	1:A:993:PHE:HA	1:A:996:ASN:H	15	0.11
(1,2780)	1:A:993:PHE:H	1:A:995:ARG:H	18	0.11
(1,2776)	1:A:993:PHE:H	1:A:994:LYS:HD3	2	0.11
(1,2773)	1:A:993:PHE:HB2	1:A:994:LYS:H	2	0.11
(1,2773)	1:A:993:PHE:HB2	1:A:994:LYS:H	6	0.11
(1,2773)	1:A:993:PHE:HB2	1:A:994:LYS:H	18	0.11
(1,2773)	1:A:993:PHE:HB2	1:A:994:LYS:H	19	0.11
(1,2767)	1:A:993:PHE:HB3	1:A:993:PHE:H	3	0.11
(1,2767)	1:A:993:PHE:HB3	1:A:993:PHE:H	19	0.11
(1,2755)	1:A:992:PHE:HB3	1:A:993:PHE:H	6	0.11
(1,275)	1:A:974:LEU:HB2	1:A:975:GLY:H	9	0.11
(1,275)	1:A:974:LEU:HB2	1:A:975:GLY:H	12	0.11
(1,2730)	1:A:991:GLY:H	1:A:992:PHE:H	3	0.11
(1,2730)	1:A:991:GLY:H	1:A:992:PHE:H	12	0.11
(1,2730)	1:A:991:GLY:H	1:A:992:PHE:H	19	0.11
(1,2721)	1:A:990:VAL:H	1:A:992:PHE:H	7	0.11
(1,2694)	1:A:989:LYS:HE3	1:A:993:PHE:HE1	9	0.11
(1,2659)	1:A:989:LYS:H	1:A:989:LYS:HD3	4	0.11
(1,2659)	1:A:989:LYS:H	1:A:989:LYS:HD3	16	0.11
(1,2640)	1:A:988:TRP:H	1:A:988:TRP:HB3	1	0.11
(1,2640)	1:A:988:TRP:H	1:A:988:TRP:HB3	4	0.11
(1,2640)	1:A:988:TRP:H	1:A:988:TRP:HB3	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2631)	1:A:987:MET:HA	1:A:990:VAL:H	3	0.11
(1,2631)	1:A:987:MET:HA	1:A:990:VAL:H	5	0.11
(1,2631)	1:A:987:MET:HA	1:A:990:VAL:H	12	0.11
(1,2631)	1:A:987:MET:HA	1:A:990:VAL:H	17	0.11
(1,2631)	1:A:987:MET:HA	1:A:990:VAL:H	19	0.11
(1,2629)	1:A:987:MET:HA	1:A:989:LYS:H	15	0.11
(1,2571)	1:A:985:LEU:H	1:A:987:MET:HG3	10	0.11
(1,2534)	1:A:984:VAL:H	1:A:987:MET:H	12	0.11
(1,2520)	1:A:984:VAL:H	1:A:984:VAL:HG11	2	0.11
(1,2520)	1:A:984:VAL:H	1:A:984:VAL:HG12	2	0.11
(1,2520)	1:A:984:VAL:H	1:A:984:VAL:HG13	2	0.11
(1,2515)	1:A:983:LEU:HB2	1:A:987:MET:H	1	0.11
(1,2515)	1:A:983:LEU:HB2	1:A:987:MET:H	3	0.11
(1,2515)	1:A:983:LEU:HB2	1:A:987:MET:H	9	0.11
(1,2515)	1:A:983:LEU:HB2	1:A:987:MET:H	12	0.11
(1,2515)	1:A:983:LEU:HB2	1:A:987:MET:H	17	0.11
(1,2491)	1:A:983:LEU:H	1:A:983:LEU:HB3	2	0.11
(1,2491)	1:A:983:LEU:H	1:A:983:LEU:HB3	12	0.11
(1,2478)	1:A:982:ILE:HA	1:A:985:LEU:HB3	6	0.11
(1,2478)	1:A:982:ILE:HA	1:A:985:LEU:HB3	15	0.11
(1,2478)	1:A:982:ILE:HA	1:A:985:LEU:HB3	16	0.11
(1,2404)	1:A:977:LEU:HB2	1:A:981:THR:H	7	0.11
(1,2358)	1:A:974:LEU:HB2	1:A:975:GLY:H	9	0.11
(1,2358)	1:A:974:LEU:HB2	1:A:975:GLY:H	12	0.11
(1,2313)	1:A:971:VAL:HA	1:A:974:LEU:HB3	2	0.11
(1,2313)	1:A:971:VAL:HA	1:A:974:LEU:HB3	15	0.11
(1,2313)	1:A:971:VAL:HA	1:A:974:LEU:HB3	17	0.11
(1,2313)	1:A:971:VAL:HA	1:A:974:LEU:HB3	20	0.11
(1,2308)	1:A:971:VAL:H	1:A:973:VAL:H	16	0.11
(1,230)	1:A:971:VAL:HA	1:A:974:LEU:HB3	2	0.11
(1,230)	1:A:971:VAL:HA	1:A:974:LEU:HB3	15	0.11
(1,230)	1:A:971:VAL:HA	1:A:974:LEU:HB3	17	0.11
(1,230)	1:A:971:VAL:HA	1:A:974:LEU:HB3	20	0.11
(1,2291)	1:A:970:LEU:HB3	1:A:974:LEU:H	12	0.11
(1,225)	1:A:971:VAL:H	1:A:973:VAL:H	16	0.11
(1,2238)	1:A:968:TRP:HA	1:A:971:VAL:H	1	0.11
(1,2215)	1:A:968:TRP:H	1:A:968:TRP:HB3	12	0.11
(1,2203)	1:A:967:TRP:HB3	1:A:968:TRP:HB3	6	0.11
(1,2203)	1:A:967:TRP:HB3	1:A:968:TRP:HB3	11	0.11
(1,2203)	1:A:967:TRP:HB3	1:A:968:TRP:HB3	17	0.11
(1,2194)	1:A:967:TRP:HB3	1:A:967:TRP:HZ3	14	0.11
(1,2187)	1:A:966:ILE:HA	1:A:970:LEU:H	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2182)	1:A:966:ILE:HA	1:A:969:VAL:H	10	0.11
(1,2182)	1:A:966:ILE:HA	1:A:969:VAL:H	15	0.11
(1,2173)	1:A:966:ILE:HB	1:A:967:TRP:H	8	0.11
(1,2167)	1:A:966:ILE:H	1:A:966:ILE:HD11	15	0.11
(1,2167)	1:A:966:ILE:H	1:A:966:ILE:HD12	15	0.11
(1,2167)	1:A:966:ILE:H	1:A:966:ILE:HD13	15	0.11
(1,2094)	1:A:961:GLU:H	1:A:962:ARG:H	3	0.11
(1,2091)	1:A:961:GLU:H	1:A:961:GLU:HB3	1	0.11
(1,2091)	1:A:961:GLU:H	1:A:961:GLU:HB3	10	0.11
(1,2091)	1:A:961:GLU:H	1:A:961:GLU:HB3	13	0.11
(1,2091)	1:A:961:GLU:H	1:A:961:GLU:HB3	19	0.11
(1,2090)	1:A:960:GLU:HB2	1:A:961:GLU:H	11	0.11
(1,2090)	1:A:960:GLU:HB2	1:A:961:GLU:H	20	0.11
(1,208)	1:A:970:LEU:HB3	1:A:974:LEU:H	12	0.11
(1,2079)	1:A:988:TRP:HE1	2:B:719:ILE:HB	11	0.11
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG21	8	0.11
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG22	8	0.11
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG23	8	0.11
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG21	10	0.11
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG22	10	0.11
(1,2077)	1:A:988:TRP:H	2:B:719:ILE:HG23	10	0.11
(1,2074)	1:A:988:TRP:HE1	2:B:715:TRP:HH2	2	0.11
(1,2073)	1:A:988:TRP:HE1	2:B:715:TRP:HD1	9	0.11
(1,2073)	1:A:988:TRP:HE1	2:B:715:TRP:HD1	10	0.11
(1,2068)	1:A:985:LEU:HB2	2:B:715:TRP:HE1	13	0.11
(1,2018)	1:A:973:VAL:H	2:B:700:VAL:HA	2	0.11
(1,2018)	1:A:973:VAL:H	2:B:700:VAL:HA	10	0.11
(1,2010)	1:A:969:VAL:HA	2:B:700:VAL:H	12	0.11
(1,2010)	1:A:969:VAL:HA	2:B:700:VAL:H	20	0.11
(1,2002)	1:A:968:TRP:HE1	2:B:693:ILE:HB	5	0.11
(1,1996)	2:B:760:ARG:HD3	2:B:760:ARG:HB2	1	0.11
(1,1987)	2:B:759:TYR:H	2:B:759:TYR:HB2	20	0.11
(1,1983)	2:B:758:THR:HB	2:B:759:TYR:H	11	0.11
(1,1966)	2:B:756:ASN:H	2:B:757:ILE:HD11	3	0.11
(1,1966)	2:B:756:ASN:H	2:B:757:ILE:HD12	3	0.11
(1,1966)	2:B:756:ASN:H	2:B:757:ILE:HD13	3	0.11
(1,1966)	2:B:756:ASN:H	2:B:757:ILE:HD11	4	0.11
(1,1966)	2:B:756:ASN:H	2:B:757:ILE:HD12	4	0.11
(1,1966)	2:B:756:ASN:H	2:B:757:ILE:HD13	4	0.11
(1,1957)	2:B:756:ASN:H	2:B:756:ASN:HB2	19	0.11
(1,1951)	2:B:755:THR:H	2:B:755:THR:HB	19	0.11
(1,1949)	2:B:754:PHE:HB3	2:B:755:THR:H	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1949)	2:B:754:PHE:HB3	2:B:755:THR:H	15	0.11
(1,1949)	2:B:754:PHE:HB3	2:B:755:THR:H	20	0.11
(1,1944)	2:B:753:THR:HA	2:B:754:PHE:H	7	0.11
(1,1944)	2:B:753:THR:HA	2:B:754:PHE:H	10	0.11
(1,1944)	2:B:753:THR:HA	2:B:754:PHE:H	19	0.11
(1,1930)	2:B:751:THR:H	2:B:752:SER:H	20	0.11
(1,1917)	2:B:749:GLU:H	2:B:749:GLU:HG3	8	0.11
(1,1917)	2:B:749:GLU:H	2:B:749:GLU:HG3	11	0.11
(1,1885)	2:B:747:TYR:H	2:B:747:TYR:HB3	2	0.11
(1,1885)	2:B:747:TYR:H	2:B:747:TYR:HB3	14	0.11
(1,1871)	2:B:746:LEU:H	2:B:746:LEU:HB2	12	0.11
(1,1852)	2:B:744:ASN:HA	2:B:747:TYR:H	16	0.11
(1,1838)	2:B:744:ASN:H	2:B:744:ASN:HB2	2	0.11
(1,1838)	2:B:744:ASN:H	2:B:744:ASN:HB2	8	0.11
(1,1814)	2:B:741:THR:HA	2:B:744:ASN:H	2	0.11
(1,1814)	2:B:741:THR:HA	2:B:744:ASN:H	5	0.11
(1,1814)	2:B:741:THR:HA	2:B:744:ASN:H	14	0.11
(1,1814)	2:B:741:THR:HA	2:B:744:ASN:H	15	0.11
(1,1811)	2:B:741:THR:HB	2:B:742:ALA:H	1	0.11
(1,1805)	2:B:740:ASP:HA	2:B:741:THR:H	16	0.11
(1,1804)	2:B:740:ASP:HB3	2:B:741:THR:H	1	0.11
(1,1798)	2:B:739:TRP:HB3	2:B:740:ASP:H	8	0.11
(1,1798)	2:B:739:TRP:HB3	2:B:740:ASP:H	9	0.11
(1,1798)	2:B:739:TRP:HB3	2:B:740:ASP:H	10	0.11
(1,1798)	2:B:739:TRP:HB3	2:B:740:ASP:H	19	0.11
(1,1798)	2:B:739:TRP:HB3	2:B:740:ASP:H	20	0.11
(1,1789)	2:B:738:LYS:HA	2:B:741:THR:H	19	0.11
(1,1786)	2:B:738:LYS:H	2:B:740:ASP:H	13	0.11
(1,1774)	2:B:738:LYS:HE3	2:B:738:LYS:HB3	2	0.11
(1,1774)	2:B:738:LYS:HE3	2:B:738:LYS:HB3	5	0.11
(1,1739)	2:B:736:ARG:H	2:B:736:ARG:HB3	11	0.11
(1,1662)	2:B:730:PHE:HE1	2:B:734:ARG:HD2	13	0.11
(1,1662)	2:B:730:PHE:HE1	2:B:734:ARG:HD2	15	0.11
(1,1662)	2:B:730:PHE:HE1	2:B:734:ARG:HD2	19	0.11
(1,1659)	2:B:730:PHE:HB3	2:B:731:GLU:HG2	19	0.11
(1,1623)	2:B:728:ALA:H	2:B:730:PHE:H	13	0.11
(1,1623)	2:B:728:ALA:H	2:B:730:PHE:H	14	0.11
(1,1623)	2:B:728:ALA:H	2:B:730:PHE:H	15	0.11
(1,1623)	2:B:728:ALA:H	2:B:730:PHE:H	17	0.11
(1,1581)	2:B:725:LYS:HA	2:B:728:ALA:H	2	0.11
(1,1581)	2:B:725:LYS:HA	2:B:728:ALA:H	11	0.11
(1,1581)	2:B:725:LYS:HA	2:B:728:ALA:H	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1572)	2:B:725:LYS:HD3	2:B:725:LYS:HB3	1	0.11
(1,1572)	2:B:725:LYS:HD3	2:B:725:LYS:HB3	2	0.11
(1,1572)	2:B:725:LYS:HD3	2:B:725:LYS:HB3	5	0.11
(1,1572)	2:B:725:LYS:HD3	2:B:725:LYS:HB3	6	0.11
(1,1572)	2:B:725:LYS:HD3	2:B:725:LYS:HB3	8	0.11
(1,1572)	2:B:725:LYS:HD3	2:B:725:LYS:HB3	9	0.11
(1,1572)	2:B:725:LYS:HD3	2:B:725:LYS:HB3	10	0.11
(1,1572)	2:B:725:LYS:HD3	2:B:725:LYS:HB3	13	0.11
(1,1572)	2:B:725:LYS:HD3	2:B:725:LYS:HB3	14	0.11
(1,1572)	2:B:725:LYS:HD3	2:B:725:LYS:HB3	15	0.11
(1,1565)	2:B:725:LYS:HE3	2:B:725:LYS:HG3	13	0.11
(1,1565)	2:B:725:LYS:HE3	2:B:725:LYS:HG3	18	0.11
(1,1555)	2:B:724:ARG:HA	2:B:728:ALA:H	4	0.11
(1,1555)	2:B:724:ARG:HA	2:B:728:ALA:H	5	0.11
(1,1555)	2:B:724:ARG:HA	2:B:728:ALA:H	12	0.11
(1,155)	1:A:968:TRP:HA	1:A:971:VAL:H	1	0.11
(1,1537)	2:B:724:ARG:HD3	2:B:724:ARG:HB3	13	0.11
(1,1534)	2:B:724:ARG:H	2:B:724:ARG:HB3	3	0.11
(1,1534)	2:B:724:ARG:H	2:B:724:ARG:HB3	9	0.11
(1,1534)	2:B:724:ARG:H	2:B:724:ARG:HB3	17	0.11
(1,1496)	2:B:721:ILE:HG12	2:B:724:ARG:HG3	8	0.11
(1,1470)	2:B:720:THR:HG21	2:B:724:ARG:HD3	4	0.11
(1,1470)	2:B:720:THR:HG22	2:B:724:ARG:HD3	4	0.11
(1,1470)	2:B:720:THR:HG23	2:B:724:ARG:HD3	4	0.11
(1,1470)	2:B:720:THR:HG21	2:B:724:ARG:HD3	8	0.11
(1,1470)	2:B:720:THR:HG22	2:B:724:ARG:HD3	8	0.11
(1,1470)	2:B:720:THR:HG23	2:B:724:ARG:HD3	8	0.11
(1,1470)	2:B:720:THR:HG21	2:B:724:ARG:HD3	18	0.11
(1,1470)	2:B:720:THR:HG22	2:B:724:ARG:HD3	18	0.11
(1,1470)	2:B:720:THR:HG23	2:B:724:ARG:HD3	18	0.11
(1,1425)	2:B:718:LEU:HD21	2:B:721:ILE:HB	19	0.11
(1,1425)	2:B:718:LEU:HD22	2:B:721:ILE:HB	19	0.11
(1,1425)	2:B:718:LEU:HD23	2:B:721:ILE:HB	19	0.11
(1,1412)	2:B:718:LEU:HB3	2:B:719:ILE:HG12	9	0.11
(1,1412)	2:B:718:LEU:HB3	2:B:719:ILE:HG12	16	0.11
(1,1387)	2:B:717:LEU:H	2:B:719:ILE:H	9	0.11
(1,1387)	2:B:717:LEU:H	2:B:719:ILE:H	12	0.11
(1,1387)	2:B:717:LEU:H	2:B:719:ILE:H	13	0.11
(1,1387)	2:B:717:LEU:H	2:B:719:ILE:H	19	0.11
(1,132)	1:A:968:TRP:H	1:A:968:TRP:HB3	12	0.11
(1,1273)	2:B:712:LEU:HB3	2:B:713:LEU:HB2	20	0.11
(1,120)	1:A:967:TRP:HB3	1:A:968:TRP:HB3	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,120)	1:A:967:TRP:HB3	1:A:968:TRP:HB3	11	0.11
(1,120)	1:A:967:TRP:HB3	1:A:968:TRP:HB3	17	0.11
(1,111)	1:A:967:TRP:HB3	1:A:967:TRP:HZ3	14	0.11
(1,1102)	2:B:703:ALA:HA	2:B:706:LEU:HB3	1	0.11
(1,1102)	2:B:703:ALA:HA	2:B:706:LEU:HB3	2	0.11
(1,1102)	2:B:703:ALA:HA	2:B:706:LEU:HB3	5	0.11
(1,1102)	2:B:703:ALA:HA	2:B:706:LEU:HB3	6	0.11
(1,1102)	2:B:703:ALA:HA	2:B:706:LEU:HB3	8	0.11
(1,1102)	2:B:703:ALA:HA	2:B:706:LEU:HB3	10	0.11
(1,1102)	2:B:703:ALA:HA	2:B:706:LEU:HB3	13	0.11
(1,1102)	2:B:703:ALA:HA	2:B:706:LEU:HB3	19	0.11
(1,11)	1:A:961:GLU:H	1:A:962:ARG:H	3	0.11
(1,1065)	2:B:701:MET:HG3	2:B:704:ILE:HG13	2	0.11
(1,104)	1:A:966:ILE:HA	1:A:970:LEU:H	6	0.11

10 Dihedral-angle violation analysis (i)

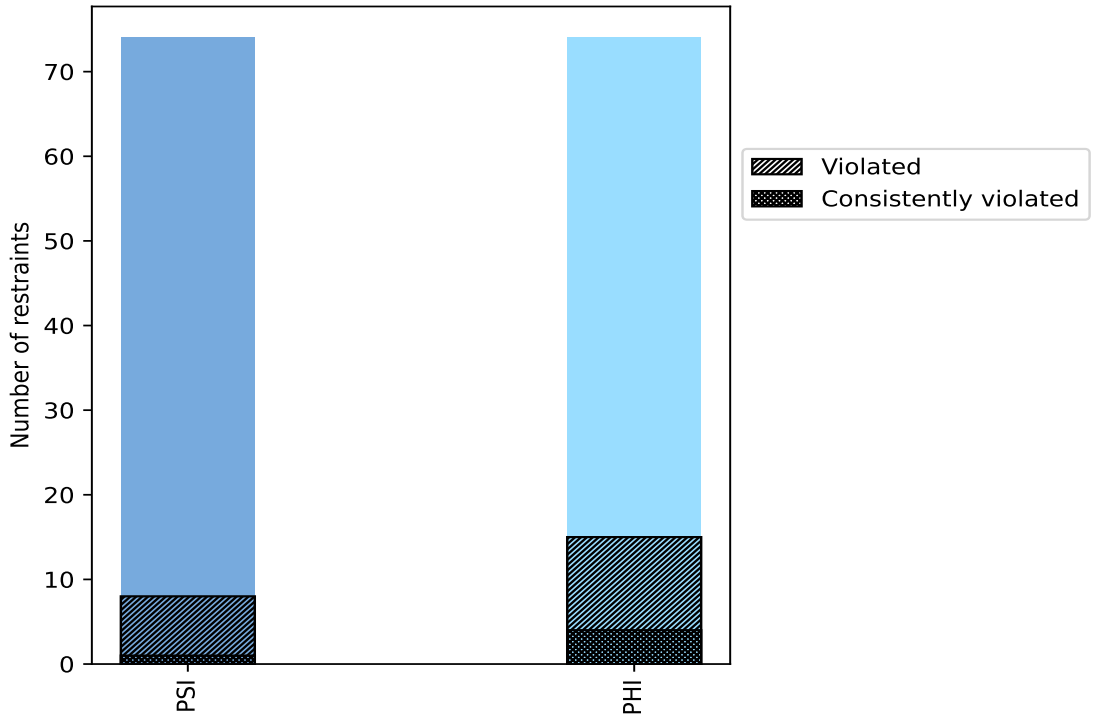
10.1 Summary of dihedral-angle violations (i)

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	74	50.0	8	10.8	5.4	1	1.4	0.7
PHI	74	50.0	15	20.3	10.1	4	5.4	2.7
Total	148	100.0	23	15.5	15.5	5	3.4	3.4

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

10.1.1 Bar chart : Distribution of dihedral-angles and violations (i)



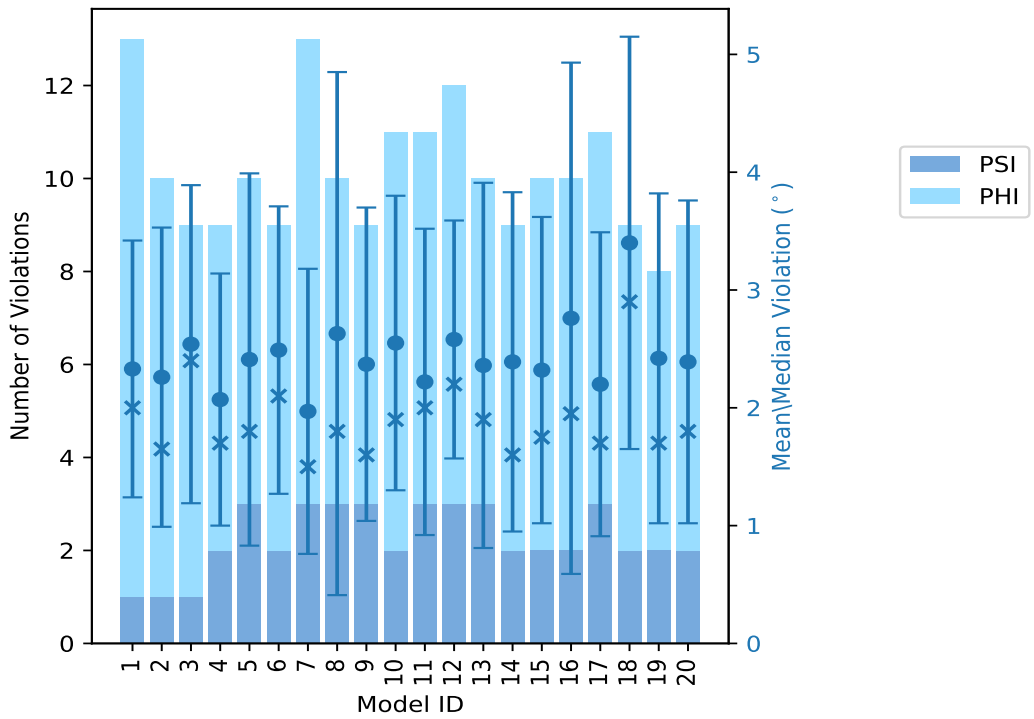
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	1	12	13	2.33	5.0	1.09	2.0
2	1	9	10	2.26	5.6	1.27	1.65
3	1	8	9	2.54	6.0	1.35	2.4
4	2	7	9	2.07	4.9	1.07	1.7
5	3	7	10	2.41	6.3	1.58	1.8
6	2	7	9	2.49	5.3	1.22	2.1
7	3	10	13	1.97	5.6	1.21	1.5
8	3	7	10	2.63	9.1	2.22	1.8
9	3	6	9	2.37	5.5	1.33	1.6
10	2	9	11	2.55	5.4	1.25	1.9
11	3	8	11	2.22	5.8	1.3	2.0
12	3	9	12	2.58	5.1	1.01	2.2
13	3	7	10	2.36	6.8	1.55	1.9
14	2	7	9	2.39	6.0	1.44	1.6
15	2	8	10	2.32	5.8	1.3	1.75
16	2	8	10	2.76	8.8	2.17	1.95
17	3	8	11	2.2	5.8	1.29	1.7
18	2	7	9	3.4	7.9	1.75	2.9
19	2	6	8	2.42	5.9	1.4	1.7
20	2	7	9	2.39	5.9	1.37	1.8

10.2.1 Bar graph : Dihedral 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

10.3 Dihedral-angle violation statistics for the ensemble (i)

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

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

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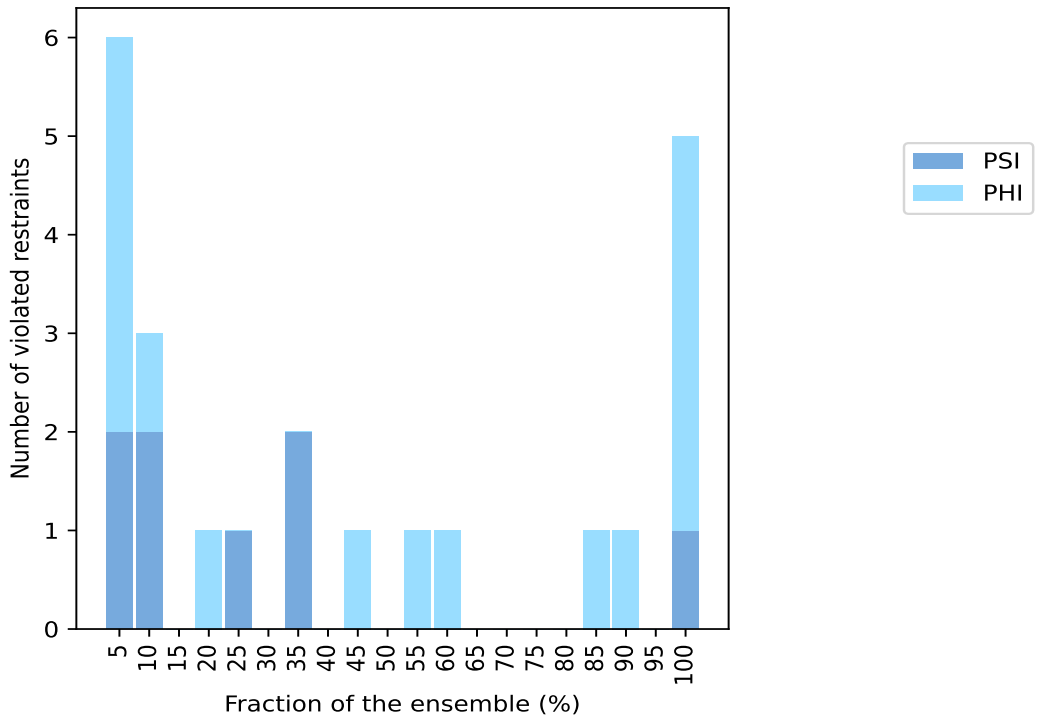
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
0	1	1	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
0	1	1	17	85.0
0	1	1	18	90.0
0	0	0	19	95.0
1	4	5	20	100.0

[1] Number of models with violations

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

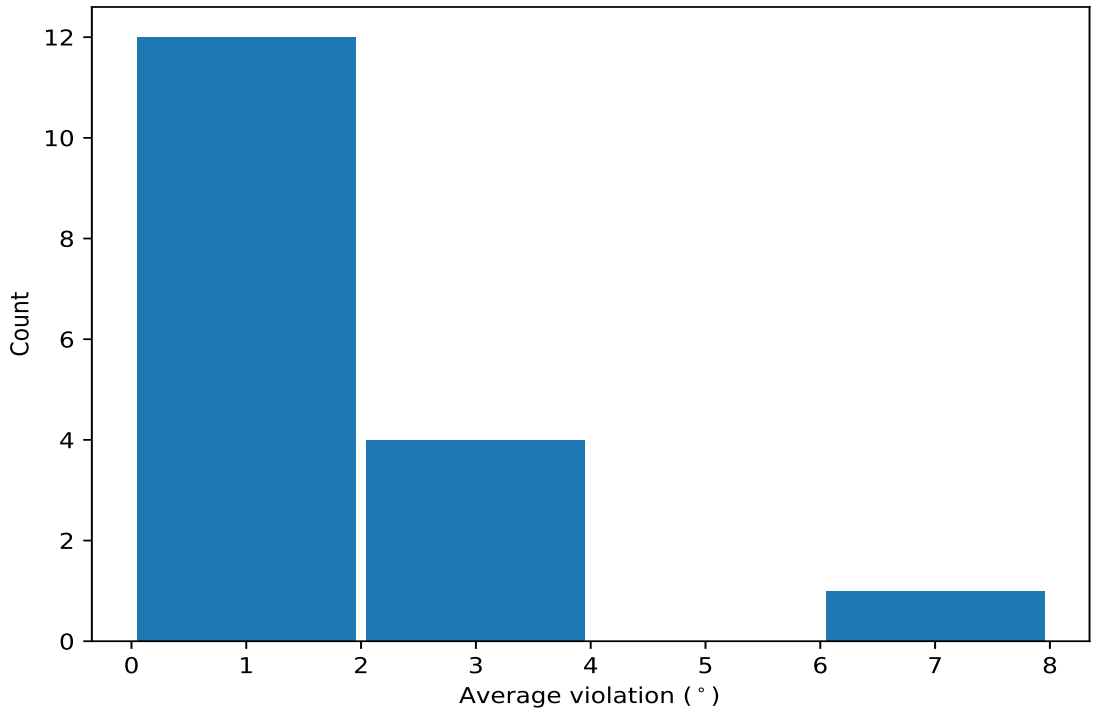


10.4 Most violated dihedral-angle restraints in the ensemble (i)

10.4.1 Histogram : Distribution of mean dihedral-angle 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



10.4.2 Table: Most violated dihedral-angle 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.

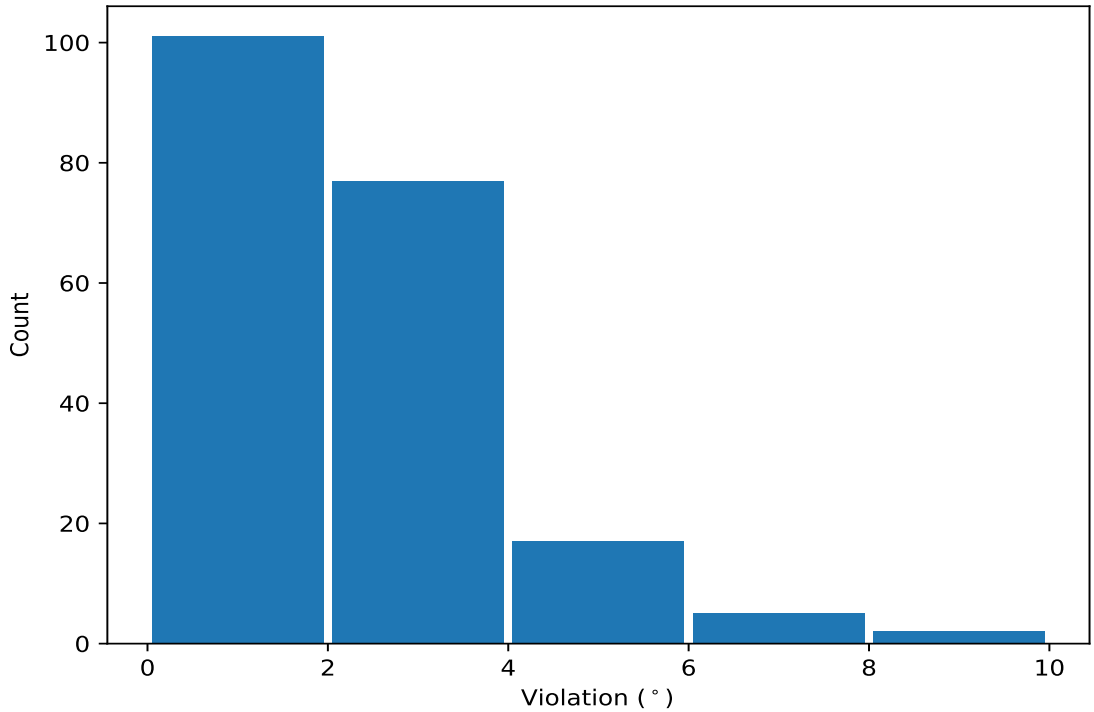
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	20	6.13	1.14	5.8
(1,116)	2:B:725:LYS:N	2:B:725:LYS:CA	2:B:725:LYS:C	2:B:726:GLU:N	20	2.98	0.49	3.05
(1,11)	1:A:970:LEU:C	1:A:971:VAL:N	1:A:971:VAL:CA	1:A:971:VAL:C	20	2.55	0.47	2.6
(1,143)	2:B:738:LYS:C	2:B:739:TRP:N	2:B:739:TRP:CA	2:B:739:TRP:C	20	2.52	0.36	2.55
(1,111)	2:B:722:HIS:C	2:B:723:ASP:N	2:B:723:ASP:CA	2:B:723:ASP:C	20	1.64	0.25	1.6
(1,49)	1:A:989:LYS:C	1:A:990:VAL:N	1:A:990:VAL:CA	1:A:990:VAL:C	18	1.83	0.7	1.7
(1,43)	1:A:986:ALA:C	1:A:987:MET:N	1:A:987:MET:CA	1:A:987:MET:C	17	1.92	0.47	1.9
(1,55)	2:B:693:ILE:C	2:B:694:LEU:N	2:B:694:LEU:CA	2:B:694:LEU:C	12	2.27	0.97	2.0
(1,73)	2:B:703:ALA:C	2:B:704:ILE:N	2:B:704:ILE:CA	2:B:704:ILE:C	11	1.5	0.34	1.4
(1,29)	1:A:979:LEU:C	1:A:980:LEU:N	1:A:980:LEU:CA	1:A:980:LEU:C	9	1.41	0.32	1.3
(1,58)	2:B:695:VAL:N	2:B:695:VAL:CA	2:B:695:VAL:C	2:B:696:VAL:N	7	1.44	0.2	1.5
(1,34)	1:A:982:ILE:N	1:A:982:ILE:CA	1:A:982:ILE:C	1:A:983:LEU:N	7	1.36	0.16	1.4
(1,90)	2:B:712:LEU:N	2:B:712:LEU:CA	2:B:712:LEU:C	2:B:713:LEU:N	5	1.36	0.19	1.4
(1,33)	1:A:981:THR:C	1:A:982:ILE:N	1:A:982:ILE:CA	1:A:982:ILE:C	4	1.38	0.18	1.35
(1,68)	2:B:700:VAL:N	2:B:700:VAL:CA	2:B:700:VAL:C	2:B:701:MET:N	2	1.3	0.1	1.3
(1,81)	2:B:707:ILE:C	2:B:708:GLY:N	2:B:708:GLY:CA	2:B:708:GLY:C	2	1.2	0.0	1.2
(1,126)	2:B:730:PHE:N	2:B:730:PHE:CA	2:B:730:PHE:C	2:B:731:GLU:N	2	1.2	0.0	1.2

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

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



10.5.2 Table: All violated dihedral-angle restraints (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.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	8	9.1
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	16	8.8
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	18	7.9
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	13	6.8
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	5	6.3
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	3	6.0
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	14	6.0
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	19	5.9
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	20	5.9
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	11	5.8
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	15	5.8
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	17	5.8
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	2	5.6
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	7	5.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	9	5.5
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	10	5.4
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	6	5.3
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	12	5.1
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	1	5.0
(1,39)	1:A:984:VAL:C	1:A:985:LEU:N	1:A:985:LEU:CA	1:A:985:LEU:C	4	4.9
(1,49)	1:A:989:LYS:C	1:A:990:VAL:N	1:A:990:VAL:CA	1:A:990:VAL:C	18	4.3
(1,37)	1:A:983:LEU:C	1:A:984:VAL:N	1:A:984:VAL:CA	1:A:984:VAL:C	1	4.1
(1,55)	2:B:693:ILE:C	2:B:694:LEU:N	2:B:694:LEU:CA	2:B:694:LEU:C	10	4.0
(1,116)	2:B:725:LYS:N	2:B:725:LYS:CA	2:B:725:LYS:C	2:B:726:GLU:N	5	4.0
(1,116)	2:B:725:LYS:N	2:B:725:LYS:CA	2:B:725:LYS:C	2:B:726:GLU:N	6	3.8
(1,55)	2:B:693:ILE:C	2:B:694:LEU:N	2:B:694:LEU:CA	2:B:694:LEU:C	16	3.6
(1,116)	2:B:725:LYS:N	2:B:725:LYS:CA	2:B:725:LYS:C	2:B:726:GLU:N	10	3.4
(1,11)	1:A:970:LEU:C	1:A:971:VAL:N	1:A:971:VAL:CA	1:A:971:VAL:C	12	3.4
(1,116)	2:B:725:LYS:N	2:B:725:LYS:CA	2:B:725:LYS:C	2:B:726:GLU:N	12	3.3
(1,55)	2:B:693:ILE:C	2:B:694:LEU:N	2:B:694:LEU:CA	2:B:694:LEU:C	18	3.2
(1,116)	2:B:725:LYS:N	2:B:725:LYS:CA	2:B:725:LYS:C	2:B:726:GLU:N	7	3.2
(1,116)	2:B:725:LYS:N	2:B:725:LYS:CA	2:B:725:LYS:C	2:B:726:GLU:N	14	3.2
(1,116)	2:B:725:LYS:N	2:B:725:LYS:CA	2:B:725:LYS:C	2:B:726:GLU:N	15	3.2
(1,116)	2:B:725:LYS:N	2:B:725:LYS:CA	2:B:725:LYS:C	2:B:726:GLU:N	18	3.2
(1,55)	2:B:693:ILE:C	2:B:694:LEU:N	2:B:694:LEU:CA	2:B:694:LEU:C	12	3.1
(1,143)	2:B:738:LYS:C	2:B:739:TRP:N	2:B:739:TRP:CA	2:B:739:TRP:C	11	3.1
(1,116)	2:B:725:LYS:N	2:B:725:LYS:CA	2:B:725:LYS:C	2:B:726:GLU:N	1	3.1
(1,116)	2:B:725:LYS:N	2:B:725:LYS:CA	2:B:725:LYS:C	2:B:726:GLU:N	16	3.1
(1,11)	1:A:970:LEU:C	1:A:971:VAL:N	1:A:971:VAL:CA	1:A:971:VAL:C	5	3.1
(1,11)	1:A:970:LEU:C	1:A:971:VAL:N	1:A:971:VAL:CA	1:A:971:VAL:C	10	3.1
(1,116)	2:B:725:LYS:N	2:B:725:LYS:CA	2:B:725:LYS:C	2:B:726:GLU:N	9	3.0
(1,116)	2:B:725:LYS:N	2:B:725:LYS:CA	2:B:725:LYS:C	2:B:726:GLU:N	20	3.0
(1,11)	1:A:970:LEU:C	1:A:971:VAL:N	1:A:971:VAL:CA	1:A:971:VAL:C	9	3.0
(1,143)	2:B:738:LYS:C	2:B:739:TRP:N	2:B:739:TRP:CA	2:B:739:TRP:C	8	2.9
(1,143)	2:B:738:LYS:C	2:B:739:TRP:N	2:B:739:TRP:CA	2:B:739:TRP:C	9	2.9
(1,143)	2:B:738:LYS:C	2:B:739:TRP:N	2:B:739:TRP:CA	2:B:739:TRP:C	12	2.9
(1,143)	2:B:738:LYS:C	2:B:739:TRP:N	2:B:739:TRP:CA	2:B:739:TRP:C	18	2.9
(1,11)	1:A:970:LEU:C	1:A:971:VAL:N	1:A:971:VAL:CA	1:A:971:VAL:C	2	2.9
(1,11)	1:A:970:LEU:C	1:A:971:VAL:N	1:A:971:VAL:CA	1:A:971:VAL:C	16	2.9
(1,11)	1:A:970:LEU:C	1:A:971:VAL:N	1:A:971:VAL:CA	1:A:971:VAL:C	17	2.9
(1,11)	1:A:970:LEU:C	1:A:971:VAL:N	1:A:971:VAL:CA	1:A:971:VAL:C	19	2.9
(1,43)	1:A:986:ALA:C	1:A:987:MET:N	1:A:987:MET:CA	1:A:987:MET:C	3	2.8
(1,43)	1:A:986:ALA:C	1:A:987:MET:N	1:A:987:MET:CA	1:A:987:MET:C	18	2.8
(1,143)	2:B:738:LYS:C	2:B:739:TRP:N	2:B:739:TRP:CA	2:B:739:TRP:C	20	2.8
(1,116)	2:B:725:LYS:N	2:B:725:LYS:CA	2:B:725:LYS:C	2:B:726:GLU:N	3	2.8
(1,116)	2:B:725:LYS:N	2:B:725:LYS:CA	2:B:725:LYS:C	2:B:726:GLU:N	8	2.8
(1,143)	2:B:738:LYS:C	2:B:739:TRP:N	2:B:739:TRP:CA	2:B:739:TRP:C	2	2.7
(1,143)	2:B:738:LYS:C	2:B:739:TRP:N	2:B:739:TRP:CA	2:B:739:TRP:C	10	2.7
(1,143)	2:B:738:LYS:C	2:B:739:TRP:N	2:B:739:TRP:CA	2:B:739:TRP:C	14	2.7
(1,116)	2:B:725:LYS:N	2:B:725:LYS:CA	2:B:725:LYS:C	2:B:726:GLU:N	2	2.7
(1,116)	2:B:725:LYS:N	2:B:725:LYS:CA	2:B:725:LYS:C	2:B:726:GLU:N	13	2.7
(1,11)	1:A:970:LEU:C	1:A:971:VAL:N	1:A:971:VAL:CA	1:A:971:VAL:C	15	2.7
(1,11)	1:A:970:LEU:C	1:A:971:VAL:N	1:A:971:VAL:CA	1:A:971:VAL:C	18	2.7
(1,55)	2:B:693:ILE:C	2:B:694:LEU:N	2:B:694:LEU:CA	2:B:694:LEU:C	1	2.6
(1,143)	2:B:738:LYS:C	2:B:739:TRP:N	2:B:739:TRP:CA	2:B:739:TRP:C	6	2.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,43)	1:A:986:ALA:C	1:A:987:MET:N	1:A:987:MET:CA	1:A:987:MET:C	17	2.5
(1,143)	2:B:738:LYS:C	2:B:739:TRP:N	2:B:739:TRP:CA	2:B:739:TRP:C	19	2.5
(1,116)	2:B:725:LYS:N	2:B:725:LYS:CA	2:B:725:LYS:C	2:B:726:GLU:N	11	2.5
(1,116)	2:B:725:LYS:N	2:B:725:LYS:CA	2:B:725:LYS:C	2:B:726:GLU:N	17	2.5
(1,11)	1:A:970:LEU:C	1:A:971:VAL:N	1:A:971:VAL:CA	1:A:971:VAL:C	14	2.5
(1,49)	1:A:989:LYS:C	1:A:990:VAL:N	1:A:990:VAL:CA	1:A:990:VAL:C	3	2.4
(1,49)	1:A:989:LYS:C	1:A:990:VAL:N	1:A:990:VAL:CA	1:A:990:VAL:C	11	2.4
(1,143)	2:B:738:LYS:C	2:B:739:TRP:N	2:B:739:TRP:CA	2:B:739:TRP:C	3	2.4
(1,143)	2:B:738:LYS:C	2:B:739:TRP:N	2:B:739:TRP:CA	2:B:739:TRP:C	5	2.4
(1,143)	2:B:738:LYS:C	2:B:739:TRP:N	2:B:739:TRP:CA	2:B:739:TRP:C	13	2.4
(1,143)	2:B:738:LYS:C	2:B:739:TRP:N	2:B:739:TRP:CA	2:B:739:TRP:C	17	2.4
(1,116)	2:B:725:LYS:N	2:B:725:LYS:CA	2:B:725:LYS:C	2:B:726:GLU:N	4	2.4
(1,11)	1:A:970:LEU:C	1:A:971:VAL:N	1:A:971:VAL:CA	1:A:971:VAL:C	3	2.4
(1,11)	1:A:970:LEU:C	1:A:971:VAL:N	1:A:971:VAL:CA	1:A:971:VAL:C	6	2.4
(1,55)	2:B:693:ILE:C	2:B:694:LEU:N	2:B:694:LEU:CA	2:B:694:LEU:C	11	2.3
(1,11)	1:A:970:LEU:C	1:A:971:VAL:N	1:A:971:VAL:CA	1:A:971:VAL:C	1	2.3
(1,11)	1:A:970:LEU:C	1:A:971:VAL:N	1:A:971:VAL:CA	1:A:971:VAL:C	7	2.3
(1,73)	2:B:703:ALA:C	2:B:704:ILE:N	2:B:704:ILE:CA	2:B:704:ILE:C	12	2.2
(1,43)	1:A:986:ALA:C	1:A:987:MET:N	1:A:987:MET:CA	1:A:987:MET:C	4	2.2
(1,43)	1:A:986:ALA:C	1:A:987:MET:N	1:A:987:MET:CA	1:A:987:MET:C	12	2.2
(1,43)	1:A:986:ALA:C	1:A:987:MET:N	1:A:987:MET:CA	1:A:987:MET:C	13	2.2
(1,143)	2:B:738:LYS:C	2:B:739:TRP:N	2:B:739:TRP:CA	2:B:739:TRP:C	7	2.2
(1,143)	2:B:738:LYS:C	2:B:739:TRP:N	2:B:739:TRP:CA	2:B:739:TRP:C	15	2.2
(1,73)	2:B:703:ALA:C	2:B:704:ILE:N	2:B:704:ILE:CA	2:B:704:ILE:C	6	2.1
(1,49)	1:A:989:LYS:C	1:A:990:VAL:N	1:A:990:VAL:CA	1:A:990:VAL:C	12	2.1
(1,43)	1:A:986:ALA:C	1:A:987:MET:N	1:A:987:MET:CA	1:A:987:MET:C	20	2.1
(1,111)	2:B:722:HIS:C	2:B:723:ASP:N	2:B:723:ASP:CA	2:B:723:ASP:C	18	2.1
(1,11)	1:A:970:LEU:C	1:A:971:VAL:N	1:A:971:VAL:CA	1:A:971:VAL:C	13	2.1
(1,43)	1:A:986:ALA:C	1:A:987:MET:N	1:A:987:MET:CA	1:A:987:MET:C	7	2.0
(1,143)	2:B:738:LYS:C	2:B:739:TRP:N	2:B:739:TRP:CA	2:B:739:TRP:C	1	2.0
(1,143)	2:B:738:LYS:C	2:B:739:TRP:N	2:B:739:TRP:CA	2:B:739:TRP:C	16	2.0
(1,111)	2:B:722:HIS:C	2:B:723:ASP:N	2:B:723:ASP:CA	2:B:723:ASP:C	1	2.0
(1,111)	2:B:722:HIS:C	2:B:723:ASP:N	2:B:723:ASP:CA	2:B:723:ASP:C	11	2.0
(1,111)	2:B:722:HIS:C	2:B:723:ASP:N	2:B:723:ASP:CA	2:B:723:ASP:C	12	2.0
(1,11)	1:A:970:LEU:C	1:A:971:VAL:N	1:A:971:VAL:CA	1:A:971:VAL:C	4	2.0
(1,11)	1:A:970:LEU:C	1:A:971:VAL:N	1:A:971:VAL:CA	1:A:971:VAL:C	8	2.0
(1,49)	1:A:989:LYS:C	1:A:990:VAL:N	1:A:990:VAL:CA	1:A:990:VAL:C	5	1.9
(1,49)	1:A:989:LYS:C	1:A:990:VAL:N	1:A:990:VAL:CA	1:A:990:VAL:C	6	1.9
(1,49)	1:A:989:LYS:C	1:A:990:VAL:N	1:A:990:VAL:CA	1:A:990:VAL:C	8	1.9
(1,43)	1:A:986:ALA:C	1:A:987:MET:N	1:A:987:MET:CA	1:A:987:MET:C	16	1.9
(1,29)	1:A:979:LEU:C	1:A:980:LEU:N	1:A:980:LEU:CA	1:A:980:LEU:C	1	1.9
(1,29)	1:A:979:LEU:C	1:A:980:LEU:N	1:A:980:LEU:CA	1:A:980:LEU:C	10	1.9
(1,88)	2:B:711:ALA:N	2:B:711:ALA:CA	2:B:711:ALA:C	2:B:712:LEU:N	12	1.8
(1,49)	1:A:989:LYS:C	1:A:990:VAL:N	1:A:990:VAL:CA	1:A:990:VAL:C	1	1.8
(1,49)	1:A:989:LYS:C	1:A:990:VAL:N	1:A:990:VAL:CA	1:A:990:VAL:C	15	1.8
(1,43)	1:A:986:ALA:C	1:A:987:MET:N	1:A:987:MET:CA	1:A:987:MET:C	1	1.8
(1,111)	2:B:722:HIS:C	2:B:723:ASP:N	2:B:723:ASP:CA	2:B:723:ASP:C	20	1.8
(1,11)	1:A:970:LEU:C	1:A:971:VAL:N	1:A:971:VAL:CA	1:A:971:VAL:C	20	1.8
(1,58)	2:B:695:VAL:N	2:B:695:VAL:CA	2:B:695:VAL:C	2:B:696:VAL:N	17	1.7
(1,58)	2:B:695:VAL:N	2:B:695:VAL:CA	2:B:695:VAL:C	2:B:696:VAL:N	19	1.7
(1,55)	2:B:693:ILE:C	2:B:694:LEU:N	2:B:694:LEU:CA	2:B:694:LEU:C	2	1.7

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,55)	2:B:693:ILE:C	2:B:694:LEU:N	2:B:694:LEU:CA	2:B:694:LEU:C	13	1.7
(1,43)	1:A:986:ALA:C	1:A:987:MET:N	1:A:987:MET:CA	1:A:987:MET:C	8	1.7
(1,143)	2:B:738:LYS:C	2:B:739:TRP:N	2:B:739:TRP:CA	2:B:739:TRP:C	4	1.7
(1,116)	2:B:725:LYS:N	2:B:725:LYS:CA	2:B:725:LYS:C	2:B:726:GLU:N	19	1.7
(1,111)	2:B:722:HIS:C	2:B:723:ASP:N	2:B:723:ASP:CA	2:B:723:ASP:C	3	1.7
(1,111)	2:B:722:HIS:C	2:B:723:ASP:N	2:B:723:ASP:CA	2:B:723:ASP:C	5	1.7
(1,111)	2:B:722:HIS:C	2:B:723:ASP:N	2:B:723:ASP:CA	2:B:723:ASP:C	7	1.7
(1,111)	2:B:722:HIS:C	2:B:723:ASP:N	2:B:723:ASP:CA	2:B:723:ASP:C	15	1.7
(1,11)	1:A:970:LEU:C	1:A:971:VAL:N	1:A:971:VAL:CA	1:A:971:VAL:C	11	1.7
(1,90)	2:B:712:LEU:N	2:B:712:LEU:CA	2:B:712:LEU:C	2:B:713:LEU:N	15	1.6
(1,73)	2:B:703:ALA:C	2:B:704:ILE:N	2:B:704:ILE:CA	2:B:704:ILE:C	20	1.6
(1,49)	1:A:989:LYS:C	1:A:990:VAL:N	1:A:990:VAL:CA	1:A:990:VAL:C	10	1.6
(1,49)	1:A:989:LYS:C	1:A:990:VAL:N	1:A:990:VAL:CA	1:A:990:VAL:C	14	1.6
(1,49)	1:A:989:LYS:C	1:A:990:VAL:N	1:A:990:VAL:CA	1:A:990:VAL:C	19	1.6
(1,43)	1:A:986:ALA:C	1:A:987:MET:N	1:A:987:MET:CA	1:A:987:MET:C	14	1.6
(1,34)	1:A:982:ILE:N	1:A:982:ILE:CA	1:A:982:ILE:C	1:A:983:LEU:N	12	1.6
(1,33)	1:A:981:THR:C	1:A:982:ILE:N	1:A:982:ILE:CA	1:A:982:ILE:C	10	1.6
(1,29)	1:A:979:LEU:C	1:A:980:LEU:N	1:A:980:LEU:CA	1:A:980:LEU:C	2	1.6
(1,29)	1:A:979:LEU:C	1:A:980:LEU:N	1:A:980:LEU:CA	1:A:980:LEU:C	9	1.6
(1,111)	2:B:722:HIS:C	2:B:723:ASP:N	2:B:723:ASP:CA	2:B:723:ASP:C	10	1.6
(1,111)	2:B:722:HIS:C	2:B:723:ASP:N	2:B:723:ASP:CA	2:B:723:ASP:C	13	1.6
(1,111)	2:B:722:HIS:C	2:B:723:ASP:N	2:B:723:ASP:CA	2:B:723:ASP:C	16	1.6
(1,111)	2:B:722:HIS:C	2:B:723:ASP:N	2:B:723:ASP:CA	2:B:723:ASP:C	19	1.6
(1,90)	2:B:712:LEU:N	2:B:712:LEU:CA	2:B:712:LEU:C	2:B:713:LEU:N	13	1.5
(1,73)	2:B:703:ALA:C	2:B:704:ILE:N	2:B:704:ILE:CA	2:B:704:ILE:C	7	1.5
(1,73)	2:B:703:ALA:C	2:B:704:ILE:N	2:B:704:ILE:CA	2:B:704:ILE:C	17	1.5
(1,58)	2:B:695:VAL:N	2:B:695:VAL:CA	2:B:695:VAL:C	2:B:696:VAL:N	6	1.5
(1,58)	2:B:695:VAL:N	2:B:695:VAL:CA	2:B:695:VAL:C	2:B:696:VAL:N	8	1.5
(1,55)	2:B:693:ILE:C	2:B:694:LEU:N	2:B:694:LEU:CA	2:B:694:LEU:C	8	1.5
(1,43)	1:A:986:ALA:C	1:A:987:MET:N	1:A:987:MET:CA	1:A:987:MET:C	19	1.5
(1,34)	1:A:982:ILE:N	1:A:982:ILE:CA	1:A:982:ILE:C	1:A:983:LEU:N	4	1.5
(1,33)	1:A:981:THR:C	1:A:982:ILE:N	1:A:982:ILE:CA	1:A:982:ILE:C	9	1.5
(1,111)	2:B:722:HIS:C	2:B:723:ASP:N	2:B:723:ASP:CA	2:B:723:ASP:C	2	1.5
(1,111)	2:B:722:HIS:C	2:B:723:ASP:N	2:B:723:ASP:CA	2:B:723:ASP:C	8	1.5
(1,105)	2:B:719:ILE:C	2:B:720:THR:N	2:B:720:THR:CA	2:B:720:THR:C	15	1.5
(1,104)	2:B:719:ILE:N	2:B:719:ILE:CA	2:B:719:ILE:C	2:B:720:THR:N	18	1.5
(1,90)	2:B:712:LEU:N	2:B:712:LEU:CA	2:B:712:LEU:C	2:B:713:LEU:N	17	1.4
(1,73)	2:B:703:ALA:C	2:B:704:ILE:N	2:B:704:ILE:CA	2:B:704:ILE:C	2	1.4
(1,68)	2:B:700:VAL:N	2:B:700:VAL:CA	2:B:700:VAL:C	2:B:701:MET:N	8	1.4
(1,49)	1:A:989:LYS:C	1:A:990:VAL:N	1:A:990:VAL:CA	1:A:990:VAL:C	13	1.4
(1,43)	1:A:986:ALA:C	1:A:987:MET:N	1:A:987:MET:CA	1:A:987:MET:C	6	1.4
(1,43)	1:A:986:ALA:C	1:A:987:MET:N	1:A:987:MET:CA	1:A:987:MET:C	15	1.4
(1,34)	1:A:982:ILE:N	1:A:982:ILE:CA	1:A:982:ILE:C	1:A:983:LEU:N	9	1.4
(1,34)	1:A:982:ILE:N	1:A:982:ILE:CA	1:A:982:ILE:C	1:A:983:LEU:N	10	1.4
(1,111)	2:B:722:HIS:C	2:B:723:ASP:N	2:B:723:ASP:CA	2:B:723:ASP:C	4	1.4
(1,111)	2:B:722:HIS:C	2:B:723:ASP:N	2:B:723:ASP:CA	2:B:723:ASP:C	6	1.4
(1,111)	2:B:722:HIS:C	2:B:723:ASP:N	2:B:723:ASP:CA	2:B:723:ASP:C	14	1.4
(1,103)	2:B:718:LEU:C	2:B:719:ILE:N	2:B:719:ILE:CA	2:B:719:ILE:C	1	1.4
(1,73)	2:B:703:ALA:C	2:B:704:ILE:N	2:B:704:ILE:CA	2:B:704:ILE:C	3	1.3
(1,73)	2:B:703:ALA:C	2:B:704:ILE:N	2:B:704:ILE:CA	2:B:704:ILE:C	10	1.3
(1,73)	2:B:703:ALA:C	2:B:704:ILE:N	2:B:704:ILE:CA	2:B:704:ILE:C	15	1.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,58)	2:B:695:VAL:N	2:B:695:VAL:CA	2:B:695:VAL:C	2:B:696:VAL:N	20	1.3
(1,49)	1:A:989:LYS:C	1:A:990:VAL:N	1:A:990:VAL:CA	1:A:990:VAL:C	7	1.3
(1,49)	1:A:989:LYS:C	1:A:990:VAL:N	1:A:990:VAL:CA	1:A:990:VAL:C	16	1.3
(1,43)	1:A:986:ALA:C	1:A:987:MET:N	1:A:987:MET:CA	1:A:987:MET:C	2	1.3
(1,43)	1:A:986:ALA:C	1:A:987:MET:N	1:A:987:MET:CA	1:A:987:MET:C	5	1.3
(1,34)	1:A:982:ILE:N	1:A:982:ILE:CA	1:A:982:ILE:C	1:A:983:LEU:N	14	1.3
(1,29)	1:A:979:LEU:C	1:A:980:LEU:N	1:A:980:LEU:CA	1:A:980:LEU:C	4	1.3
(1,90)	2:B:712:LEU:N	2:B:712:LEU:CA	2:B:712:LEU:C	2:B:713:LEU:N	5	1.2
(1,81)	2:B:707:ILE:C	2:B:708:GLY:N	2:B:708:GLY:CA	2:B:708:GLY:C	1	1.2
(1,81)	2:B:707:ILE:C	2:B:708:GLY:N	2:B:708:GLY:CA	2:B:708:GLY:C	12	1.2
(1,73)	2:B:703:ALA:C	2:B:704:ILE:N	2:B:704:ILE:CA	2:B:704:ILE:C	16	1.2
(1,68)	2:B:700:VAL:N	2:B:700:VAL:CA	2:B:700:VAL:C	2:B:701:MET:N	16	1.2
(1,58)	2:B:695:VAL:N	2:B:695:VAL:CA	2:B:695:VAL:C	2:B:696:VAL:N	7	1.2
(1,58)	2:B:695:VAL:N	2:B:695:VAL:CA	2:B:695:VAL:C	2:B:696:VAL:N	9	1.2
(1,55)	2:B:693:ILE:C	2:B:694:LEU:N	2:B:694:LEU:CA	2:B:694:LEU:C	7	1.2
(1,55)	2:B:693:ILE:C	2:B:694:LEU:N	2:B:694:LEU:CA	2:B:694:LEU:C	14	1.2
(1,49)	1:A:989:LYS:C	1:A:990:VAL:N	1:A:990:VAL:CA	1:A:990:VAL:C	4	1.2
(1,49)	1:A:989:LYS:C	1:A:990:VAL:N	1:A:990:VAL:CA	1:A:990:VAL:C	17	1.2
(1,49)	1:A:989:LYS:C	1:A:990:VAL:N	1:A:990:VAL:CA	1:A:990:VAL:C	20	1.2
(1,34)	1:A:982:ILE:N	1:A:982:ILE:CA	1:A:982:ILE:C	1:A:983:LEU:N	7	1.2
(1,33)	1:A:981:THR:C	1:A:982:ILE:N	1:A:982:ILE:CA	1:A:982:ILE:C	2	1.2
(1,33)	1:A:981:THR:C	1:A:982:ILE:N	1:A:982:ILE:CA	1:A:982:ILE:C	11	1.2
(1,126)	2:B:730:PHE:N	2:B:730:PHE:CA	2:B:730:PHE:C	2:B:731:GLU:N	11	1.2
(1,126)	2:B:730:PHE:N	2:B:730:PHE:CA	2:B:730:PHE:C	2:B:731:GLU:N	13	1.2
(1,111)	2:B:722:HIS:C	2:B:723:ASP:N	2:B:723:ASP:CA	2:B:723:ASP:C	9	1.2
(1,111)	2:B:722:HIS:C	2:B:723:ASP:N	2:B:723:ASP:CA	2:B:723:ASP:C	17	1.2
(1,90)	2:B:712:LEU:N	2:B:712:LEU:CA	2:B:712:LEU:C	2:B:713:LEU:N	11	1.1
(1,73)	2:B:703:ALA:C	2:B:704:ILE:N	2:B:704:ILE:CA	2:B:704:ILE:C	1	1.1
(1,57)	2:B:694:LEU:C	2:B:695:VAL:N	2:B:695:VAL:CA	2:B:695:VAL:C	7	1.1
(1,55)	2:B:693:ILE:C	2:B:694:LEU:N	2:B:694:LEU:CA	2:B:694:LEU:C	17	1.1
(1,34)	1:A:982:ILE:N	1:A:982:ILE:CA	1:A:982:ILE:C	1:A:983:LEU:N	5	1.1
(1,29)	1:A:979:LEU:C	1:A:980:LEU:N	1:A:980:LEU:CA	1:A:980:LEU:C	3	1.1
(1,29)	1:A:979:LEU:C	1:A:980:LEU:N	1:A:980:LEU:CA	1:A:980:LEU:C	5	1.1
(1,29)	1:A:979:LEU:C	1:A:980:LEU:N	1:A:980:LEU:CA	1:A:980:LEU:C	7	1.1
(1,29)	1:A:979:LEU:C	1:A:980:LEU:N	1:A:980:LEU:CA	1:A:980:LEU:C	11	1.1