



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 03:40 PM UTC

PDB ID : 2LW1 / pdb_00002lw1
BMRB ID : 17989
Title : The C-terminal domain of the Uup protein is a DNA-binding coiled coil motif
Authors : Carlier, L.; Haase, A.S.; Burgos Zepeda, M.Y.; Dassa, E.; Lequin, O.
Deposited on : 2012-07-19

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

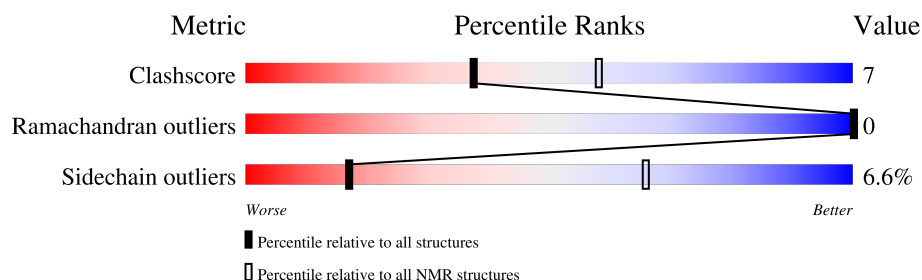
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 94%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	108	55% 10% 14% 21%

2 Ensemble composition and analysis

This entry contains 20 models. Model 18 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:563-A:632 (70)	0.51	18

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 6 clusters and 2 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1358 atoms, of which 674 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ABC transporter ATP-binding protein uup.

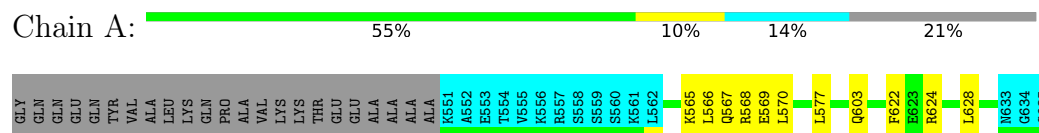
Mol	Chain	Residues	Atoms							Trace
1	A	85	Total	C	H	N	O	S		0
			1358	428	674	115	140	1		

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: ABC transporter ATP-binding protein uup

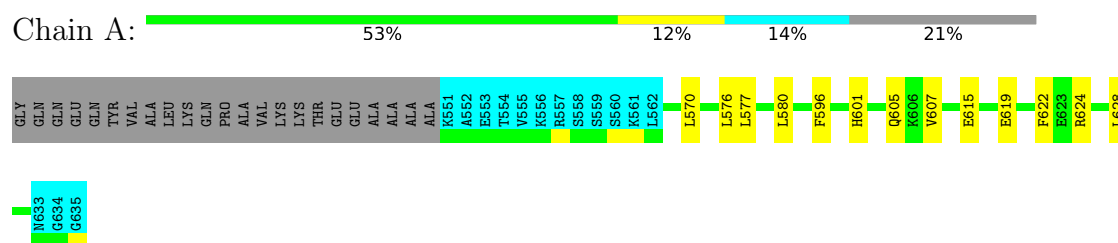


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

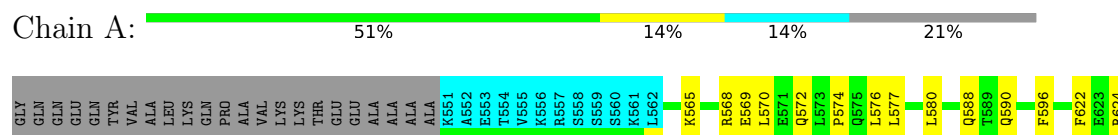
4.2.1 Score per residue for model 1

- Molecule 1: ABC transporter ATP-binding protein uup



4.2.2 Score per residue for model 2

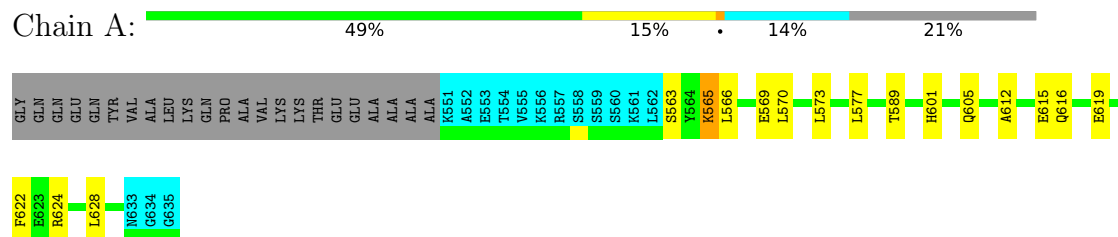
- Molecule 1: ABC transporter ATP-binding protein uup





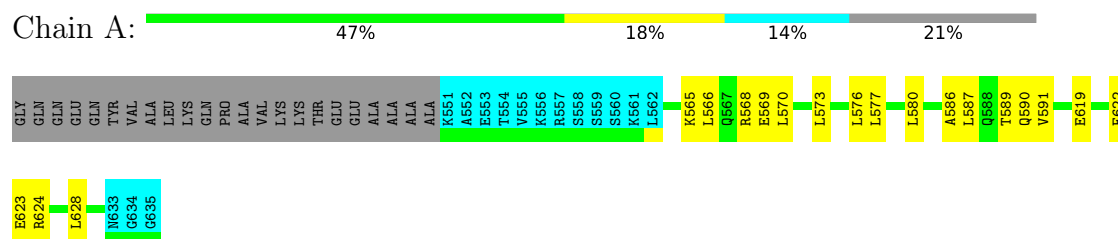
4.2.3 Score per residue for model 3

- Molecule 1: ABC transporter ATP-binding protein uup



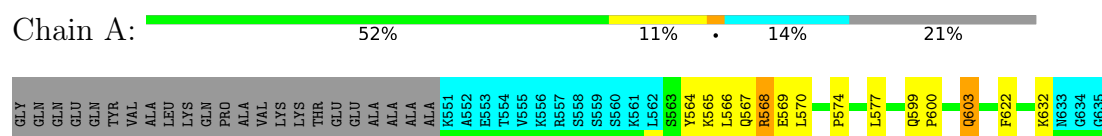
4.2.4 Score per residue for model 4

- Molecule 1: ABC transporter ATP-binding protein uup



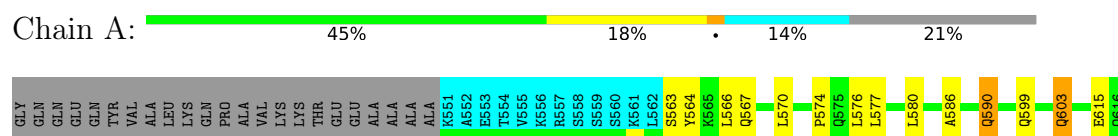
4.2.5 Score per residue for model 5

- Molecule 1: ABC transporter ATP-binding protein uup



4.2.6 Score per residue for model 6

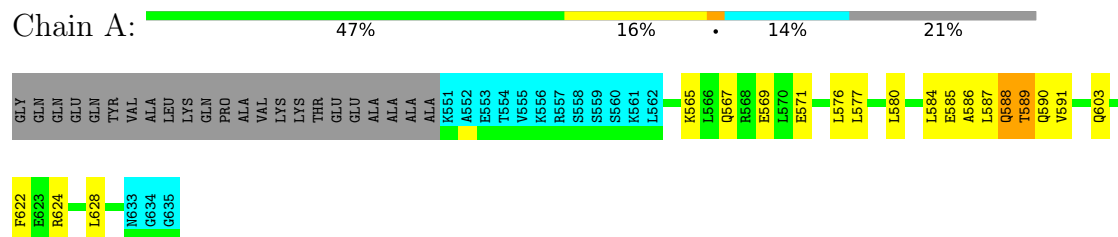
- Molecule 1: ABC transporter ATP-binding protein uup





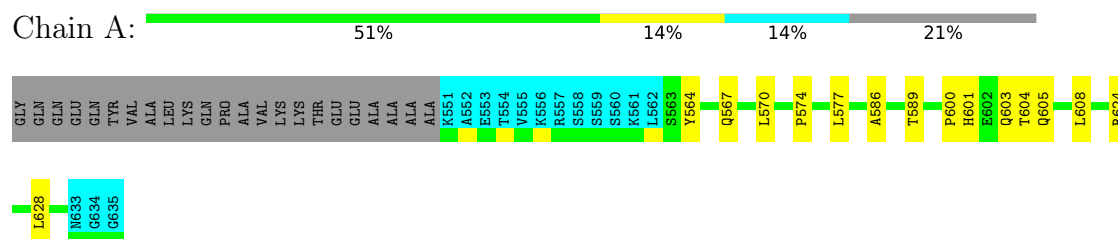
4.2.7 Score per residue for model 7

- Molecule 1: ABC transporter ATP-binding protein uup



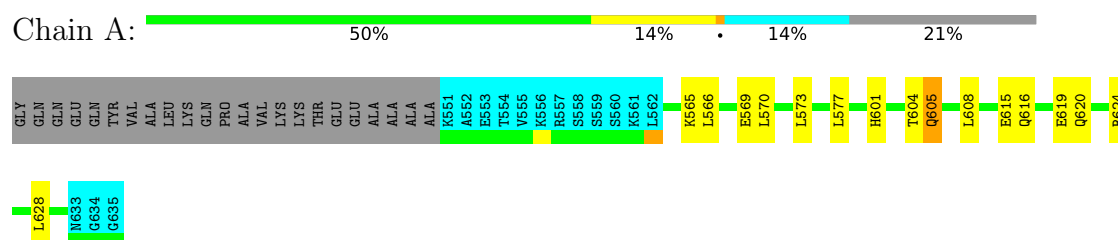
4.2.8 Score per residue for model 8

- Molecule 1: ABC transporter ATP-binding protein uup



4.2.9 Score per residue for model 9

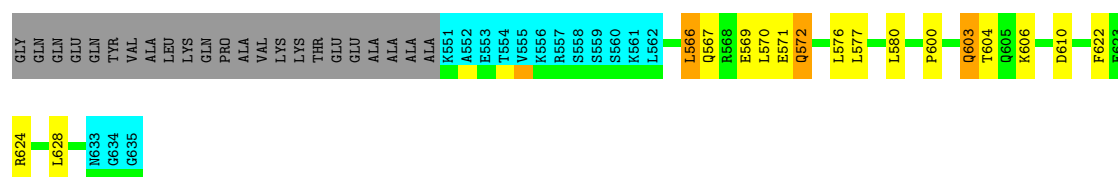
- Molecule 1: ABC transporter ATP-binding protein uup



4.2.10 Score per residue for model 10

- Molecule 1: ABC transporter ATP-binding protein uup

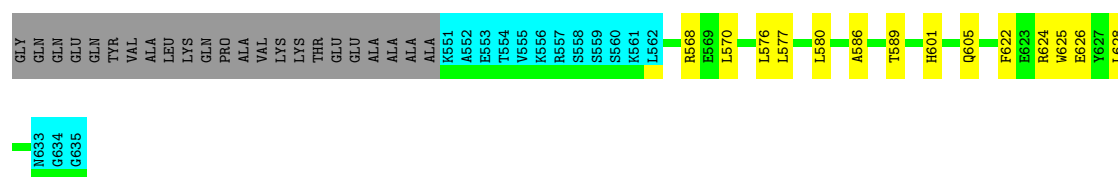




4.2.11 Score per residue for model 11

- Molecule 1: ABC transporter ATP-binding protein uup

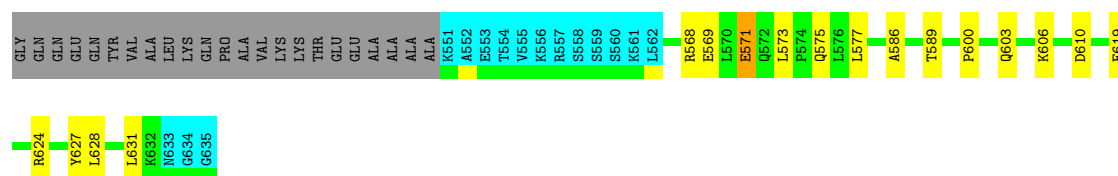
Chain A: 52% 13% 14% 21%



4.2.12 Score per residue for model 12

- Molecule 1: ABC transporter ATP-binding protein uup

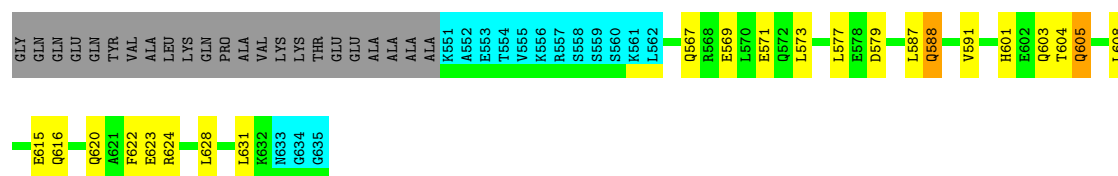
Chain A: 49% 15% 14% 21%



4.2.13 Score per residue for model 13

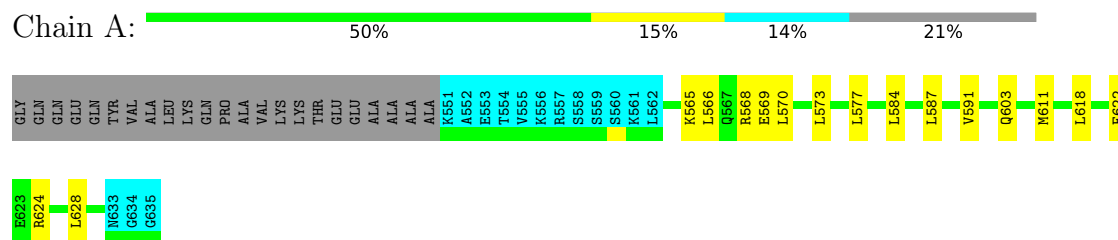
- Molecule 1: ABC transporter ATP-binding protein uup

Chain A: 44% 19% 14% 21%



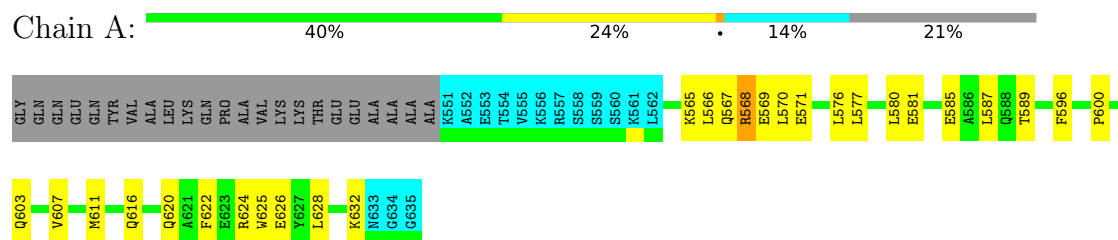
4.2.14 Score per residue for model 14

- Molecule 1: ABC transporter ATP-binding protein uup



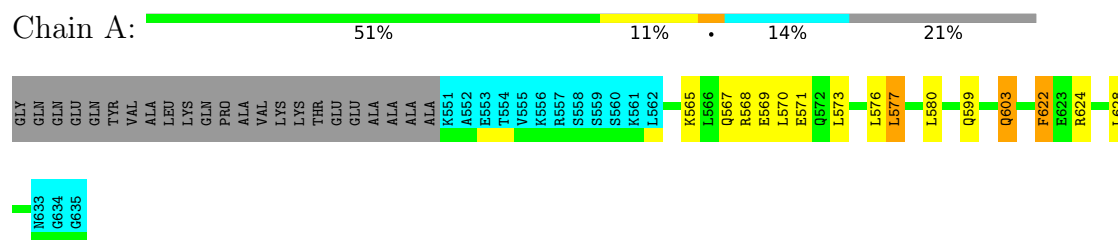
4.2.15 Score per residue for model 15

- Molecule 1: ABC transporter ATP-binding protein uup



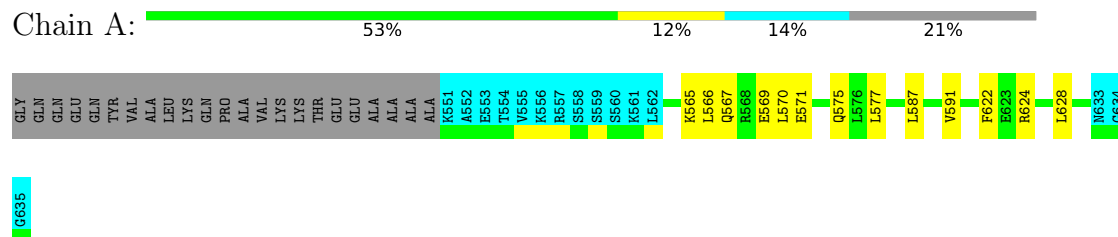
4.2.16 Score per residue for model 16

- Molecule 1: ABC transporter ATP-binding protein uup



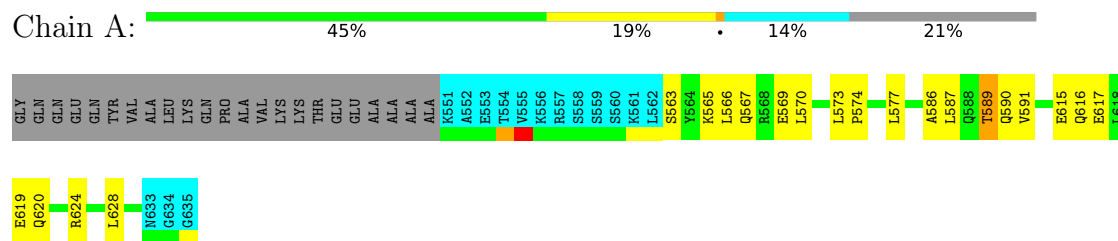
4.2.17 Score per residue for model 17

- Molecule 1: ABC transporter ATP-binding protein uup



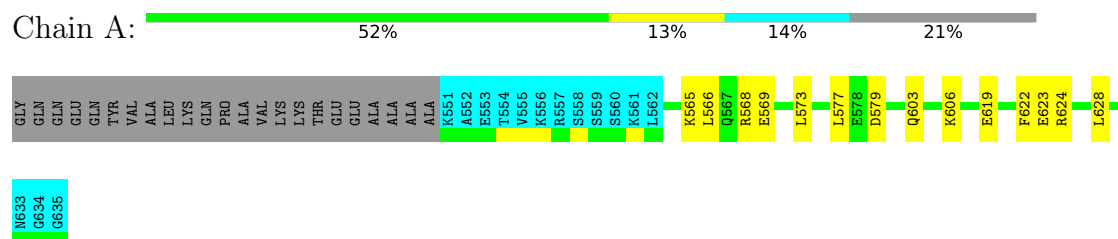
4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: ABC transporter ATP-binding protein uup



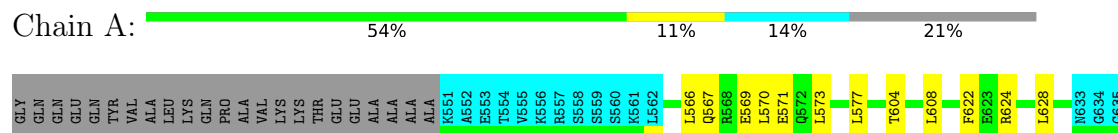
4.2.19 Score per residue for model 19

- Molecule 1: ABC transporter ATP-binding protein uup



4.2.20 Score per residue for model 20

- Molecule 1: ABC transporter ATP-binding protein uup



5 Refinement protocol and experimental data overview

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

Of the 400 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
TopSpin	geometry optimization	2.0
ARIA	structure solution	2.2
CNS	structure solution	1.1
CNS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1362
Number of shifts mapped to atoms	1096
Number of unparsed shifts	0
Number of shifts with mapping errors	266
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	94%

6 Model quality

6.1 Standard geometry

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

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	575	557	556	8±2
All	All	11500	11140	11120	169

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:563:SER:HB2	1:A:566:LEU:HD13	0.70	1.64	3	1
1:A:590:GLN:HE21	1:A:590:GLN:HA	0.69	1.47	6	1
1:A:600:PRO:HD2	1:A:603:GLN:HG2	0.67	1.63	10	2
1:A:565:LYS:O	1:A:569:GLU:HB2	0.67	1.90	2	12
1:A:624:ARG:O	1:A:628:LEU:HG	0.66	1.91	7	19
1:A:570:LEU:O	1:A:574:PRO:HD3	0.64	1.92	8	5
1:A:617:GLU:HA	1:A:620:GLN:HE21	0.63	1.53	18	2
1:A:601:HIS:O	1:A:605:GLN:HG3	0.63	1.94	9	2
1:A:566:LEU:HD23	1:A:628:LEU:HD22	0.62	1.71	4	7
1:A:601:HIS:CD2	1:A:605:GLN:HG2	0.60	2.32	9	2
1:A:615:GLU:O	1:A:619:GLU:HG3	0.60	1.96	6	5
1:A:569:GLU:O	1:A:573:LEU:HB2	0.60	1.95	13	9
1:A:603:GLN:O	1:A:606:LYS:HG3	0.60	1.97	19	1
1:A:567:GLN:O	1:A:571:GLU:HG2	0.59	1.98	13	6

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:564:TYR:CZ	1:A:568:ARG:HD3	0.58	2.33	5	1
1:A:572:GLN:HE21	1:A:572:GLN:HA	0.56	1.60	10	1
1:A:600:PRO:HG2	1:A:603:GLN:HG2	0.55	1.79	15	1
1:A:563:SER:HB3	1:A:566:LEU:HD13	0.55	1.77	6	1
1:A:570:LEU:HD23	1:A:570:LEU:O	0.55	2.02	2	5
1:A:599:GLN:HB3	1:A:603:GLN:HG2	0.54	1.80	6	2
1:A:565:LYS:O	1:A:568:ARG:HD3	0.54	2.02	14	3
1:A:618:LEU:HD13	1:A:618:LEU:C	0.53	2.29	14	1
1:A:568:ARG:N	1:A:568:ARG:HD2	0.52	2.19	5	1
1:A:568:ARG:HA	1:A:571:GLU:HB3	0.51	1.83	12	1
1:A:576:LEU:O	1:A:580:LEU:HG	0.51	2.06	7	9
1:A:625:TRP:CE3	1:A:626:GLU:HG2	0.51	2.41	11	2
1:A:586:ALA:O	1:A:589:THR:HG22	0.50	2.06	18	5
1:A:627:TYR:CE1	1:A:631:LEU:HD13	0.50	2.41	12	1
1:A:606:LYS:O	1:A:610:ASP:HB2	0.50	2.06	12	2
1:A:570:LEU:O	1:A:570:LEU:HD23	0.50	2.07	18	1
1:A:586:ALA:O	1:A:590:GLN:HG2	0.49	2.08	7	4
1:A:616:GLN:O	1:A:620:GLN:HG2	0.49	2.08	18	4
1:A:565:LYS:HA	1:A:568:ARG:CZ	0.49	2.37	15	1
1:A:567:GLN:O	1:A:571:GLU:HG3	0.49	2.07	7	1
1:A:587:LEU:O	1:A:591:VAL:HG23	0.48	2.08	4	6
1:A:564:TYR:O	1:A:567:GLN:HB2	0.48	2.08	5	3
1:A:604:THR:O	1:A:608:LEU:HG	0.48	2.07	13	4
1:A:590:GLN:HE21	1:A:590:GLN:CA	0.48	2.20	6	1
1:A:600:PRO:HB2	1:A:603:GLN:HG2	0.47	1.87	12	1
1:A:566:LEU:HA	1:A:569:GLU:CB	0.46	2.40	10	1
1:A:584:LEU:O	1:A:588:GLN:HB2	0.46	2.11	7	1
1:A:585:GLU:O	1:A:589:THR:HB	0.45	2.11	7	1
1:A:619:GLU:O	1:A:623:GLU:HG2	0.45	2.11	4	2
1:A:565:LYS:H	1:A:565:LYS:HD2	0.45	1.71	3	1
1:A:565:LYS:HG3	1:A:566:LEU:HD12	0.45	1.89	18	1
1:A:581:GLU:O	1:A:585:GLU:HG2	0.44	2.13	15	1
1:A:601:HIS:NE2	1:A:605:GLN:HG3	0.44	2.27	11	3
1:A:566:LEU:HD23	1:A:628:LEU:CD2	0.44	2.43	9	2
1:A:588:GLN:HE21	1:A:588:GLN:HA	0.43	1.73	13	1
1:A:587:LEU:HD13	1:A:611:MET:HA	0.43	1.89	15	1
1:A:603:GLN:HG3	1:A:604:THR:N	0.43	2.28	10	1
1:A:590:GLN:O	1:A:596:PHE:HB2	0.43	2.14	2	1
1:A:601:HIS:CE1	1:A:605:GLN:HG3	0.42	2.49	8	1
1:A:584:LEU:HD13	1:A:584:LEU:C	0.42	2.39	14	2
1:A:566:LEU:HA	1:A:569:GLU:HB3	0.42	1.91	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:575:GLN:HA	1:A:575:GLN:OE1	0.41	2.16	17	1
1:A:566:LEU:HD12	1:A:566:LEU:N	0.41	2.30	3	1
1:A:596:PHE:CZ	1:A:607:VAL:HB	0.41	2.50	15	2
1:A:600:PRO:HD2	1:A:603:GLN:HG3	0.41	1.92	8	1
1:A:600:PRO:HD2	1:A:603:GLN:CG	0.41	2.46	8	1
1:A:599:GLN:HB3	1:A:600:PRO:CD	0.41	2.45	5	1
1:A:566:LEU:HD13	1:A:628:LEU:HD22	0.41	1.92	15	1
1:A:612:ALA:O	1:A:616:GLN:HG2	0.41	2.15	3	1
1:A:577:LEU:HG	1:A:622:PHE:CD2	0.40	2.50	16	1
1:A:599:GLN:HB3	1:A:603:GLN:CG	0.40	2.47	16	1
1:A:563:SER:HB3	1:A:566:LEU:CD1	0.40	2.46	18	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	70/108 (65%)	70±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	1400/2160 (65%)	1398 (100%)	2 (0%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	60/88 (68%)	56±2 (93±3%)	4±2 (7±3%)	17	66
All	All	1200/1760 (68%)	1121 (93%)	79 (7%)	17	66

All 21 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	577	LEU	20
1	A	622	PHE	16
1	A	570	LEU	7
1	A	603	GLN	7
1	A	568	ARG	5
1	A	589	THR	4
1	A	588	GLN	3
1	A	572	GLN	2
1	A	605	GLN	2
1	A	579	ASP	2
1	A	565	LYS	1
1	A	590	GLN	1
1	A	566	LEU	1
1	A	571	GLU	1
1	A	575	GLN	1
1	A	619	GLU	1
1	A	615	GLU	1
1	A	623	GLU	1
1	A	573	LEU	1
1	A	611	MET	1
1	A	567	GLN	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 94% for the well-defined parts and 93% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1362
Number of shifts mapped to atoms	1096
Number of unparsed shifts	0
Number of shifts with mapping errors	266
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atom found in the structure. All 266 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	528	GLY	H	8.44	0.02	1
1	A	528	GLY	HA2	3.97	0.02	1
1	A	528	GLY	HA3	3.97	0.02	1
1	A	528	GLY	C	174.19	0.1	1
1	A	528	GLY	CA	45.39	0.1	1
1	A	528	GLY	N	110.14	0.1	1
1	A	529	GLN	H	8.25	0.02	1
1	A	529	GLN	HA	4.33	0.02	1
1	A	529	GLN	HB2	2.12	0.02	2
1	A	529	GLN	HB3	1.99	0.02	2
1	A	529	GLN	HG2	2.35	0.02	1
1	A	529	GLN	HG3	2.35	0.02	1
1	A	529	GLN	C	176.22	0.1	1
1	A	529	GLN	CA	56.17	0.1	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	529	GLN	CB	29.41	0.1	1
1	A	529	GLN	CG	33.82	0.1	1
1	A	529	GLN	N	119.93	0.1	1
1	A	530	GLN	H	8.46	0.02	1
1	A	530	GLN	HA	4.3	0.02	1
1	A	530	GLN	HB2	2.11	0.02	2
1	A	530	GLN	HB3	1.99	0.02	2
1	A	530	GLN	HG2	2.37	0.02	1
1	A	530	GLN	HG3	2.37	0.02	1
1	A	530	GLN	C	176.21	0.1	1
1	A	530	GLN	CA	56.37	0.1	1
1	A	530	GLN	CB	29.38	0.1	1
1	A	530	GLN	CG	33.86	0.1	1
1	A	530	GLN	N	121.27	0.1	1
1	A	531	GLU	H	8.47	0.02	1
1	A	531	GLU	HA	4.21	0.02	1
1	A	531	GLU	HB2	2.02	0.02	2
1	A	531	GLU	HB3	1.92	0.02	2
1	A	531	GLU	HG2	2.24	0.02	1
1	A	531	GLU	HG3	2.24	0.02	1
1	A	531	GLU	C	176.51	0.1	1
1	A	531	GLU	CA	57.1	0.1	1
1	A	531	GLU	CB	30.09	0.1	1
1	A	531	GLU	CG	36.32	0.1	1
1	A	531	GLU	N	121.99	0.1	1
1	A	532	GLN	H	8.31	0.02	1
1	A	532	GLN	HA	4.24	0.02	1
1	A	532	GLN	HB2	1.91	0.02	2
1	A	532	GLN	HB3	1.99	0.02	2
1	A	532	GLN	HG2	2.23	0.02	1
1	A	532	GLN	HG3	2.23	0.02	1
1	A	532	GLN	C	175.66	0.1	1
1	A	532	GLN	CA	56.07	0.1	1
1	A	532	GLN	CB	29.45	0.1	1
1	A	532	GLN	CG	33.68	0.1	1
1	A	532	GLN	N	120.57	0.1	1
1	A	533	TYR	H	8.16	0.02	1
1	A	533	TYR	HA	4.55	0.02	1
1	A	533	TYR	HB2	2.96	0.02	2
1	A	533	TYR	HB3	3.04	0.02	2
1	A	533	TYR	C	175.66	0.1	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	533	TYR	CA	58.19	0.1	1
1	A	533	TYR	CB	38.64	0.1	1
1	A	533	TYR	N	121.34	0.1	1
1	A	534	VAL	H	7.85	0.02	1
1	A	534	VAL	HA	3.98	0.02	1
1	A	534	VAL	HB	1.97	0.02	1
1	A	534	VAL	HG11	0.89	0.02	1
1	A	534	VAL	HG12	0.89	0.02	1
1	A	534	VAL	HG13	0.89	0.02	1
1	A	534	VAL	HG21	0.89	0.02	1
1	A	534	VAL	HG22	0.89	0.02	1
1	A	534	VAL	HG23	0.89	0.02	1
1	A	534	VAL	C	175.36	0.1	1
1	A	534	VAL	CA	62.35	0.1	1
1	A	534	VAL	CB	32.89	0.1	1
1	A	534	VAL	CG1	20.53	0.1	2
1	A	534	VAL	CG2	20.94	0.1	2
1	A	534	VAL	N	122.84	0.1	1
1	A	535	ALA	H	8.17	0.02	1
1	A	535	ALA	HA	4.23	0.02	1
1	A	535	ALA	HB1	1.37	0.02	1
1	A	535	ALA	HB2	1.37	0.02	1
1	A	535	ALA	HB3	1.37	0.02	1
1	A	535	ALA	C	177.54	0.1	1
1	A	535	ALA	CA	52.48	0.1	1
1	A	535	ALA	CB	19.1	0.1	1
1	A	535	ALA	N	127.19	0.1	1
1	A	536	LEU	H	8.03	0.02	1
1	A	536	LEU	HA	4.29	0.02	1
1	A	536	LEU	HB2	1.56	0.02	2
1	A	536	LEU	HB3	1.62	0.02	2
1	A	536	LEU	HD11	0.89	0.02	1
1	A	536	LEU	HD12	0.89	0.02	1
1	A	536	LEU	HD13	0.89	0.02	1
1	A	536	LEU	HD21	0.89	0.02	1
1	A	536	LEU	HD22	0.89	0.02	1
1	A	536	LEU	HD23	0.89	0.02	1
1	A	536	LEU	HG	1.58	0.02	1
1	A	536	LEU	C	177.25	0.1	1
1	A	536	LEU	CA	55.16	0.1	1
1	A	536	LEU	CB	42.46	0.1	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	536	LEU	CD1	24.84	0.1	2
1	A	536	LEU	CD2	23.55	0.1	2
1	A	536	LEU	CG	26.92	0.1	1
1	A	536	LEU	N	121.27	0.1	1
1	A	537	LYS	H	8.19	0.02	1
1	A	537	LYS	HA	4.29	0.02	1
1	A	537	LYS	HB2	1.79	0.02	2
1	A	537	LYS	HB3	1.74	0.02	2
1	A	537	LYS	HD2	1.69	0.02	1
1	A	537	LYS	HD3	1.69	0.02	1
1	A	537	LYS	HE2	2.98	0.02	1
1	A	537	LYS	HE3	2.98	0.02	1
1	A	537	LYS	HG2	1.39	0.02	1
1	A	537	LYS	HG3	1.39	0.02	1
1	A	537	LYS	C	176.18	0.1	1
1	A	537	LYS	CA	56.11	0.1	1
1	A	537	LYS	CB	32.96	0.1	1
1	A	537	LYS	CD	29.01	0.1	1
1	A	537	LYS	CE	42.24	0.1	1
1	A	537	LYS	CG	24.71	0.1	1
1	A	537	LYS	N	122.14	0.1	1
1	A	538	GLN	H	8.3	0.02	1
1	A	538	GLN	HA	4.33	0.02	1
1	A	538	GLN	HB2	1.92	0.02	2
1	A	538	GLN	HB3	2.12	0.02	2
1	A	538	GLN	HG2	2.37	0.02	1
1	A	538	GLN	HG3	2.37	0.02	1
1	A	538	GLN	C	173.86	0.1	1
1	A	538	GLN	CA	53.69	0.1	1
1	A	538	GLN	CB	28.96	0.1	1
1	A	538	GLN	N	122.55	0.1	1
1	A	539	PRO	HA	4.39	0.02	1
1	A	539	PRO	HB2	2.29	0.02	2
1	A	539	PRO	HB3	1.89	0.02	2
1	A	539	PRO	HD2	3.66	0.02	2
1	A	539	PRO	HD3	3.73	0.02	2
1	A	539	PRO	HG2	1.97	0.02	2
1	A	539	PRO	HG3	2.04	0.02	2
1	A	539	PRO	C	176.49	0.1	1
1	A	539	PRO	CA	63.17	0.1	1
1	A	539	PRO	CB	32.03	0.1	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	539	PRO	CD	50.77	0.1	1
1	A	539	PRO	CG	27.29	0.1	1
1	A	540	ALA	H	8.37	0.02	1
1	A	540	ALA	HA	4.31	0.02	1
1	A	540	ALA	HB1	1.37	0.02	1
1	A	540	ALA	HB2	1.37	0.02	1
1	A	540	ALA	HB3	1.37	0.02	1
1	A	540	ALA	C	177.76	0.1	1
1	A	540	ALA	CA	52.48	0.1	1
1	A	540	ALA	CB	19.25	0.1	1
1	A	540	ALA	N	124.44	0.1	1
1	A	541	VAL	H	8.05	0.02	1
1	A	541	VAL	HA	4.07	0.02	1
1	A	541	VAL	HB	2.03	0.02	1
1	A	541	VAL	HG11	0.93	0.02	1
1	A	541	VAL	HG12	0.93	0.02	1
1	A	541	VAL	HG13	0.93	0.02	1
1	A	541	VAL	HG21	0.93	0.02	1
1	A	541	VAL	HG22	0.93	0.02	1
1	A	541	VAL	HG23	0.93	0.02	1
1	A	541	VAL	C	176.06	0.1	1
1	A	541	VAL	CA	62.25	0.1	1
1	A	541	VAL	CB	32.83	0.1	1
1	A	541	VAL	CG1	20.84	0.1	2
1	A	541	VAL	CG2	21.08	0.1	2
1	A	541	VAL	N	119.72	0.1	1
1	A	542	LYS	H	8.36	0.02	1
1	A	542	LYS	HA	4.32	0.02	1
1	A	542	LYS	HB2	1.81	0.02	2
1	A	542	LYS	HB3	1.77	0.02	2
1	A	542	LYS	HD2	1.72	0.02	1
1	A	542	LYS	HD3	1.72	0.02	1
1	A	542	LYS	HE2	2.99	0.02	1
1	A	542	LYS	HE3	2.99	0.02	1
1	A	542	LYS	HG2	1.42	0.02	1
1	A	542	LYS	HG3	1.42	0.02	1
1	A	542	LYS	C	176.47	0.1	1
1	A	542	LYS	CA	56.29	0.1	1
1	A	542	LYS	CB	33.06	0.1	1
1	A	542	LYS	CD	29.05	0.1	1
1	A	542	LYS	CE	42.17	0.1	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	542	LYS	CG	24.7	0.1	1
1	A	542	LYS	N	125.63	0.1	1
1	A	543	LYS	H	8.44	0.02	1
1	A	543	LYS	HA	4.36	0.02	1
1	A	543	LYS	HB2	1.85	0.02	2
1	A	543	LYS	HB3	1.71	0.02	2
1	A	543	LYS	HD2	1.71	0.02	1
1	A	543	LYS	HD3	1.71	0.02	1
1	A	543	LYS	HE2	3.0	0.02	1
1	A	543	LYS	HE3	3.0	0.02	1
1	A	543	LYS	HG2	1.44	0.02	2
1	A	543	LYS	HG3	1.41	0.02	2
1	A	543	LYS	C	176.96	0.1	1
1	A	543	LYS	CA	56.44	0.1	1
1	A	543	LYS	CB	33.07	0.1	1
1	A	543	LYS	CD	29.07	0.1	1
1	A	543	LYS	CE	42.19	0.1	1
1	A	543	LYS	CG	24.7	0.1	1
1	A	543	LYS	N	123.73	0.1	1
1	A	544	THR	H	8.18	0.02	1
1	A	544	THR	HA	4.25	0.02	1
1	A	544	THR	HB	4.21	0.02	1
1	A	544	THR	HG21	1.2	0.02	1
1	A	544	THR	HG22	1.2	0.02	1
1	A	544	THR	HG23	1.2	0.02	1
1	A	544	THR	C	174.78	0.1	1
1	A	544	THR	CA	62.36	0.1	1
1	A	544	THR	CB	69.77	0.1	1
1	A	544	THR	CG2	21.69	0.1	1
1	A	544	THR	N	115.9	0.1	1
1	A	545	GLU	H	8.48	0.02	1
1	A	545	GLU	HA	4.31	0.02	1
1	A	545	GLU	HB2	1.97	0.02	2
1	A	545	GLU	HB3	2.03	0.02	2
1	A	545	GLU	HG2	2.27	0.02	1
1	A	545	GLU	HG3	2.27	0.02	1
1	A	545	GLU	C	176.79	0.1	1
1	A	545	GLU	CA	56.89	0.1	1
1	A	545	GLU	CB	30.23	0.1	1
1	A	545	GLU	CG	36.29	0.1	1
1	A	545	GLU	N	123.17	0.1	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	546	GLU	H	8.39	0.02	1
1	A	546	GLU	HA	4.22	0.02	1
1	A	546	GLU	HB2	2.03	0.02	2
1	A	546	GLU	HB3	1.97	0.02	2
1	A	546	GLU	HG2	2.28	0.02	1
1	A	546	GLU	HG3	2.28	0.02	1
1	A	546	GLU	C	176.75	0.1	1
1	A	546	GLU	CA	57.05	0.1	1
1	A	546	GLU	CB	30.25	0.1	1
1	A	546	GLU	CG	36.34	0.1	1
1	A	546	GLU	N	122.22	0.1	1
1	A	547	ALA	H	8.3	0.02	1
1	A	547	ALA	HA	4.27	0.02	1
1	A	547	ALA	HB1	1.41	0.02	1
1	A	547	ALA	HB2	1.41	0.02	1
1	A	547	ALA	HB3	1.41	0.02	1
1	A	547	ALA	C	178.02	0.1	1
1	A	547	ALA	CA	52.94	0.1	1
1	A	547	ALA	CB	19.0	0.1	1
1	A	547	ALA	N	124.9	0.1	1
1	A	548	ALA	H	8.17	0.02	1
1	A	548	ALA	HA	4.21	0.02	1
1	A	548	ALA	HB1	1.41	0.02	1
1	A	548	ALA	HB2	1.41	0.02	1
1	A	548	ALA	HB3	1.41	0.02	1
1	A	548	ALA	C	178.09	0.1	1
1	A	548	ALA	CA	52.83	0.1	1
1	A	548	ALA	CB	19.12	0.1	1
1	A	548	ALA	N	122.82	0.1	1
1	A	549	ALA	H	8.1	0.02	1
1	A	549	ALA	HA	4.28	0.02	1
1	A	549	ALA	HB1	1.41	0.02	1
1	A	549	ALA	HB2	1.41	0.02	1
1	A	549	ALA	HB3	1.41	0.02	1
1	A	549	ALA	C	177.91	0.1	1
1	A	549	ALA	CA	52.84	0.1	1
1	A	549	ALA	CB	18.97	0.1	1
1	A	549	ALA	N	122.68	0.1	1
1	A	550	ALA	H	8.08	0.02	1
1	A	550	ALA	HA	4.27	0.02	1
1	A	550	ALA	HB1	1.4	0.02	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	550	ALA	HB2	1.4	0.02	1
1	A	550	ALA	HB3	1.4	0.02	1
1	A	550	ALA	C	178.1	0.1	1
1	A	550	ALA	CA	52.75	0.1	1
1	A	550	ALA	CB	19.09	0.1	1
1	A	550	ALA	N	122.67	0.1	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	108	-0.59 ± 0.09	Should be checked
$^{13}\text{C}_\beta$	105	0.14 ± 0.05	None needed (< 0.5 ppm)
$^{13}\text{C}'$	106	-0.64 ± 0.10	Should be applied
^{15}N	102	-0.63 ± 0.22	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 94%, i.e. 925 atoms were assigned a chemical shift out of a possible 984. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	343/346 (99%)	137/138 (99%)	139/140 (99%)	67/68 (99%)
Sidechain	520/570 (91%)	355/367 (97%)	156/183 (85%)	9/20 (45%)
Aromatic	62/68 (91%)	31/33 (94%)	30/32 (94%)	1/3 (33%)
Overall	925/984 (94%)	523/538 (97%)	325/355 (92%)	77/91 (85%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 93%, i.e. 1096 atoms were assigned a chemical shift out of a possible 1174. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	415/423 (98%)	167/170 (98%)	168/170 (99%)	80/83 (96%)
Sidechain	619/683 (91%)	422/439 (96%)	187/217 (86%)	10/27 (37%)
Aromatic	62/68 (91%)	31/33 (94%)	30/32 (94%)	1/3 (33%)
Overall	1096/1174 (93%)	620/642 (97%)	385/419 (92%)	91/113 (81%)

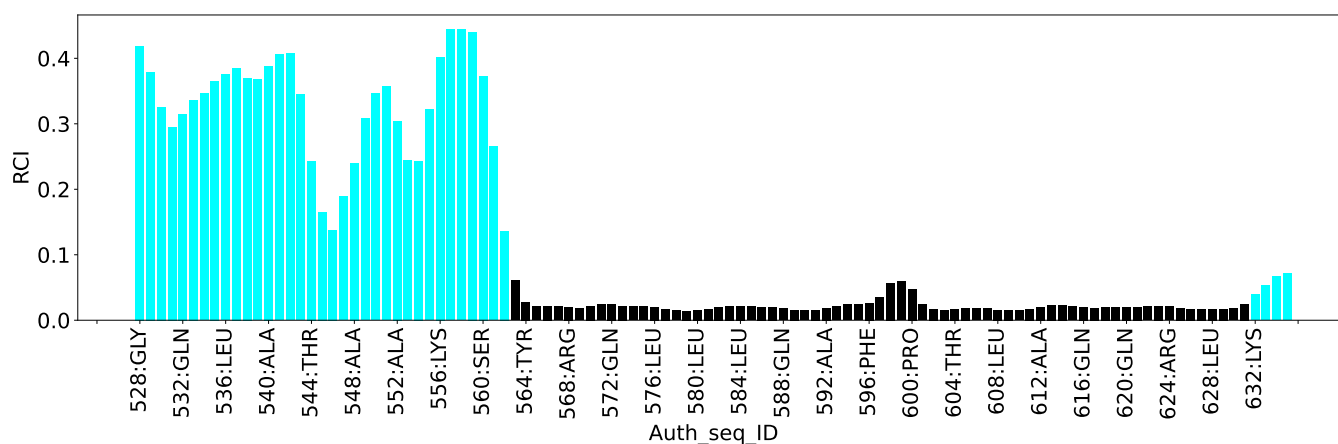
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2215
Intra-residue ($ i-j =0$)	802
Sequential ($ i-j =1$)	424
Medium range ($ i-j >1$ and $ i-j <5$)	594
Long range ($ i-j \geq 5$)	355
Inter-chain	0
Hydrogen bond restraints	40
Disulfide bond restraints	0
Total dihedral-angle restraints	158
Number of unmapped restraints	0
Number of restraints per residue	22.0
Number of long range restraints per residue ¹	3.3

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	57.4	0.2
0.2-0.5 (Medium)	142.9	0.5
>0.5 (Large)	174.2	3.95

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)	4.5	4.62
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

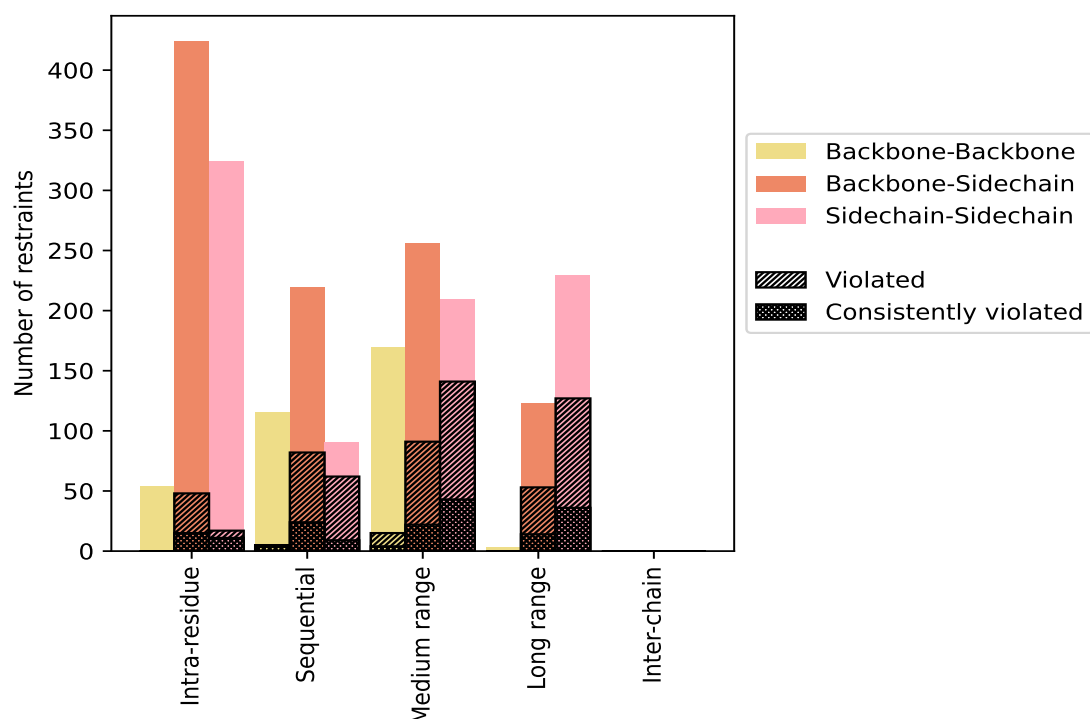
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	802	36.2	65	8.1	2.9	26	3.2	1.2
Backbone-Backbone	54	2.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	424	19.1	48	11.3	2.2	15	3.5	0.7
Sidechain-Sidechain	324	14.6	17	5.2	0.8	11	3.4	0.5
Sequential ($i-j =1$)	424	19.1	149	35.1	6.7	37	8.7	1.7
Backbone-Backbone	115	5.2	5	4.3	0.2	4	3.5	0.2
Backbone-Sidechain	219	9.9	82	37.4	3.7	24	11.0	1.1
Sidechain-Sidechain	90	4.1	62	68.9	2.8	9	10.0	0.4
Medium range ($i-j >1$ & $i-j <5$)	594	26.8	244	41.1	11.0	69	11.6	3.1
Backbone-Backbone	169	7.6	15	8.9	0.7	4	2.4	0.2
Backbone-Sidechain	216	9.8	88	40.7	4.0	22	10.2	1.0
Sidechain-Sidechain	209	9.4	141	67.5	6.4	43	20.6	1.9
Long range ($i-j \geq 5$)	355	16.0	180	50.7	8.1	50	14.1	2.3
Backbone-Backbone	3	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	123	5.6	53	43.1	2.4	14	11.4	0.6
Sidechain-Sidechain	229	10.3	127	55.5	5.7	36	15.7	1.6
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	40	1.8	3	7.5	0.1	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2215	100.0	641	28.9	28.9	182	8.2	8.2
Backbone-Backbone	341	15.4	20	5.9	0.9	8	2.3	0.4
Backbone-Sidechain	1022	46.1	274	26.8	12.4	75	7.3	3.4
Sidechain-Sidechain	852	38.5	347	40.7	15.7	99	11.6	4.5

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	44	81	149	111	0	385	0.65	3.76	0.53	0.47
2	44	95	142	115	0	396	0.6	3.76	0.53	0.44
3	38	95	137	105	0	375	0.59	3.6	0.47	0.46
4	42	79	142	101	0	364	0.6	3.64	0.48	0.47
5	41	87	139	111	0	378	0.66	3.74	0.58	0.47
6	42	86	146	100	0	374	0.6	3.43	0.47	0.44
7	40	85	134	105	0	364	0.64	3.75	0.53	0.5
8	39	92	151	102	0	384	0.59	3.62	0.48	0.46
9	46	97	142	99	0	384	0.59	3.7	0.49	0.44
10	39	88	172	102	0	401	0.67	3.83	0.59	0.49

Continued on next page...

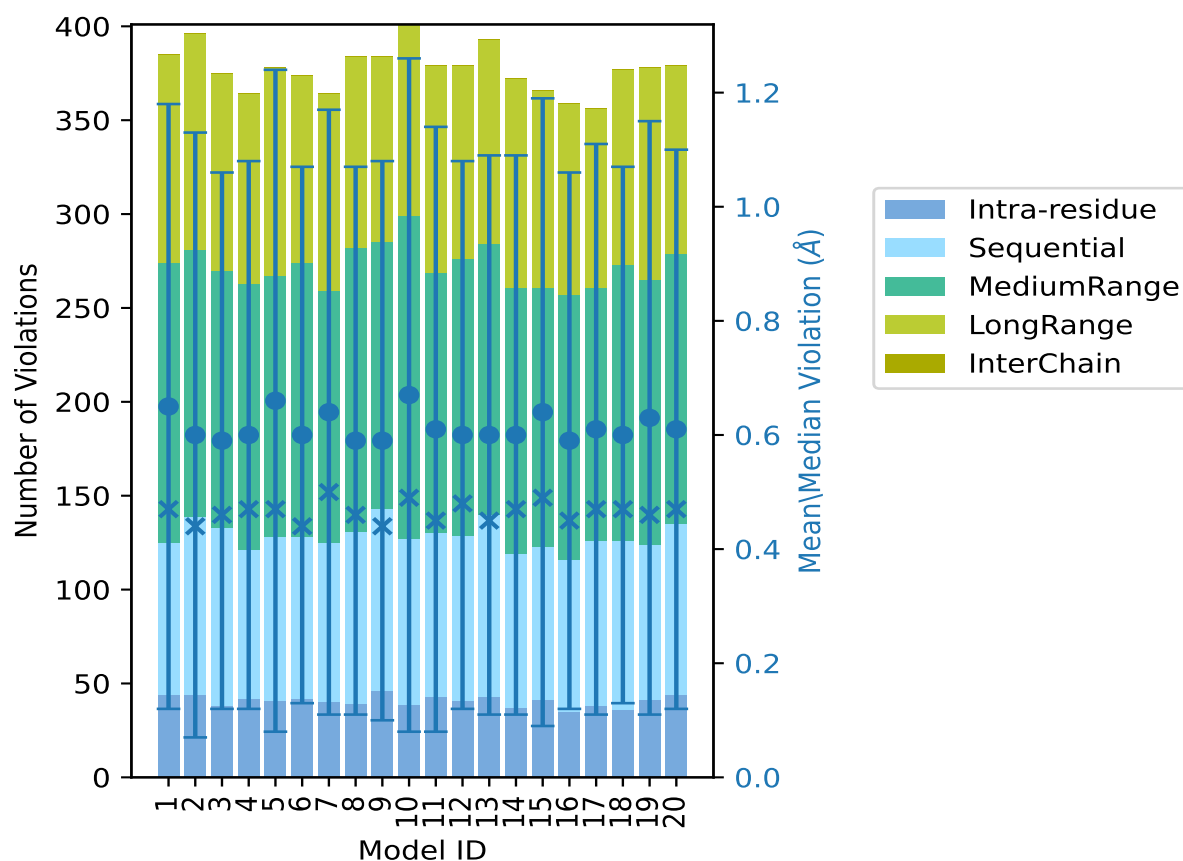
Continued from previous page...

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	43	87	139	110	0	379	0.61	3.91	0.53	0.45
12	41	88	147	103	0	379	0.6	3.67	0.48	0.48
13	43	97	144	109	0	393	0.6	3.95	0.49	0.45
14	37	82	142	111	0	372	0.6	3.65	0.49	0.47
15	41	82	138	105	0	366	0.64	3.85	0.55	0.49
16	35	81	141	102	0	359	0.59	3.52	0.47	0.45
17	38	88	135	95	0	356	0.61	3.81	0.5	0.47
18	36	90	147	104	0	377	0.6	3.46	0.47	0.47
19	41	83	141	113	0	378	0.63	3.54	0.52	0.46
20	44	91	144	100	0	379	0.61	3.68	0.49	0.47

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

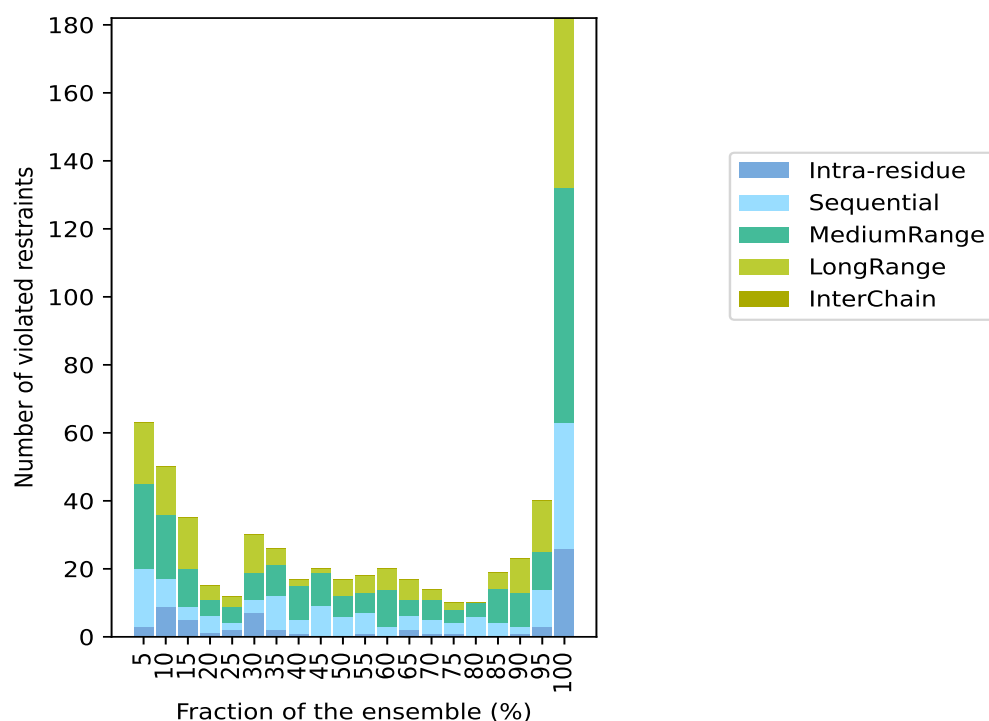
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1537(IR:737, SQ:275, MR:350, LR:175, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
3	17	25	18	0	63	1	5.0
9	8	19	14	0	50	2	10.0
5	4	11	15	0	35	3	15.0
1	5	5	4	0	15	4	20.0
2	2	5	3	0	12	5	25.0
7	4	8	11	0	30	6	30.0
2	10	9	5	0	26	7	35.0
1	4	10	2	0	17	8	40.0
0	9	10	1	0	20	9	45.0
0	6	6	5	0	17	10	50.0
1	6	6	5	0	18	11	55.0
0	3	11	6	0	20	12	60.0
2	4	5	6	0	17	13	65.0
1	4	6	3	0	14	14	70.0
1	3	4	2	0	10	15	75.0
0	6	4	0	0	10	16	80.0
0	4	10	5	0	19	17	85.0
1	2	10	10	0	23	18	90.0
3	11	11	15	0	40	19	95.0
26	37	69	50	0	182	20	100.0

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

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

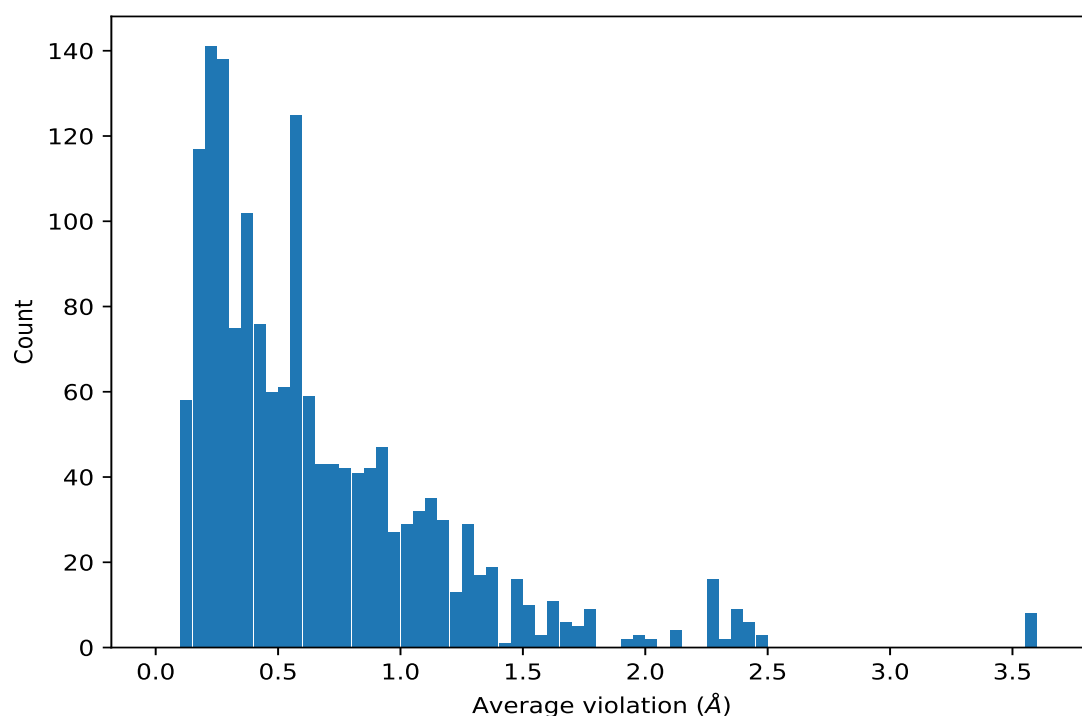
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1274)	1:618:A:LEU:HD21	1:577:A:LEU:HD21	20	3.57	0.53	3.68
(1,1274)	1:618:A:LEU:HD21	1:577:A:LEU:HD23	20	3.57	0.53	3.68
(1,1274)	1:618:A:LEU:HD22	1:577:A:LEU:HD23	20	3.57	0.53	3.68
(1,1274)	1:618:A:LEU:HD21	1:577:A:LEU:HD22	20	3.57	0.53	3.68
(1,1274)	1:618:A:LEU:HD23	1:577:A:LEU:HD22	20	3.57	0.53	3.68
(1,1274)	1:618:A:LEU:HD22	1:577:A:LEU:HD22	20	3.57	0.53	3.68
(1,1274)	1:618:A:LEU:HD23	1:577:A:LEU:HD23	20	3.57	0.53	3.68
(1,1274)	1:618:A:LEU:HD23	1:577:A:LEU:HD21	20	3.57	0.53	3.68
(1,1936)	1:588:A:GLN:HG3	1:591:A:VAL:HG21	20	2.41	0.1	2.44
(1,1936)	1:588:A:GLN:HG3	1:591:A:VAL:HG23	20	2.41	0.1	2.44
(1,1936)	1:588:A:GLN:HG3	1:591:A:VAL:HG13	20	2.41	0.1	2.44
(1,1936)	1:588:A:GLN:HG3	1:591:A:VAL:HG22	20	2.41	0.1	2.44
(1,1936)	1:588:A:GLN:HG3	1:591:A:VAL:HG12	20	2.41	0.1	2.44
(1,1936)	1:588:A:GLN:HG3	1:591:A:VAL:HG11	20	2.41	0.1	2.44
(1,1746)	1:612:A:ALA:HB2	1:584:A:LEU:HD22	20	2.38	0.12	2.4
(1,1746)	1:612:A:ALA:HB3	1:584:A:LEU:HD22	20	2.38	0.12	2.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1746)	1:612:A:ALA:HB1	1:584:A:LEU:HD23	20	2.38	0.12	2.4
(1,1746)	1:612:A:ALA:HB1	1:584:A:LEU:HD22	20	2.38	0.12	2.4
(1,1746)	1:612:A:ALA:HB2	1:584:A:LEU:HD21	20	2.38	0.12	2.4
(1,1746)	1:612:A:ALA:HB2	1:584:A:LEU:HD23	20	2.38	0.12	2.4
(1,1746)	1:612:A:ALA:HB3	1:584:A:LEU:HD23	20	2.38	0.12	2.4
(1,1746)	1:612:A:ALA:HB3	1:584:A:LEU:HD21	20	2.38	0.12	2.4
(1,1746)	1:612:A:ALA:HB1	1:584:A:LEU:HD21	20	2.38	0.12	2.4
(1,1969)	1:579:A:ASP:HB3	1:578:A:GLU:HB2	20	2.3	0.1	2.32
(1,1969)	1:579:A:ASP:HB3	1:575:A:GLN:HB2	20	2.3	0.1	2.32
(1,1747)	1:613:A:ALA:HB1	1:580:A:LEU:HD21	20	2.28	0.2	2.26
(1,1747)	1:613:A:ALA:HB2	1:580:A:LEU:HD21	20	2.28	0.2	2.26
(1,1747)	1:613:A:ALA:HB3	1:580:A:LEU:HD23	20	2.28	0.2	2.26
(1,1747)	1:613:A:ALA:HB2	1:580:A:LEU:HD22	20	2.28	0.2	2.26
(1,1747)	1:613:A:ALA:HB1	1:580:A:LEU:HD22	20	2.28	0.2	2.26
(1,1747)	1:613:A:ALA:HB1	1:580:A:LEU:HD23	20	2.28	0.2	2.26
(1,1747)	1:613:A:ALA:HB3	1:580:A:LEU:HD21	20	2.28	0.2	2.26
(1,1747)	1:613:A:ALA:HB2	1:580:A:LEU:HD23	20	2.28	0.2	2.26
(1,1748)	1:613:A:ALA:HB1	1:580:A:LEU:HD21	20	2.28	0.2	2.26
(1,1748)	1:613:A:ALA:HB2	1:580:A:LEU:HD21	20	2.28	0.2	2.26
(1,1748)	1:613:A:ALA:HB3	1:580:A:LEU:HD23	20	2.28	0.2	2.26
(1,1748)	1:613:A:ALA:HB2	1:580:A:LEU:HD22	20	2.28	0.2	2.26
(1,1748)	1:613:A:ALA:HB1	1:580:A:LEU:HD22	20	2.28	0.2	2.26
(1,1748)	1:613:A:ALA:HB1	1:580:A:LEU:HD23	20	2.28	0.2	2.26
(1,1748)	1:613:A:ALA:HB3	1:580:A:LEU:HD21	20	2.28	0.2	2.26
(1,1748)	1:613:A:ALA:HB2	1:580:A:LEU:HD23	20	2.28	0.2	2.26
(1,1846)	1:622:A:PHE:HA	1:576:A:LEU:HD23	20	2.1	0.39	2.15
(1,1846)	1:622:A:PHE:HA	1:576:A:LEU:HD21	20	2.1	0.39	2.15
(1,1846)	1:622:A:PHE:HA	1:576:A:LEU:HD22	20	2.1	0.39	2.15
(1,1846)	1:622:A:PHE:HA	1:618:A:LEU:HD21	20	2.1	0.39	2.15
(1,1753)	1:614:A:ALA:HB2	1:617:A:GLU:HB2	20	1.79	0.16	1.81
(1,1753)	1:614:A:ALA:HB3	1:616:A:GLN:HB2	20	1.79	0.16	1.81
(1,1753)	1:614:A:ALA:HB1	1:617:A:GLU:HB2	20	1.79	0.16	1.81
(1,1753)	1:614:A:ALA:HB1	1:616:A:GLN:HB3	20	1.79	0.16	1.81
(1,1753)	1:614:A:ALA:HB3	1:617:A:GLU:HB2	20	1.79	0.16	1.81
(1,1753)	1:614:A:ALA:HB3	1:616:A:GLN:HB3	20	1.79	0.16	1.81
(1,1069)	1:579:A:ASP:HB2	1:583:A:LYS:HB2	20	1.72	0.08	1.72
(1,1930)	1:556:A:LYS:HB3	1:555:A:VAL:HB	20	1.72	0.62	1.61
(1,1930)	1:565:A:LYS:HB3	1:569:A:GLU:HB3	20	1.72	0.62	1.61
(1,1928)	1:583:A:LYS:HB3	1:584:A:LEU:HD22	20	1.69	0.08	1.69
(1,1928)	1:583:A:LYS:HB3	1:584:A:LEU:HD23	20	1.69	0.08	1.69
(1,1928)	1:583:A:LYS:HB3	1:584:A:LEU:HD21	20	1.69	0.08	1.69
(1,1366)	1:566:A:LEU:HD22	1:631:A:LEU:HD12	20	1.62	1.1	1.05

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1366)	1:566:A:LEU:HD22	1:631:A:LEU:HD13	20	1.62	1.1	1.05
(1,1366)	1:566:A:LEU:HD21	1:631:A:LEU:HD12	20	1.62	1.1	1.05
(1,1366)	1:566:A:LEU:HD23	1:631:A:LEU:HD12	20	1.62	1.1	1.05
(1,1366)	1:566:A:LEU:HD23	1:631:A:LEU:HD11	20	1.62	1.1	1.05
(1,1366)	1:566:A:LEU:HD21	1:631:A:LEU:HD11	20	1.62	1.1	1.05
(1,1366)	1:566:A:LEU:HD23	1:631:A:LEU:HD13	20	1.62	1.1	1.05
(1,1366)	1:566:A:LEU:HD21	1:631:A:LEU:HD13	20	1.62	1.1	1.05
(1,2033)	1:577:A:LEU:HG	1:578:A:GLU:HA	20	1.58	0.4	1.7
(1,2033)	1:562:A:LEU:HG	1:563:A:SER:HB3	20	1.58	0.4	1.7
(1,1385)	1:622:A:PHE:HB2	1:625:A:TRP:HB2	20	1.5	0.11	1.52
(1,2138)	1:584:A:LEU:HD11	1:582:A:ALA:HA	20	1.48	0.14	1.51
(1,2138)	1:584:A:LEU:HD13	1:589:A:THR:HB	20	1.48	0.14	1.51
(1,2138)	1:618:A:LEU:HD13	1:614:A:ALA:HA	20	1.48	0.14	1.51
(1,2138)	1:584:A:LEU:HD12	1:589:A:THR:HB	20	1.48	0.14	1.51
(1,2138)	1:584:A:LEU:HD13	1:582:A:ALA:HA	20	1.48	0.14	1.51
(1,2138)	1:584:A:LEU:HD12	1:582:A:ALA:HA	20	1.48	0.14	1.51
(1,2138)	1:618:A:LEU:HD11	1:614:A:ALA:HA	20	1.48	0.14	1.51
(1,2074)	1:576:A:LEU:HB2	1:574:A:PRO:HA	20	1.47	0.07	1.46
(1,1715)	1:577:A:LEU:HD13	1:619:A:GLU:HG2	20	1.45	0.28	1.56
(1,1715)	1:577:A:LEU:HD12	1:617:A:GLU:HG2	20	1.45	0.28	1.56
(1,1715)	1:577:A:LEU:HD11	1:620:A:GLN:HG3	20	1.45	0.28	1.56
(1,1715)	1:577:A:LEU:HD12	1:620:A:GLN:HG3	20	1.45	0.28	1.56
(1,1715)	1:577:A:LEU:HD13	1:617:A:GLU:HG2	20	1.45	0.28	1.56
(1,1715)	1:577:A:LEU:HD13	1:620:A:GLN:HG3	20	1.45	0.28	1.56
(1,1715)	1:577:A:LEU:HD11	1:617:A:GLU:HG2	20	1.45	0.28	1.56
(1,1715)	1:577:A:LEU:HD11	1:619:A:GLU:HG2	20	1.45	0.28	1.56
(1,611)	1:625:A:TRP:HH2	1:626:A:GLU:HG3	20	1.4	0.13	1.42
(1,1393)	1:630:A:ALA:HB1	1:626:A:GLU:HB2	20	1.33	0.15	1.27
(1,1393)	1:630:A:ALA:HB3	1:626:A:GLU:HB2	20	1.33	0.15	1.27
(1,1393)	1:630:A:ALA:HB2	1:626:A:GLU:HB2	20	1.33	0.15	1.27
(1,2140)	1:628:A:LEU:HD13	1:625:A:TRP:HB3	20	1.26	0.14	1.26
(1,2140)	1:628:A:LEU:HD11	1:625:A:TRP:HB3	20	1.26	0.14	1.26
(1,2140)	1:628:A:LEU:HD12	1:625:A:TRP:HB3	20	1.26	0.14	1.26
(1,1902)	1:567:A:GLN:HB2	1:562:A:LEU:HB3	20	1.25	0.5	1.1
(1,1902)	1:567:A:GLN:HB2	1:562:A:LEU:HB2	20	1.25	0.5	1.1
(1,1902)	1:567:A:GLN:HB3	1:562:A:LEU:HB3	20	1.25	0.5	1.1
(1,1902)	1:567:A:GLN:HB2	1:562:A:LEU:HG	20	1.25	0.5	1.1
(1,1902)	1:567:A:GLN:HB2	1:570:A:LEU:HB3	20	1.25	0.5	1.1
(1,1902)	1:609:A:ALA:HB3	1:608:A:LEU:HG	20	1.25	0.5	1.1
(1,1873)	1:613:A:ALA:HB2	1:587:A:LEU:HD12	20	1.25	0.14	1.25
(1,1873)	1:613:A:ALA:HB3	1:587:A:LEU:HD11	20	1.25	0.14	1.25
(1,1873)	1:613:A:ALA:HB1	1:587:A:LEU:HD13	20	1.25	0.14	1.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1873)	1:613:A:ALA:HB2	1:587:A:LEU:HD13	20	1.25	0.14	1.25
(1,1873)	1:613:A:ALA:HB1	1:587:A:LEU:HD11	20	1.25	0.14	1.25
(1,1873)	1:613:A:ALA:HB1	1:587:A:LEU:HD12	20	1.25	0.14	1.25
(1,1873)	1:613:A:ALA:HB3	1:587:A:LEU:HD12	20	1.25	0.14	1.25
(1,1873)	1:613:A:ALA:HB3	1:587:A:LEU:HD13	20	1.25	0.14	1.25
(1,1518)	1:578:A:GLU:H	1:576:A:LEU:HD13	20	1.24	0.25	1.25
(1,1518)	1:578:A:GLU:H	1:576:A:LEU:HD12	20	1.24	0.25	1.25
(1,1518)	1:578:A:GLU:H	1:576:A:LEU:HD11	20	1.24	0.25	1.25
(1,1518)	1:578:A:GLU:H	1:618:A:LEU:HD22	20	1.24	0.25	1.25
(1,1956)	1:627:A:TYR:HB3	1:630:A:ALA:HB3	20	1.22	0.13	1.29
(1,1956)	1:627:A:TYR:HB3	1:630:A:ALA:HB2	20	1.22	0.13	1.29
(1,1956)	1:627:A:TYR:HB3	1:630:A:ALA:HB1	20	1.22	0.13	1.29
(1,1713)	1:577:A:LEU:HD13	1:581:A:GLU:HB2	20	1.16	0.13	1.16
(1,1713)	1:577:A:LEU:HD13	1:617:A:GLU:HG3	20	1.16	0.13	1.16
(1,1713)	1:577:A:LEU:HD11	1:617:A:GLU:HG3	20	1.16	0.13	1.16
(1,1713)	1:577:A:LEU:HD11	1:581:A:GLU:HB2	20	1.16	0.13	1.16
(1,1713)	1:577:A:LEU:HD12	1:581:A:GLU:HB2	20	1.16	0.13	1.16
(1,2149)	1:628:A:LEU:HD23	1:631:A:LEU:HD13	20	1.15	0.25	1.17
(1,2149)	1:628:A:LEU:HD22	1:631:A:LEU:HD13	20	1.15	0.25	1.17
(1,2149)	1:628:A:LEU:HD21	1:631:A:LEU:HD12	20	1.15	0.25	1.17
(1,2149)	1:628:A:LEU:HD21	1:631:A:LEU:HD11	20	1.15	0.25	1.17
(1,2149)	1:628:A:LEU:HD21	1:631:A:LEU:HD13	20	1.15	0.25	1.17
(1,2149)	1:631:A:LEU:HD11	1:566:A:LEU:HD13	20	1.15	0.25	1.17
(1,2149)	1:628:A:LEU:HD23	1:631:A:LEU:HD12	20	1.15	0.25	1.17
(1,2149)	1:631:A:LEU:HD13	1:566:A:LEU:HD11	20	1.15	0.25	1.17
(1,2149)	1:628:A:LEU:HD23	1:631:A:LEU:HD11	20	1.15	0.25	1.17
(1,2149)	1:631:A:LEU:HD13	1:566:A:LEU:HD12	20	1.15	0.25	1.17
(1,2149)	1:628:A:LEU:HD22	1:631:A:LEU:HD11	20	1.15	0.25	1.17
(1,1590)	1:583:A:LYS:H	1:618:A:LEU:HD23	20	1.15	0.08	1.16
(1,1590)	1:583:A:LYS:H	1:618:A:LEU:HD21	20	1.15	0.08	1.16
(1,1590)	1:583:A:LYS:H	1:618:A:LEU:HD13	20	1.15	0.08	1.16
(1,1590)	1:583:A:LYS:H	1:618:A:LEU:HD22	20	1.15	0.08	1.16
(1,1590)	1:583:A:LYS:H	1:618:A:LEU:HD11	20	1.15	0.08	1.16
(1,1590)	1:583:A:LYS:H	1:618:A:LEU:HD12	20	1.15	0.08	1.16
(1,1280)	1:573:A:LEU:HD21	1:580:A:LEU:HD12	20	1.12	0.84	0.85
(1,1280)	1:573:A:LEU:HD21	1:580:A:LEU:HD13	20	1.12	0.84	0.85
(1,1280)	1:573:A:LEU:HD23	1:580:A:LEU:HD13	20	1.12	0.84	0.85
(1,1280)	1:573:A:LEU:HD22	1:580:A:LEU:HD13	20	1.12	0.84	0.85
(1,1280)	1:573:A:LEU:HD23	1:580:A:LEU:HD12	20	1.12	0.84	0.85
(1,1280)	1:573:A:LEU:HD22	1:580:A:LEU:HD11	20	1.12	0.84	0.85
(1,1280)	1:573:A:LEU:HD23	1:580:A:LEU:HD11	20	1.12	0.84	0.85
(1,1280)	1:573:A:LEU:HD22	1:580:A:LEU:HD12	20	1.12	0.84	0.85

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2125)	1:607:A:VAL:HG11	1:590:A:GLN:HA	20	1.12	0.11	1.14
(1,2125)	1:580:A:LEU:HD21	1:617:A:GLU:HA	20	1.12	0.11	1.14
(1,2125)	1:580:A:LEU:HD23	1:617:A:GLU:HA	20	1.12	0.11	1.14
(1,2125)	1:580:A:LEU:HD22	1:617:A:GLU:HA	20	1.12	0.11	1.14
(1,2125)	1:607:A:VAL:HG13	1:590:A:GLN:HA	20	1.12	0.11	1.14
(1,2125)	1:607:A:VAL:HG12	1:590:A:GLN:HA	20	1.12	0.11	1.14
(1,1850)	1:589:A:THR:HA	1:590:A:GLN:HB2	20	1.1	0.32	1.03
(1,1850)	1:589:A:THR:HA	1:590:A:GLN:HG3	20	1.1	0.32	1.03
(1,1630)	1:621:A:ALA:H	1:576:A:LEU:HD22	20	1.1	0.21	1.14
(1,1630)	1:621:A:ALA:H	1:576:A:LEU:HD23	20	1.1	0.21	1.14
(1,1630)	1:621:A:ALA:H	1:576:A:LEU:HD21	20	1.1	0.21	1.14
(1,1630)	1:621:A:ALA:H	1:618:A:LEU:HD21	20	1.1	0.21	1.14
(1,1684)	1:625:A:TRP:HE3	1:573:A:LEU:HD21	20	1.1	0.12	1.1
(1,1684)	1:625:A:TRP:HE3	1:573:A:LEU:HD22	20	1.1	0.12	1.1
(1,1684)	1:625:A:TRP:HE3	1:573:A:LEU:HD23	20	1.1	0.12	1.1
(1,1945)	1:585:A:GLU:HG2	1:582:A:ALA:HB3	20	1.09	0.3	1.14
(1,1945)	1:585:A:GLU:HG2	1:582:A:ALA:HB2	20	1.09	0.3	1.14
(1,1945)	1:585:A:GLU:HG2	1:586:A:ALA:HB2	20	1.09	0.3	1.14
(1,1945)	1:585:A:GLU:HG2	1:582:A:ALA:HB1	20	1.09	0.3	1.14
(1,1612)	1:616:A:GLN:H	1:618:A:LEU:HD22	20	1.09	0.17	1.1
(1,1612)	1:616:A:GLN:H	1:618:A:LEU:HD23	20	1.09	0.17	1.1
(1,1612)	1:616:A:GLN:H	1:618:A:LEU:HD21	20	1.09	0.17	1.1
(1,1612)	1:616:A:GLN:H	1:618:A:LEU:HD11	20	1.09	0.17	1.1
(1,1583)	1:611:A:MET:H	1:609:A:ALA:HB2	20	1.07	0.06	1.08
(1,1583)	1:611:A:MET:H	1:609:A:ALA:HB1	20	1.07	0.06	1.08
(1,1583)	1:611:A:MET:H	1:609:A:ALA:HB3	20	1.07	0.06	1.08
(1,1583)	1:611:A:MET:H	1:612:A:ALA:HB1	20	1.07	0.06	1.08
(1,1583)	1:611:A:MET:H	1:613:A:ALA:HB1	20	1.07	0.06	1.08
(1,1583)	1:611:A:MET:H	1:612:A:ALA:HB2	20	1.07	0.06	1.08
(1,1583)	1:611:A:MET:H	1:613:A:ALA:HB3	20	1.07	0.06	1.08
(1,1392)	1:621:A:ALA:HB3	1:625:A:TRP:HB3	20	1.07	0.11	1.08
(1,1392)	1:621:A:ALA:HB2	1:625:A:TRP:HB3	20	1.07	0.11	1.08
(1,1392)	1:621:A:ALA:HB1	1:625:A:TRP:HB3	20	1.07	0.11	1.08
(1,1252)	1:580:A:LEU:HA	1:579:A:ASP:HB2	20	1.03	0.04	1.04
(1,637)	1:604:A:THR:HG23	1:607:A:VAL:HG22	20	1.02	0.13	1.08
(1,637)	1:604:A:THR:HG21	1:607:A:VAL:HG23	20	1.02	0.13	1.08
(1,637)	1:604:A:THR:HG23	1:607:A:VAL:HG21	20	1.02	0.13	1.08
(1,637)	1:604:A:THR:HG22	1:607:A:VAL:HG22	20	1.02	0.13	1.08
(1,637)	1:604:A:THR:HG22	1:607:A:VAL:HG23	20	1.02	0.13	1.08
(1,637)	1:604:A:THR:HG21	1:607:A:VAL:HG22	20	1.02	0.13	1.08
(1,637)	1:604:A:THR:HG22	1:607:A:VAL:HG21	20	1.02	0.13	1.08
(1,637)	1:604:A:THR:HG23	1:607:A:VAL:HG23	20	1.02	0.13	1.08

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,637)	1:604:A:THR:HG21	1:607:A:VAL:HG21	20	1.02	0.13	1.08
(1,649)	1:591:A:VAL:HG11	1:596:A:PHE:HB2	20	1.02	0.13	1.06
(1,649)	1:591:A:VAL:HG12	1:596:A:PHE:HB2	20	1.02	0.13	1.06
(1,649)	1:591:A:VAL:HG13	1:596:A:PHE:HB2	20	1.02	0.13	1.06
(1,2161)	1:628:A:LEU:HA	1:630:A:ALA:HB3	20	1.01	0.1	0.98
(1,2161)	1:628:A:LEU:HA	1:630:A:ALA:HB2	20	1.01	0.1	0.98
(1,2161)	1:628:A:LEU:HA	1:630:A:ALA:HB1	20	1.01	0.1	0.98
(1,1015)	1:609:A:ALA:HB3	1:605:A:GLN:HG3	20	1.01	0.09	0.99
(1,1015)	1:609:A:ALA:HB2	1:605:A:GLN:HG3	20	1.01	0.09	0.99
(1,1015)	1:609:A:ALA:HB1	1:605:A:GLN:HG3	20	1.01	0.09	0.99
(1,2155)	1:628:A:LEU:HD11	1:624:A:ARG:HB2	20	0.99	0.35	0.94
(1,2155)	1:628:A:LEU:HD12	1:624:A:ARG:HB2	20	0.99	0.35	0.94
(1,2155)	1:624:A:ARG:HB2	1:628:A:LEU:HD23	20	0.99	0.35	0.94
(1,2155)	1:628:A:LEU:HD13	1:624:A:ARG:HB2	20	0.99	0.35	0.94
(1,644)	1:591:A:VAL:HG11	1:607:A:VAL:HG13	20	0.98	0.12	0.98
(1,644)	1:591:A:VAL:HG13	1:607:A:VAL:HG11	20	0.98	0.12	0.98
(1,644)	1:591:A:VAL:HG13	1:607:A:VAL:HG12	20	0.98	0.12	0.98
(1,644)	1:591:A:VAL:HG11	1:607:A:VAL:HG11	20	0.98	0.12	0.98
(1,644)	1:591:A:VAL:HG13	1:607:A:VAL:HG13	20	0.98	0.12	0.98
(1,644)	1:591:A:VAL:HG11	1:607:A:VAL:HG12	20	0.98	0.12	0.98
(1,644)	1:591:A:VAL:HG12	1:607:A:VAL:HG11	20	0.98	0.12	0.98
(1,644)	1:591:A:VAL:HG12	1:607:A:VAL:HG12	20	0.98	0.12	0.98
(1,1856)	1:580:A:LEU:HA	1:583:A:LYS:HE3	20	0.97	0.09	1.0
(1,1856)	1:580:A:LEU:HA	1:583:A:LYS:HE2	20	0.97	0.09	1.0
(1,1856)	1:580:A:LEU:HA	1:579:A:ASP:HB2	20	0.97	0.09	1.0
(1,1898)	1:628:A:LEU:HG	1:631:A:LEU:HB2	20	0.96	0.21	0.94
(1,1067)	1:579:A:ASP:HB2	1:580:A:LEU:HD23	20	0.96	0.07	0.94
(1,1067)	1:579:A:ASP:HB2	1:580:A:LEU:HD22	20	0.96	0.07	0.94
(1,1067)	1:579:A:ASP:HB2	1:580:A:LEU:HD21	20	0.96	0.07	0.94
(1,1722)	1:591:A:VAL:HG13	1:611:A:MET:HB2	20	0.96	0.17	0.92
(1,1722)	1:591:A:VAL:HG11	1:611:A:MET:HB2	20	0.96	0.17	0.92
(1,1722)	1:591:A:VAL:HG12	1:611:A:MET:HB2	20	0.96	0.17	0.92
(1,1968)	1:579:A:ASP:HB3	1:583:A:LYS:HD2	20	0.94	0.12	0.97
(1,1968)	1:579:A:ASP:HB3	1:576:A:LEU:HB3	20	0.94	0.12	0.97
(1,1053)	1:577:A:LEU:HD12	1:617:A:GLU:HG3	20	0.94	0.41	0.9
(1,1053)	1:577:A:LEU:HD13	1:617:A:GLU:HG3	20	0.94	0.41	0.9
(1,1053)	1:577:A:LEU:HD11	1:617:A:GLU:HG3	20	0.94	0.41	0.9
(1,1495)	1:584:A:LEU:H	1:584:A:LEU:HD13	20	0.94	0.05	0.94
(1,1495)	1:584:A:LEU:H	1:584:A:LEU:HD11	20	0.94	0.05	0.94
(1,1495)	1:584:A:LEU:H	1:584:A:LEU:HD12	20	0.94	0.05	0.94
(1,975)	1:615:A:GLU:HB2	1:584:A:LEU:HD12	20	0.94	0.22	0.89
(1,975)	1:615:A:GLU:HB2	1:584:A:LEU:HD13	20	0.94	0.22	0.89

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,975)	1:615:A:GLU:HB2	1:584:A:LEU:HD11	20	0.94	0.22	0.89
(1,1489)	1:586:A:ALA:H	1:584:A:LEU:HD23	20	0.93	0.08	0.92
(1,1489)	1:586:A:ALA:H	1:584:A:LEU:HD21	20	0.93	0.08	0.92
(1,1489)	1:586:A:ALA:H	1:584:A:LEU:HD22	20	0.93	0.08	0.92
(1,1743)	1:628:A:LEU:HD22	1:625:A:TRP:HA	20	0.93	0.2	0.98
(1,1743)	1:628:A:LEU:HD23	1:570:A:LEU:HA	20	0.93	0.2	0.98
(1,1743)	1:628:A:LEU:HD23	1:625:A:TRP:HA	20	0.93	0.2	0.98
(1,1743)	1:628:A:LEU:HD22	1:570:A:LEU:HA	20	0.93	0.2	0.98
(1,1743)	1:628:A:LEU:HD21	1:570:A:LEU:HA	20	0.93	0.2	0.98
(1,1743)	1:628:A:LEU:HD21	1:625:A:TRP:HA	20	0.93	0.2	0.98
(1,2172)	1:625:A:TRP:HE3	1:573:A:LEU:HD21	20	0.91	0.12	0.91
(1,2172)	1:625:A:TRP:HE3	1:573:A:LEU:HD22	20	0.91	0.12	0.91
(1,2172)	1:625:A:TRP:HE3	1:573:A:LEU:HD23	20	0.91	0.12	0.91
(1,695)	1:586:A:ALA:HB3	1:583:A:LYS:HB2	20	0.9	0.05	0.92
(1,695)	1:586:A:ALA:HB2	1:583:A:LYS:HB2	20	0.9	0.05	0.92
(1,695)	1:586:A:ALA:HB1	1:583:A:LYS:HB2	20	0.9	0.05	0.92
(1,1681)	1:622:A:PHE:HD1	1:577:A:LEU:HD23	20	0.9	0.11	0.9
(1,1681)	1:622:A:PHE:HD1	1:577:A:LEU:HD22	20	0.9	0.11	0.9
(1,1681)	1:625:A:TRP:HE3	1:577:A:LEU:HD21	20	0.9	0.11	0.9
(1,1681)	1:622:A:PHE:HE1	1:577:A:LEU:HD22	20	0.9	0.11	0.9
(1,1681)	1:625:A:TRP:HE3	1:577:A:LEU:HD23	20	0.9	0.11	0.9
(1,1681)	1:622:A:PHE:HE1	1:577:A:LEU:HD23	20	0.9	0.11	0.9
(1,1681)	1:622:A:PHE:HD1	1:577:A:LEU:HD21	20	0.9	0.11	0.9
(1,1681)	1:625:A:TRP:HE3	1:577:A:LEU:HD22	20	0.9	0.11	0.9
(1,1761)	1:621:A:ALA:HB3	1:624:A:ARG:HG2	20	0.89	0.16	0.9
(1,1761)	1:621:A:ALA:HB2	1:624:A:ARG:HG2	20	0.89	0.16	0.9
(1,1761)	1:621:A:ALA:HB1	1:624:A:ARG:HG2	20	0.89	0.16	0.9
(1,1761)	1:621:A:ALA:HB2	1:580:A:LEU:HG	20	0.89	0.16	0.9
(1,1761)	1:621:A:ALA:HB3	1:580:A:LEU:HG	20	0.89	0.16	0.9
(1,1761)	1:621:A:ALA:HB1	1:580:A:LEU:HG	20	0.89	0.16	0.9
(1,43)	1:597:A:PHE:H	1:596:A:PHE:HB2	20	0.89	0.05	0.9
(1,1947)	1:581:A:GLU:HG2	1:584:A:LEU:HD11	20	0.88	0.27	0.88
(1,1947)	1:581:A:GLU:HG2	1:618:A:LEU:HD13	20	0.88	0.27	0.88
(1,1947)	1:581:A:GLU:HG2	1:584:A:LEU:HD12	20	0.88	0.27	0.88
(1,1947)	1:615:A:GLU:HG2	1:584:A:LEU:HD11	20	0.88	0.27	0.88
(1,1947)	1:581:A:GLU:HG2	1:618:A:LEU:HD12	20	0.88	0.27	0.88
(1,1947)	1:581:A:GLU:HG2	1:584:A:LEU:HD13	20	0.88	0.27	0.88
(1,1947)	1:615:A:GLU:HG2	1:584:A:LEU:HD12	20	0.88	0.27	0.88
(1,1619)	1:618:A:LEU:H	1:618:A:LEU:HD11	20	0.88	0.03	0.88
(1,1619)	1:618:A:LEU:H	1:618:A:LEU:HD12	20	0.88	0.03	0.88
(1,1619)	1:618:A:LEU:H	1:618:A:LEU:HD13	20	0.88	0.03	0.88
(1,1619)	1:618:A:LEU:H	1:618:A:LEU:HD21	20	0.88	0.03	0.88

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1024)	1:590:A:GLN:HG3	1:589:A:THR:HG22	20	0.85	0.5	0.8
(1,1024)	1:590:A:GLN:HG3	1:589:A:THR:HG21	20	0.85	0.5	0.8
(1,1024)	1:590:A:GLN:HG3	1:589:A:THR:HG23	20	0.85	0.5	0.8
(1,1271)	1:576:A:LEU:HD11	1:621:A:ALA:HB2	20	0.83	0.19	0.86
(1,1271)	1:576:A:LEU:HD13	1:621:A:ALA:HB1	20	0.83	0.19	0.86
(1,1271)	1:576:A:LEU:HD12	1:621:A:ALA:HB3	20	0.83	0.19	0.86
(1,1271)	1:576:A:LEU:HD13	1:621:A:ALA:HB3	20	0.83	0.19	0.86
(1,1271)	1:576:A:LEU:HD11	1:621:A:ALA:HB1	20	0.83	0.19	0.86
(1,1271)	1:576:A:LEU:HD12	1:621:A:ALA:HB1	20	0.83	0.19	0.86
(1,1271)	1:576:A:LEU:HD12	1:621:A:ALA:HB2	20	0.83	0.19	0.86
(1,1271)	1:576:A:LEU:HD13	1:621:A:ALA:HB2	20	0.83	0.19	0.86
(1,1720)	1:604:A:THR:HG21	1:597:A:PHE:HB2	20	0.81	0.1	0.85
(1,1720)	1:604:A:THR:HG22	1:597:A:PHE:HB2	20	0.81	0.1	0.85
(1,1720)	1:604:A:THR:HG21	1:600:A:PRO:HD3	20	0.81	0.1	0.85
(1,1720)	1:604:A:THR:HG23	1:600:A:PRO:HD3	20	0.81	0.1	0.85
(1,1720)	1:604:A:THR:HG23	1:597:A:PHE:HB2	20	0.81	0.1	0.85
(1,1720)	1:604:A:THR:HG22	1:600:A:PRO:HD3	20	0.81	0.1	0.85
(1,2037)	1:609:A:ALA:HA	1:605:A:GLN:HB3	20	0.81	0.13	0.79
(1,2037)	1:603:A:GLN:HA	1:605:A:GLN:HB2	20	0.81	0.13	0.79
(1,2037)	1:609:A:ALA:HA	1:605:A:GLN:HB2	20	0.81	0.13	0.79
(1,2037)	1:603:A:GLN:HA	1:599:A:GLN:HB2	20	0.81	0.13	0.79
(1,1792)	1:610:A:ASP:HA	1:587:A:LEU:HD23	20	0.8	0.05	0.8
(1,1792)	1:610:A:ASP:HA	1:587:A:LEU:HD21	20	0.8	0.05	0.8
(1,1792)	1:610:A:ASP:HA	1:587:A:LEU:HD22	20	0.8	0.05	0.8
(1,1733)	1:607:A:VAL:HG21	1:610:A:ASP:HB3	20	0.79	0.15	0.77
(1,1733)	1:607:A:VAL:HG22	1:610:A:ASP:HB3	20	0.79	0.15	0.77
(1,1733)	1:607:A:VAL:HG23	1:610:A:ASP:HB3	20	0.79	0.15	0.77
(1,1966)	1:579:A:ASP:HB2	1:576:A:LEU:HB3	20	0.78	0.06	0.78
(1,670)	1:591:A:VAL:HG23	1:607:A:VAL:HG22	20	0.77	0.12	0.78
(1,670)	1:591:A:VAL:HG22	1:607:A:VAL:HG23	20	0.77	0.12	0.78
(1,670)	1:591:A:VAL:HG23	1:607:A:VAL:HG21	20	0.77	0.12	0.78
(1,670)	1:591:A:VAL:HG21	1:607:A:VAL:HG22	20	0.77	0.12	0.78
(1,670)	1:591:A:VAL:HG21	1:607:A:VAL:HG23	20	0.77	0.12	0.78
(1,670)	1:591:A:VAL:HG23	1:607:A:VAL:HG23	20	0.77	0.12	0.78
(1,670)	1:591:A:VAL:HG22	1:607:A:VAL:HG22	20	0.77	0.12	0.78
(1,670)	1:591:A:VAL:HG21	1:607:A:VAL:HG21	20	0.77	0.12	0.78
(1,1467)	1:593:A:ASP:H	1:591:A:VAL:HG12	20	0.76	0.16	0.72
(1,1467)	1:593:A:ASP:H	1:591:A:VAL:HG13	20	0.76	0.16	0.72
(1,1467)	1:593:A:ASP:H	1:591:A:VAL:HG11	20	0.76	0.16	0.72
(1,125)	1:589:A:THR:H	1:586:A:ALA:HB2	20	0.76	0.15	0.82
(1,125)	1:589:A:THR:H	1:586:A:ALA:HB1	20	0.76	0.15	0.82
(1,125)	1:589:A:THR:H	1:586:A:ALA:HB3	20	0.76	0.15	0.82

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1545)	1:569:A:GLU:H	1:628:A:LEU:HD12	20	0.74	0.13	0.7
(1,1545)	1:569:A:GLU:H	1:628:A:LEU:HD13	20	0.74	0.13	0.7
(1,1545)	1:569:A:GLU:H	1:628:A:LEU:HD11	20	0.74	0.13	0.7
(1,989)	1:611:A:MET:HG2	1:587:A:LEU:HD12	20	0.74	0.2	0.8
(1,989)	1:611:A:MET:HG2	1:587:A:LEU:HD11	20	0.74	0.2	0.8
(1,989)	1:611:A:MET:HG2	1:587:A:LEU:HD13	20	0.74	0.2	0.8
(1,2158)	1:591:A:VAL:HG23	1:596:A:PHE:HB2	20	0.73	0.11	0.75
(1,2158)	1:591:A:VAL:HG22	1:596:A:PHE:HB2	20	0.73	0.11	0.75
(1,2158)	1:591:A:VAL:HG21	1:596:A:PHE:HB2	20	0.73	0.11	0.75
(1,35)	1:598:A:SER:H	1:599:A:GLN:HB3	20	0.72	0.16	0.74
(1,1466)	1:606:A:LYS:H	1:609:A:ALA:HB2	20	0.71	0.07	0.7
(1,1466)	1:606:A:LYS:H	1:609:A:ALA:HB1	20	0.71	0.07	0.7
(1,1466)	1:606:A:LYS:H	1:609:A:ALA:HB3	20	0.71	0.07	0.7
(1,1690)	1:564:A:TYR:HE1	1:567:A:GLN:HB3	20	0.68	0.11	0.71
(1,1690)	1:564:A:TYR:HE1	1:567:A:GLN:HB2	20	0.68	0.11	0.71
(1,1690)	1:564:A:TYR:HE2	1:567:A:GLN:HB2	20	0.68	0.11	0.71
(1,1958)	1:622:A:PHE:HB3	1:623:A:GLU:HB2	20	0.68	0.26	0.59
(1,1958)	1:622:A:PHE:HB3	1:619:A:GLU:HB2	20	0.68	0.26	0.59
(1,1291)	1:608:A:LEU:HD12	1:604:A:THR:HG21	20	0.67	0.18	0.69
(1,1291)	1:608:A:LEU:HD11	1:604:A:THR:HG22	20	0.67	0.18	0.69
(1,1291)	1:608:A:LEU:HD13	1:604:A:THR:HG22	20	0.67	0.18	0.69
(1,1291)	1:608:A:LEU:HD12	1:604:A:THR:HG22	20	0.67	0.18	0.69
(1,1291)	1:608:A:LEU:HD11	1:604:A:THR:HG21	20	0.67	0.18	0.69
(1,1291)	1:608:A:LEU:HD12	1:604:A:THR:HG23	20	0.67	0.18	0.69
(1,1291)	1:608:A:LEU:HD11	1:604:A:THR:HG23	20	0.67	0.18	0.69
(1,1291)	1:608:A:LEU:HD13	1:604:A:THR:HG21	20	0.67	0.18	0.69
(1,1449)	1:603:A:GLN:H	1:605:A:GLN:HB2	20	0.66	0.19	0.69
(1,1449)	1:603:A:GLN:H	1:599:A:GLN:HB2	20	0.66	0.19	0.69
(1,1506)	1:582:A:ALA:H	1:618:A:LEU:HD13	20	0.64	0.13	0.65
(1,1506)	1:582:A:ALA:H	1:618:A:LEU:HD11	20	0.64	0.13	0.65
(1,1506)	1:582:A:ALA:H	1:618:A:LEU:HD21	20	0.64	0.13	0.65
(1,1506)	1:582:A:ALA:H	1:618:A:LEU:HD12	20	0.64	0.13	0.65
(1,1506)	1:582:A:ALA:H	1:618:A:LEU:HD23	20	0.64	0.13	0.65
(1,1704)	1:622:A:PHE:HD2	1:618:A:LEU:HB3	20	0.64	0.09	0.62
(1,1513)	1:579:A:ASP:H	1:576:A:LEU:HG	20	0.63	0.06	0.62
(1,1944)	1:585:A:GLU:HG3	1:586:A:ALA:HB1	20	0.63	0.23	0.68
(1,1944)	1:582:A:ALA:HB2	1:585:A:GLU:HG3	20	0.63	0.23	0.68
(1,1944)	1:582:A:ALA:HB3	1:585:A:GLU:HG3	20	0.63	0.23	0.68
(1,1944)	1:582:A:ALA:HB1	1:578:A:GLU:HG3	20	0.63	0.23	0.68
(1,1944)	1:582:A:ALA:HB1	1:585:A:GLU:HG3	20	0.63	0.23	0.68
(1,1944)	1:585:A:GLU:HG3	1:586:A:ALA:HB2	20	0.63	0.23	0.68
(1,1944)	1:582:A:ALA:HB3	1:578:A:GLU:HG3	20	0.63	0.23	0.68

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2014)	1:601:A:HIS:HB3	1:602:A:GLU:HB2	20	0.63	0.09	0.64
(1,1306)	1:589:A:THR:HG22	1:590:A:GLN:HB2	20	0.62	0.1	0.6
(1,1306)	1:589:A:THR:HG23	1:590:A:GLN:HB2	20	0.62	0.1	0.6
(1,1306)	1:589:A:THR:HG21	1:590:A:GLN:HB2	20	0.62	0.1	0.6
(1,1469)	1:592:A:ALA:H	1:591:A:VAL:HG22	20	0.62	0.1	0.64
(1,1469)	1:592:A:ALA:H	1:591:A:VAL:HG12	20	0.62	0.1	0.64
(1,1469)	1:592:A:ALA:H	1:591:A:VAL:HG23	20	0.62	0.1	0.64
(1,1469)	1:592:A:ALA:H	1:591:A:VAL:HG11	20	0.62	0.1	0.64
(1,1469)	1:592:A:ALA:H	1:591:A:VAL:HG13	20	0.62	0.1	0.64
(1,586)	1:625:A:TRP:HD1	1:577:A:LEU:HD22	20	0.62	0.13	0.65
(1,586)	1:625:A:TRP:HD1	1:577:A:LEU:HD21	20	0.62	0.13	0.65
(1,586)	1:625:A:TRP:HD1	1:577:A:LEU:HD23	20	0.62	0.13	0.65
(1,2093)	1:570:A:LEU:HD22	1:570:A:LEU:HD13	20	0.61	0.02	0.61
(1,2093)	1:570:A:LEU:HD21	1:570:A:LEU:HD11	20	0.61	0.02	0.61
(1,2093)	1:570:A:LEU:HD21	1:570:A:LEU:HD12	20	0.61	0.02	0.61
(1,2093)	1:570:A:LEU:HD22	1:570:A:LEU:HD11	20	0.61	0.02	0.61
(1,2093)	1:570:A:LEU:HD23	1:570:A:LEU:HD12	20	0.61	0.02	0.61
(1,2093)	1:570:A:LEU:HD22	1:570:A:LEU:HD12	20	0.61	0.02	0.61
(1,2093)	1:570:A:LEU:HD21	1:570:A:LEU:HD13	20	0.61	0.02	0.61
(1,2093)	1:587:A:LEU:HD23	1:587:A:LEU:HD12	20	0.61	0.02	0.61
(1,2093)	1:587:A:LEU:HD22	1:587:A:LEU:HD12	20	0.61	0.02	0.61
(1,1712)	1:577:A:LEU:HD23	1:625:A:TRP:HA	20	0.6	0.09	0.62
(1,1712)	1:577:A:LEU:HD22	1:625:A:TRP:HA	20	0.6	0.09	0.62
(1,1712)	1:577:A:LEU:HD21	1:625:A:TRP:HA	20	0.6	0.09	0.62
(1,1532)	1:573:A:LEU:H	1:573:A:LEU:HD11	20	0.6	0.06	0.6
(1,1532)	1:573:A:LEU:H	1:573:A:LEU:HD13	20	0.6	0.06	0.6
(1,1532)	1:573:A:LEU:H	1:573:A:LEU:HD12	20	0.6	0.06	0.6
(1,1532)	1:573:A:LEU:H	1:573:A:LEU:HD21	20	0.6	0.06	0.6
(1,1758)	1:609:A:ALA:HB1	1:609:A:ALA:HA	20	0.6	0.01	0.6
(1,1758)	1:609:A:ALA:HB3	1:609:A:ALA:HA	20	0.6	0.01	0.6
(1,1758)	1:582:A:ALA:HB3	1:582:A:ALA:HA	20	0.6	0.01	0.6
(1,1758)	1:609:A:ALA:HB2	1:609:A:ALA:HA	20	0.6	0.01	0.6
(1,1758)	1:612:A:ALA:HB1	1:612:A:ALA:HA	20	0.6	0.01	0.6
(1,1758)	1:582:A:ALA:HB2	1:582:A:ALA:HA	20	0.6	0.01	0.6
(1,1758)	1:612:A:ALA:HB2	1:612:A:ALA:HA	20	0.6	0.01	0.6
(1,1758)	1:582:A:ALA:HB1	1:582:A:ALA:HA	20	0.6	0.01	0.6
(1,1812)	1:632:A:LYS:HA	1:631:A:LEU:HD23	20	0.59	0.1	0.58
(1,1812)	1:632:A:LYS:HA	1:631:A:LEU:HD21	20	0.59	0.1	0.58
(1,1812)	1:632:A:LYS:HA	1:631:A:LEU:HD22	20	0.59	0.1	0.58
(1,1834)	1:583:A:LYS:HA	1:587:A:LEU:HD21	20	0.59	0.13	0.64
(1,1834)	1:583:A:LYS:HA	1:587:A:LEU:HD22	20	0.59	0.13	0.64
(1,1834)	1:583:A:LYS:HA	1:587:A:LEU:HD23	20	0.59	0.13	0.64

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1387)	1:577:A:LEU:HD22	1:574:A:PRO:HB2	20	0.59	0.07	0.62
(1,1387)	1:577:A:LEU:HD21	1:574:A:PRO:HB2	20	0.59	0.07	0.62
(1,1387)	1:577:A:LEU:HD23	1:574:A:PRO:HB2	20	0.59	0.07	0.62
(1,1611)	1:616:A:GLN:H	1:612:A:ALA:HB3	20	0.57	0.11	0.56
(1,1611)	1:616:A:GLN:H	1:612:A:ALA:HB1	20	0.57	0.11	0.56
(1,1611)	1:616:A:GLN:H	1:612:A:ALA:HB2	20	0.57	0.11	0.56
(1,1879)	1:561:A:LYS:HG3	1:561:A:LYS:HD2	20	0.57	0.03	0.57
(1,1879)	1:565:A:LYS:HG2	1:565:A:LYS:HD3	20	0.57	0.03	0.57
(1,1879)	1:551:A:LYS:HG3	1:551:A:LYS:HD2	20	0.57	0.03	0.57
(1,1879)	1:565:A:LYS:HG2	1:565:A:LYS:HD2	20	0.57	0.03	0.57
(1,1879)	1:556:A:LYS:HG2	1:556:A:LYS:HD3	20	0.57	0.03	0.57
(1,1879)	1:551:A:LYS:HG3	1:551:A:LYS:HD3	20	0.57	0.03	0.57
(1,2117)	1:561:A:LYS:HG3	1:561:A:LYS:HD2	20	0.57	0.02	0.58
(1,2117)	1:551:A:LYS:HG3	1:551:A:LYS:HD2	20	0.57	0.02	0.58
(1,2117)	1:551:A:LYS:HG2	1:551:A:LYS:HD3	20	0.57	0.02	0.58
(1,2117)	1:556:A:LYS:HG2	1:556:A:LYS:HD3	20	0.57	0.02	0.58
(1,2117)	1:551:A:LYS:HG2	1:551:A:LYS:HD2	20	0.57	0.02	0.58
(1,2117)	1:551:A:LYS:HG3	1:551:A:LYS:HD3	20	0.57	0.02	0.58
(1,2117)	1:556:A:LYS:HG2	1:556:A:LYS:HD2	20	0.57	0.02	0.58
(1,1705)	1:622:A:PHE:HD1	1:577:A:LEU:HD23	20	0.57	0.12	0.55
(1,1705)	1:622:A:PHE:HD1	1:577:A:LEU:HD22	20	0.57	0.12	0.55
(1,1705)	1:622:A:PHE:HD1	1:577:A:LEU:HD21	20	0.57	0.12	0.55
(1,1705)	1:622:A:PHE:HE1	1:577:A:LEU:HD22	20	0.57	0.12	0.55
(1,1705)	1:622:A:PHE:HE1	1:577:A:LEU:HD23	20	0.57	0.12	0.55
(1,1705)	1:622:A:PHE:HE1	1:577:A:LEU:HD21	20	0.57	0.12	0.55
(1,1891)	1:562:A:LEU:HG	1:562:A:LEU:HD13	20	0.57	0.03	0.56
(1,1891)	1:562:A:LEU:HG	1:562:A:LEU:HD11	20	0.57	0.03	0.56
(1,1891)	1:562:A:LEU:HG	1:562:A:LEU:HD23	20	0.57	0.03	0.56
(1,1891)	1:576:A:LEU:HG	1:580:A:LEU:HD13	20	0.57	0.03	0.56
(1,1891)	1:576:A:LEU:HG	1:580:A:LEU:HD12	20	0.57	0.03	0.56
(1,1891)	1:562:A:LEU:HG	1:562:A:LEU:HD12	20	0.57	0.03	0.56
(1,1891)	1:562:A:LEU:HG	1:562:A:LEU:HD22	20	0.57	0.03	0.56
(1,1982)	1:632:A:LYS:HE3	1:632:A:LYS:HD2	20	0.57	0.02	0.57
(1,1982)	1:632:A:LYS:HE2	1:632:A:LYS:HD3	20	0.57	0.02	0.57
(1,1982)	1:583:A:LYS:HE2	1:583:A:LYS:HD3	20	0.57	0.02	0.57
(1,1982)	1:632:A:LYS:HE2	1:632:A:LYS:HD2	20	0.57	0.02	0.57
(1,1741)	1:628:A:LEU:HD22	1:624:A:ARG:HA	20	0.57	0.28	0.5
(1,1741)	1:628:A:LEU:HD21	1:624:A:ARG:HA	20	0.57	0.28	0.5
(1,1741)	1:628:A:LEU:HD23	1:624:A:ARG:HA	20	0.57	0.28	0.5
(1,1741)	1:628:A:LEU:HD21	1:627:A:TYR:HA	20	0.57	0.28	0.5
(1,2010)	1:561:A:LYS:HE2	1:561:A:LYS:HD3	20	0.56	0.02	0.56
(1,2010)	1:561:A:LYS:HE3	1:561:A:LYS:HD2	20	0.56	0.02	0.56

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2010)	1:556:A:LYS:HE3	1:556:A:LYS:HD3	20	0.56	0.02	0.56
(1,2010)	1:556:A:LYS:HE3	1:556:A:LYS:HD2	20	0.56	0.02	0.56
(1,2010)	1:551:A:LYS:HE3	1:551:A:LYS:HD2	20	0.56	0.02	0.56
(1,2010)	1:551:A:LYS:HE2	1:551:A:LYS:HD3	20	0.56	0.02	0.56
(1,2010)	1:551:A:LYS:HE2	1:551:A:LYS:HD2	20	0.56	0.02	0.56
(1,2010)	1:556:A:LYS:HE2	1:556:A:LYS:HD3	20	0.56	0.02	0.56
(1,2010)	1:561:A:LYS:HE2	1:561:A:LYS:HD2	20	0.56	0.02	0.56
(1,1019)	1:604:A:THR:HG22	1:599:A:GLN:HG2	20	0.56	0.1	0.56
(1,1019)	1:604:A:THR:HG23	1:599:A:GLN:HG2	20	0.56	0.1	0.56
(1,1019)	1:604:A:THR:HG21	1:599:A:GLN:HG2	20	0.56	0.1	0.56
(1,1880)	1:632:A:LYS:HG2	1:632:A:LYS:HD2	20	0.56	0.03	0.56
(1,1880)	1:565:A:LYS:HG3	1:565:A:LYS:HD2	20	0.56	0.03	0.56
(1,1880)	1:551:A:LYS:HG2	1:551:A:LYS:HD3	20	0.56	0.03	0.56
(1,1880)	1:556:A:LYS:HG3	1:556:A:LYS:HD2	20	0.56	0.03	0.56
(1,1880)	1:551:A:LYS:HG2	1:551:A:LYS:HD2	20	0.56	0.03	0.56
(1,1880)	1:632:A:LYS:HG2	1:632:A:LYS:HD3	20	0.56	0.03	0.56
(1,2163)	1:567:A:GLN:HA	1:570:A:LEU:HD11	20	0.56	0.36	0.52
(1,2163)	1:567:A:GLN:HA	1:570:A:LEU:HD12	20	0.56	0.36	0.52
(1,2163)	1:567:A:GLN:HA	1:570:A:LEU:HD13	20	0.56	0.36	0.52
(1,2163)	1:588:A:GLN:HA	1:607:A:VAL:HG11	20	0.56	0.36	0.52
(1,1309)	1:573:A:LEU:HD23	1:576:A:LEU:HB2	20	0.56	0.75	0.32
(1,1309)	1:573:A:LEU:HD21	1:576:A:LEU:HB2	20	0.56	0.75	0.32
(1,1309)	1:573:A:LEU:HD22	1:576:A:LEU:HB2	20	0.56	0.75	0.32
(1,1980)	1:561:A:LYS:HE2	1:561:A:LYS:HD3	20	0.56	0.02	0.56
(1,1980)	1:565:A:LYS:HE2	1:565:A:LYS:HD3	20	0.56	0.02	0.56
(1,1980)	1:556:A:LYS:HE3	1:556:A:LYS:HD3	20	0.56	0.02	0.56
(1,1980)	1:556:A:LYS:HE3	1:556:A:LYS:HD2	20	0.56	0.02	0.56
(1,1980)	1:551:A:LYS:HE2	1:551:A:LYS:HD3	20	0.56	0.02	0.56
(1,1980)	1:565:A:LYS:HE2	1:565:A:LYS:HD2	20	0.56	0.02	0.56
(1,1980)	1:565:A:LYS:HE3	1:565:A:LYS:HD2	20	0.56	0.02	0.56
(1,1980)	1:556:A:LYS:HE2	1:556:A:LYS:HD3	20	0.56	0.02	0.56
(1,1980)	1:561:A:LYS:HE3	1:561:A:LYS:HD2	20	0.56	0.02	0.56
(1,1980)	1:561:A:LYS:HE2	1:561:A:LYS:HD2	20	0.56	0.02	0.56
(1,1980)	1:551:A:LYS:HE3	1:551:A:LYS:HD2	20	0.56	0.02	0.56
(1,2103)	1:562:A:LEU:HG	1:562:A:LEU:HD21	20	0.55	0.04	0.56
(1,2103)	1:562:A:LEU:HB3	1:562:A:LEU:HD23	20	0.55	0.04	0.56
(1,2103)	1:562:A:LEU:HG	1:562:A:LEU:HD23	20	0.55	0.04	0.56
(1,2103)	1:562:A:LEU:HG	1:562:A:LEU:HD22	20	0.55	0.04	0.56
(1,2103)	1:562:A:LEU:HB3	1:562:A:LEU:HD21	20	0.55	0.04	0.56
(1,2103)	1:562:A:LEU:HB3	1:562:A:LEU:HD22	20	0.55	0.04	0.56
(1,238)	1:575:A:GLN:H	1:575:A:GLN:HB3	20	0.54	0.03	0.55
(1,1575)	1:621:A:ALA:H	1:622:A:PHE:HA	20	0.54	0.03	0.54

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,572)	1:625:A:TRP:HE3	1:625:A:TRP:HB2	20	0.53	0.03	0.53
(1,2160)	1:630:A:ALA:HB3	1:627:A:TYR:HB2	20	0.53	0.16	0.58
(1,2160)	1:630:A:ALA:HB2	1:627:A:TYR:HB2	20	0.53	0.16	0.58
(1,2160)	1:630:A:ALA:HB1	1:627:A:TYR:HB2	20	0.53	0.16	0.58
(1,348)	1:607:A:VAL:H	1:607:A:VAL:HG13	20	0.53	0.02	0.53
(1,348)	1:607:A:VAL:H	1:607:A:VAL:HG11	20	0.53	0.02	0.53
(1,348)	1:607:A:VAL:H	1:607:A:VAL:HG12	20	0.53	0.02	0.53
(1,1054)	1:604:A:THR:HG21	1:597:A:PHE:HB2	20	0.53	0.07	0.51
(1,1054)	1:604:A:THR:HG22	1:597:A:PHE:HB2	20	0.53	0.07	0.51
(1,1054)	1:604:A:THR:HG23	1:597:A:PHE:HB2	20	0.53	0.07	0.51
(1,1397)	1:587:A:LEU:HD11	1:583:A:LYS:HA	20	0.52	0.07	0.52
(1,1397)	1:587:A:LEU:HD12	1:583:A:LYS:HA	20	0.52	0.07	0.52
(1,1397)	1:587:A:LEU:HD13	1:583:A:LYS:HA	20	0.52	0.07	0.52
(1,631)	1:577:A:LEU:HD11	1:622:A:PHE:HB3	20	0.52	0.11	0.49
(1,631)	1:577:A:LEU:HD12	1:622:A:PHE:HB3	20	0.52	0.11	0.49
(1,631)	1:577:A:LEU:HD13	1:622:A:PHE:HB3	20	0.52	0.11	0.49
(1,44)	1:597:A:PHE:H	1:597:A:PHE:HB3	20	0.52	0.01	0.52
(1,1480)	1:588:A:GLN:H	1:586:A:ALA:HB3	20	0.51	0.09	0.52
(1,1480)	1:588:A:GLN:H	1:586:A:ALA:HB2	20	0.51	0.09	0.52
(1,1480)	1:588:A:GLN:H	1:586:A:ALA:HB1	20	0.51	0.09	0.52
(1,630)	1:577:A:LEU:HD12	1:580:A:LEU:HG	20	0.51	0.12	0.54
(1,630)	1:577:A:LEU:HD11	1:580:A:LEU:HG	20	0.51	0.12	0.54
(1,630)	1:577:A:LEU:HD13	1:580:A:LEU:HG	20	0.51	0.12	0.54
(1,1865)	1:622:A:PHE:HA	1:623:A:GLU:HA	20	0.5	0.07	0.5
(1,1865)	1:622:A:PHE:HA	1:619:A:GLU:HA	20	0.5	0.07	0.5
(1,92)	1:592:A:ALA:H	1:589:A:THR:HG22	20	0.49	0.08	0.5
(1,92)	1:592:A:ALA:H	1:589:A:THR:HG23	20	0.49	0.08	0.5
(1,92)	1:592:A:ALA:H	1:589:A:THR:HG21	20	0.49	0.08	0.5
(1,1457)	1:597:A:PHE:H	1:598:A:SER:HB2	20	0.48	0.13	0.55
(1,1230)	1:612:A:ALA:HA	1:611:A:MET:HG3	20	0.48	0.04	0.47
(1,2109)	1:608:A:LEU:HD12	1:591:A:VAL:HG11	20	0.48	0.14	0.5
(1,2109)	1:608:A:LEU:HD11	1:591:A:VAL:HG11	20	0.48	0.14	0.5
(1,2109)	1:608:A:LEU:HD13	1:591:A:VAL:HG11	20	0.48	0.14	0.5
(1,2109)	1:608:A:LEU:HD11	1:591:A:VAL:HG12	20	0.48	0.14	0.5
(1,2109)	1:608:A:LEU:HD12	1:591:A:VAL:HG12	20	0.48	0.14	0.5
(1,2109)	1:608:A:LEU:HD11	1:591:A:VAL:HG13	20	0.48	0.14	0.5
(1,2109)	1:608:A:LEU:HD13	1:591:A:VAL:HG13	20	0.48	0.14	0.5
(1,2109)	1:608:A:LEU:HD12	1:591:A:VAL:HG13	20	0.48	0.14	0.5
(1,2109)	1:608:A:LEU:HD13	1:591:A:VAL:HG12	20	0.48	0.14	0.5
(1,2168)	1:626:A:GLU:HA	1:625:A:TRP:HA	20	0.46	0.03	0.46
(1,2168)	1:626:A:GLU:HA	1:627:A:TYR:HA	20	0.46	0.03	0.46
(1,1510)	1:581:A:GLU:H	1:582:A:ALA:HB1	20	0.46	0.06	0.47

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1510)	1:581:A:GLU:H	1:582:A:ALA:HB2	20	0.46	0.06	0.47
(1,1510)	1:581:A:GLU:H	1:582:A:ALA:HB3	20	0.46	0.06	0.47
(1,154)	1:585:A:GLU:H	1:584:A:LEU:HB2	20	0.46	0.03	0.45
(1,755)	1:621:A:ALA:HA	1:576:A:LEU:HD23	20	0.45	0.07	0.47
(1,755)	1:621:A:ALA:HA	1:576:A:LEU:HD21	20	0.45	0.07	0.47
(1,755)	1:621:A:ALA:HA	1:576:A:LEU:HD22	20	0.45	0.07	0.47
(1,1852)	1:604:A:THR:HB	1:599:A:GLN:HB2	20	0.45	0.1	0.44
(1,1852)	1:604:A:THR:HB	1:608:A:LEU:HB2	20	0.45	0.1	0.44
(1,1701)	1:622:A:PHE:HE2	1:577:A:LEU:HA	20	0.45	0.04	0.46
(1,1468)	1:592:A:ALA:H	1:593:A:ASP:HB2	20	0.45	0.1	0.44
(1,1468)	1:592:A:ALA:H	1:593:A:ASP:HB3	20	0.45	0.1	0.44
(1,1854)	1:612:A:ALA:HA	1:611:A:MET:HA	20	0.44	0.02	0.44
(1,1854)	1:614:A:ALA:HA	1:615:A:GLU:HA	20	0.44	0.02	0.44
(1,1526)	1:576:A:LEU:H	1:576:A:LEU:HD23	20	0.44	0.05	0.45
(1,1526)	1:576:A:LEU:H	1:576:A:LEU:HD21	20	0.44	0.05	0.45
(1,1526)	1:576:A:LEU:H	1:576:A:LEU:HD22	20	0.44	0.05	0.45
(1,893)	1:583:A:LYS:HA	1:583:A:LYS:HE2	20	0.44	0.05	0.44
(1,893)	1:583:A:LYS:HA	1:583:A:LYS:HE3	20	0.44	0.05	0.44
(1,1136)	1:600:A:PRO:HD3	1:603:A:GLN:HB2	20	0.44	0.21	0.39
(1,1136)	1:600:A:PRO:HD3	1:603:A:GLN:HB3	20	0.44	0.21	0.39
(1,926)	1:583:A:LYS:HG3	1:580:A:LEU:HD23	20	0.43	0.03	0.44
(1,926)	1:583:A:LYS:HG3	1:580:A:LEU:HD22	20	0.43	0.03	0.44
(1,926)	1:583:A:LYS:HG3	1:580:A:LEU:HD21	20	0.43	0.03	0.44
(1,2159)	1:627:A:TYR:HB3	1:628:A:LEU:HA	20	0.43	0.05	0.43
(1,1965)	1:579:A:ASP:HB2	1:576:A:LEU:HG	20	0.42	0.08	0.4
(1,1711)	1:577:A:LEU:HD23	1:626:A:GLU:HG3	20	0.42	0.19	0.39
(1,1711)	1:577:A:LEU:HD22	1:626:A:GLU:HG3	20	0.42	0.19	0.39
(1,1711)	1:577:A:LEU:HD21	1:626:A:GLU:HG3	20	0.42	0.19	0.39
(1,1711)	1:577:A:LEU:HD22	1:624:A:ARG:HB3	20	0.42	0.19	0.39
(1,1711)	1:577:A:LEU:HD23	1:624:A:ARG:HB3	20	0.42	0.19	0.39
(1,1711)	1:577:A:LEU:HD21	1:624:A:ARG:HB3	20	0.42	0.19	0.39
(1,172)	1:582:A:ALA:H	1:579:A:ASP:HB2	20	0.41	0.03	0.41
(1,26)	1:599:A:GLN:H	1:599:A:GLN:HB3	20	0.4	0.04	0.41
(1,2171)	1:591:A:VAL:HG23	1:597:A:PHE:HZ	20	0.4	0.12	0.38
(1,2171)	1:591:A:VAL:HG22	1:597:A:PHE:HZ	20	0.4	0.12	0.38
(1,2171)	1:591:A:VAL:HG21	1:597:A:PHE:HZ	20	0.4	0.12	0.38
(1,416)	1:616:A:GLN:H	1:615:A:GLU:HB3	20	0.4	0.04	0.39
(1,1325)	1:628:A:LEU:HD12	1:569:A:GLU:HA	20	0.4	0.15	0.38
(1,1325)	1:628:A:LEU:HD13	1:569:A:GLU:HA	20	0.4	0.15	0.38
(1,1325)	1:628:A:LEU:HD11	1:569:A:GLU:HA	20	0.4	0.15	0.38
(1,1399)	1:583:A:LYS:HG2	1:580:A:LEU:HD23	20	0.4	0.08	0.39
(1,1399)	1:583:A:LYS:HG2	1:580:A:LEU:HD22	20	0.4	0.08	0.39

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1399)	1:583:A:LYS:HG2	1:580:A:LEU:HD21	20	0.4	0.08	0.39
(1,1535)	1:572:A:GLN:H	1:573:A:LEU:HD22	20	0.4	0.16	0.37
(1,1535)	1:572:A:GLN:H	1:573:A:LEU:HD11	20	0.4	0.16	0.37
(1,1535)	1:572:A:GLN:H	1:573:A:LEU:HD13	20	0.4	0.16	0.37
(1,1535)	1:572:A:GLN:H	1:573:A:LEU:HD12	20	0.4	0.16	0.37
(1,1535)	1:572:A:GLN:H	1:573:A:LEU:HD21	20	0.4	0.16	0.37
(1,368)	1:609:A:ALA:H	1:608:A:LEU:HD21	20	0.39	0.03	0.4
(1,368)	1:609:A:ALA:H	1:608:A:LEU:HD22	20	0.39	0.03	0.4
(1,368)	1:609:A:ALA:H	1:608:A:LEU:HD23	20	0.39	0.03	0.4
(1,550)	1:596:A:PHE:HD1	1:604:A:THR:HG23	20	0.39	0.1	0.42
(1,550)	1:596:A:PHE:HD2	1:604:A:THR:HG21	20	0.39	0.1	0.42
(1,550)	1:596:A:PHE:HD1	1:604:A:THR:HG22	20	0.39	0.1	0.42
(1,550)	1:596:A:PHE:HD1	1:604:A:THR:HG21	20	0.39	0.1	0.42
(1,550)	1:596:A:PHE:HD2	1:604:A:THR:HG23	20	0.39	0.1	0.42
(1,1517)	1:578:A:GLU:H	1:577:A:LEU:HG	20	0.38	0.04	0.38
(1,1057)	1:622:A:PHE:HB3	1:577:A:LEU:HD23	20	0.37	0.02	0.37
(1,1057)	1:622:A:PHE:HB3	1:577:A:LEU:HD22	20	0.37	0.02	0.37
(1,1057)	1:622:A:PHE:HB3	1:577:A:LEU:HD21	20	0.37	0.02	0.37
(1,658)	1:591:A:VAL:HG23	1:596:A:PHE:HB3	20	0.37	0.09	0.4
(1,658)	1:591:A:VAL:HG22	1:596:A:PHE:HB3	20	0.37	0.09	0.4
(1,658)	1:591:A:VAL:HG21	1:596:A:PHE:HB3	20	0.37	0.09	0.4
(1,569)	1:625:A:TRP:HZ2	1:629:A:GLU:HG2	20	0.36	0.04	0.35
(1,1678)	1:627:A:TYR:HE1	1:631:A:LEU:HG	20	0.36	0.08	0.34
(1,1774)	1:592:A:ALA:HA	1:589:A:THR:HA	20	0.34	0.06	0.33
(1,1567)	1:607:A:VAL:H	1:606:A:LYS:HB2	20	0.32	0.1	0.3
(1,1016)	1:588:A:GLN:HG2	1:584:A:LEU:HG	20	0.31	0.06	0.31
(1,850)	1:604:A:THR:HA	1:607:A:VAL:HG11	20	0.31	0.08	0.31
(1,850)	1:604:A:THR:HA	1:607:A:VAL:HG12	20	0.31	0.08	0.31
(1,850)	1:604:A:THR:HA	1:607:A:VAL:HG13	20	0.31	0.08	0.31
(1,1625)	1:620:A:GLN:H	1:618:A:LEU:HB3	20	0.31	0.05	0.3
(1,1625)	1:620:A:GLN:H	1:621:A:ALA:HB3	20	0.31	0.05	0.3
(1,1625)	1:620:A:GLN:H	1:621:A:ALA:HB2	20	0.31	0.05	0.3
(1,1625)	1:620:A:GLN:H	1:621:A:ALA:HB1	20	0.31	0.05	0.3
(1,1323)	1:576:A:LEU:HA	1:576:A:LEU:HD21	20	0.3	0.03	0.3
(1,1323)	1:576:A:LEU:HA	1:576:A:LEU:HD22	20	0.3	0.03	0.3
(1,1323)	1:576:A:LEU:HA	1:576:A:LEU:HD23	20	0.3	0.03	0.3
(1,1608)	1:616:A:GLN:H	1:612:A:ALA:HA	20	0.3	0.08	0.29
(1,1797)	1:576:A:LEU:HA	1:576:A:LEU:HD21	20	0.29	0.05	0.3
(1,1797)	1:576:A:LEU:HA	1:576:A:LEU:HD22	20	0.29	0.05	0.3
(1,1797)	1:628:A:LEU:HD23	1:624:A:ARG:HA	20	0.29	0.05	0.3
(1,1797)	1:576:A:LEU:HA	1:576:A:LEU:HD23	20	0.29	0.05	0.3
(1,1797)	1:628:A:LEU:HD22	1:624:A:ARG:HA	20	0.29	0.05	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1855)	1:572:A:GLN:HA	1:571:A:GLU:HA	20	0.29	0.04	0.29
(1,1443)	1:564:A:TYR:HE1	1:564:A:TYR:HA	20	0.28	0.03	0.29
(1,1443)	1:564:A:TYR:HE2	1:564:A:TYR:HA	20	0.28	0.03	0.29
(1,1796)	1:580:A:LEU:HA	1:580:A:LEU:HD23	20	0.28	0.03	0.28
(1,1796)	1:580:A:LEU:HA	1:580:A:LEU:HD22	20	0.28	0.03	0.28
(1,1796)	1:580:A:LEU:HA	1:580:A:LEU:HD21	20	0.28	0.03	0.28
(1,1420)	1:627:A:TYR:HE1	1:631:A:LEU:HD21	20	0.28	0.09	0.26
(1,1420)	1:627:A:TYR:HE1	1:631:A:LEU:HD22	20	0.28	0.09	0.26
(1,1420)	1:627:A:TYR:HE1	1:631:A:LEU:HD23	20	0.28	0.09	0.26
(1,1420)	1:627:A:TYR:HE2	1:631:A:LEU:HD22	20	0.28	0.09	0.26
(1,1795)	1:579:A:ASP:HA	1:583:A:LYS:HB2	20	0.27	0.07	0.27
(1,339)	1:605:A:GLN:H	1:604:A:THR:HG22	20	0.27	0.08	0.26
(1,339)	1:605:A:GLN:H	1:604:A:THR:HG23	20	0.27	0.08	0.26
(1,339)	1:605:A:GLN:H	1:604:A:THR:HG21	20	0.27	0.08	0.26
(1,1806)	1:577:A:LEU:HA	1:581:A:GLU:HB2	20	0.26	0.08	0.29
(1,58)	1:596:A:PHE:H	1:594:A:ALA:HB3	20	0.26	0.03	0.26
(1,58)	1:596:A:PHE:H	1:594:A:ALA:HB1	20	0.26	0.03	0.26
(1,58)	1:596:A:PHE:H	1:594:A:ALA:HB2	20	0.26	0.03	0.26
(1,2027)	1:564:A:TYR:HB3	1:567:A:GLN:HB2	20	0.25	0.05	0.25
(1,1693)	1:627:A:TYR:HD1	1:631:A:LEU:HD13	20	0.25	0.02	0.25
(1,1693)	1:627:A:TYR:HD1	1:631:A:LEU:HD12	20	0.25	0.02	0.25
(1,1693)	1:627:A:TYR:HD1	1:631:A:LEU:HD11	20	0.25	0.02	0.25
(1,665)	1:631:A:LEU:HD23	1:631:A:LEU:HA	20	0.24	0.03	0.24
(1,665)	1:631:A:LEU:HD21	1:631:A:LEU:HA	20	0.24	0.03	0.24
(1,665)	1:631:A:LEU:HD22	1:631:A:LEU:HA	20	0.24	0.03	0.24
(1,545)	1:577:A:LEU:HD22	1:577:A:LEU:HD21	20	0.24	0.0	0.24
(1,545)	1:577:A:LEU:HD21	1:577:A:LEU:HD23	20	0.24	0.0	0.24
(1,545)	1:577:A:LEU:HD22	1:577:A:LEU:HD23	20	0.24	0.0	0.24
(1,998)	1:583:A:LYS:HB3	1:587:A:LEU:HD13	20	0.24	0.09	0.2
(1,998)	1:583:A:LYS:HB3	1:587:A:LEU:HD12	20	0.24	0.09	0.2
(1,998)	1:583:A:LYS:HB3	1:587:A:LEU:HD11	20	0.24	0.09	0.2
(1,1591)	1:583:A:LYS:H	1:583:A:LYS:HG3	20	0.24	0.02	0.24
(1,1459)	1:593:A:ASP:H	1:594:A:ALA:H	20	0.23	0.03	0.23
(1,1422)	1:627:A:TYR:HD1	1:631:A:LEU:HD13	20	0.23	0.02	0.22
(1,1422)	1:627:A:TYR:HD1	1:631:A:LEU:HD12	20	0.23	0.02	0.22
(1,1422)	1:627:A:TYR:HD1	1:631:A:LEU:HD11	20	0.23	0.02	0.22
(1,1491)	1:585:A:GLU:H	1:584:A:LEU:HG	20	0.22	0.04	0.22
(1,1503)	1:582:A:ALA:H	1:581:A:GLU:HB2	20	0.22	0.03	0.23
(1,1384)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	20	0.22	0.06	0.22
(1,1384)	1:602:A:GLU:HG2	1:601:A:HIS:HB2	20	0.22	0.06	0.22
(1,1430)	1:596:A:PHE:HD2	1:608:A:LEU:HD23	20	0.19	0.02	0.19
(1,1430)	1:596:A:PHE:HD2	1:608:A:LEU:HD21	20	0.19	0.02	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1430)	1:596:A:PHE:HD2	1:608:A:LEU:HD22	20	0.19	0.02	0.19
(1,712)	1:594:A:ALA:HB1	1:593:A:ASP:HA	20	0.19	0.03	0.18
(1,712)	1:594:A:ALA:HB2	1:593:A:ASP:HA	20	0.19	0.03	0.18
(1,712)	1:594:A:ALA:HB3	1:593:A:ASP:HA	20	0.19	0.03	0.18
(1,1955)	1:622:A:PHE:HB3	1:618:A:LEU:HD11	19	1.69	0.08	1.7
(1,1955)	1:622:A:PHE:HB3	1:618:A:LEU:HD12	19	1.69	0.08	1.7
(1,1955)	1:622:A:PHE:HB3	1:618:A:LEU:HD13	19	1.69	0.08	1.7
(1,1279)	1:618:A:LEU:HD23	1:580:A:LEU:HD12	19	1.39	0.14	1.39
(1,1279)	1:618:A:LEU:HD21	1:580:A:LEU:HD13	19	1.39	0.14	1.39
(1,1279)	1:618:A:LEU:HD23	1:580:A:LEU:HD13	19	1.39	0.14	1.39
(1,1279)	1:618:A:LEU:HD22	1:580:A:LEU:HD12	19	1.39	0.14	1.39
(1,1279)	1:618:A:LEU:HD21	1:580:A:LEU:HD12	19	1.39	0.14	1.39
(1,1279)	1:618:A:LEU:HD23	1:580:A:LEU:HD11	19	1.39	0.14	1.39
(1,1279)	1:618:A:LEU:HD21	1:580:A:LEU:HD11	19	1.39	0.14	1.39
(1,1279)	1:618:A:LEU:HD22	1:580:A:LEU:HD11	19	1.39	0.14	1.39
(1,1279)	1:618:A:LEU:HD22	1:580:A:LEU:HD13	19	1.39	0.14	1.39
(1,1794)	1:566:A:LEU:HA	1:570:A:LEU:HB3	19	1.37	0.34	1.49
(1,1794)	1:566:A:LEU:HA	1:562:A:LEU:HG	19	1.37	0.34	1.49
(1,2156)	1:634:A:GLY:HA3	1:633:A:ASN:HB2	19	1.31	0.27	1.38
(1,2156)	1:634:A:GLY:HA2	1:633:A:ASN:HB2	19	1.31	0.27	1.38
(1,1634)	1:622:A:PHE:H	1:576:A:LEU:HD23	19	1.3	0.14	1.31
(1,1634)	1:622:A:PHE:H	1:576:A:LEU:HD21	19	1.3	0.14	1.31
(1,1634)	1:622:A:PHE:H	1:576:A:LEU:HD22	19	1.3	0.14	1.31
(1,1344)	1:577:A:LEU:HB3	1:618:A:LEU:HD21	19	1.29	0.11	1.28
(1,1344)	1:577:A:LEU:HB3	1:618:A:LEU:HD22	19	1.29	0.11	1.28
(1,1344)	1:577:A:LEU:HB3	1:618:A:LEU:HD23	19	1.29	0.11	1.28
(1,2139)	1:566:A:LEU:HD23	1:632:A:LYS:HA	19	1.28	0.62	1.42
(1,2139)	1:566:A:LEU:HD21	1:565:A:LYS:HA	19	1.28	0.62	1.42
(1,2139)	1:566:A:LEU:HD22	1:632:A:LYS:HA	19	1.28	0.62	1.42
(1,2139)	1:566:A:LEU:HD22	1:565:A:LYS:HA	19	1.28	0.62	1.42
(1,2139)	1:566:A:LEU:HD21	1:632:A:LYS:HA	19	1.28	0.62	1.42
(1,796)	1:577:A:LEU:HA	1:618:A:LEU:HD23	19	1.17	0.14	1.19
(1,796)	1:577:A:LEU:HA	1:618:A:LEU:HD21	19	1.17	0.14	1.19
(1,796)	1:577:A:LEU:HA	1:618:A:LEU:HD22	19	1.17	0.14	1.19
(1,623)	1:577:A:LEU:HD13	1:618:A:LEU:HD21	19	1.09	0.05	1.1
(1,623)	1:577:A:LEU:HD13	1:618:A:LEU:HD22	19	1.09	0.05	1.1
(1,623)	1:577:A:LEU:HD13	1:618:A:LEU:HD23	19	1.09	0.05	1.1
(1,623)	1:577:A:LEU:HD11	1:618:A:LEU:HD22	19	1.09	0.05	1.1
(1,623)	1:577:A:LEU:HD11	1:618:A:LEU:HD21	19	1.09	0.05	1.1
(1,623)	1:577:A:LEU:HD12	1:618:A:LEU:HD23	19	1.09	0.05	1.1
(1,623)	1:577:A:LEU:HD12	1:618:A:LEU:HD22	19	1.09	0.05	1.1
(1,623)	1:577:A:LEU:HD11	1:618:A:LEU:HD23	19	1.09	0.05	1.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2119)	1:569:A:GLU:HB3	1:566:A:LEU:HD11	19	1.02	0.28	1.08
(1,2119)	1:569:A:GLU:HB3	1:566:A:LEU:HD12	19	1.02	0.28	1.08
(1,2119)	1:569:A:GLU:HB3	1:566:A:LEU:HD13	19	1.02	0.28	1.08
(1,1962)	1:610:A:ASP:HB3	1:609:A:ALA:HB2	19	0.77	0.1	0.77
(1,1962)	1:610:A:ASP:HB3	1:609:A:ALA:HB1	19	0.77	0.1	0.77
(1,1962)	1:610:A:ASP:HB3	1:613:A:ALA:HB3	19	0.77	0.1	0.77
(1,1962)	1:610:A:ASP:HB3	1:609:A:ALA:HB3	19	0.77	0.1	0.77
(1,1962)	1:610:A:ASP:HB3	1:613:A:ALA:HB2	19	0.77	0.1	0.77
(1,1962)	1:610:A:ASP:HB3	1:606:A:LYS:HG2	19	0.77	0.1	0.77
(1,1962)	1:610:A:ASP:HB3	1:613:A:ALA:HB1	19	0.77	0.1	0.77
(1,1250)	1:626:A:GLU:HG2	1:623:A:GLU:HA	19	0.73	0.39	0.81
(1,1836)	1:619:A:GLU:HA	1:618:A:LEU:HD11	19	0.58	0.12	0.58
(1,1836)	1:619:A:GLU:HA	1:618:A:LEU:HD12	19	0.58	0.12	0.58
(1,1836)	1:619:A:GLU:HA	1:618:A:LEU:HD13	19	0.58	0.12	0.58
(1,1836)	1:619:A:GLU:HA	1:618:A:LEU:HD23	19	0.58	0.12	0.58
(1,1538)	1:571:A:GLU:H	1:570:A:LEU:HD11	19	0.55	0.21	0.58
(1,1538)	1:571:A:GLU:H	1:628:A:LEU:HD13	19	0.55	0.21	0.58
(1,1538)	1:571:A:GLU:H	1:628:A:LEU:HD12	19	0.55	0.21	0.58
(1,1538)	1:571:A:GLU:H	1:570:A:LEU:HD12	19	0.55	0.21	0.58
(1,1538)	1:571:A:GLU:H	1:628:A:LEU:HD11	19	0.55	0.21	0.58
(1,1723)	1:591:A:VAL:HG13	1:611:A:MET:HG3	19	0.54	0.13	0.58
(1,1723)	1:591:A:VAL:HG11	1:611:A:MET:HG3	19	0.54	0.13	0.58
(1,1723)	1:591:A:VAL:HG12	1:607:A:VAL:HB	19	0.54	0.13	0.58
(1,1723)	1:591:A:VAL:HG12	1:611:A:MET:HG3	19	0.54	0.13	0.58
(1,1621)	1:619:A:GLU:H	1:618:A:LEU:HD22	19	0.52	0.12	0.53
(1,1621)	1:619:A:GLU:H	1:618:A:LEU:HD23	19	0.52	0.12	0.53
(1,1621)	1:619:A:GLU:H	1:618:A:LEU:HD21	19	0.52	0.12	0.53
(1,1621)	1:619:A:GLU:H	1:618:A:LEU:HD12	19	0.52	0.12	0.53
(1,2135)	1:567:A:GLN:HA	1:570:A:LEU:HD11	19	0.5	0.28	0.48
(1,2135)	1:567:A:GLN:HA	1:570:A:LEU:HD12	19	0.5	0.28	0.48
(1,2135)	1:567:A:GLN:HA	1:570:A:LEU:HD13	19	0.5	0.28	0.48
(1,1465)	1:606:A:LYS:H	1:606:A:LYS:HG2	19	0.5	0.02	0.5
(1,1691)	1:627:A:TYR:HE2	1:624:A:ARG:HA	19	0.43	0.08	0.4
(1,1691)	1:627:A:TYR:HE1	1:627:A:TYR:HA	19	0.43	0.08	0.4
(1,1062)	1:610:A:ASP:HB2	1:587:A:LEU:HD23	19	0.39	0.11	0.42
(1,1062)	1:610:A:ASP:HB2	1:587:A:LEU:HD21	19	0.39	0.11	0.42
(1,1062)	1:610:A:ASP:HB2	1:587:A:LEU:HD22	19	0.39	0.11	0.42
(1,559)	1:596:A:PHE:HE1	1:604:A:THR:HG23	19	0.39	0.11	0.41
(1,559)	1:596:A:PHE:HE2	1:604:A:THR:HG21	19	0.39	0.11	0.41
(1,559)	1:596:A:PHE:HE1	1:604:A:THR:HG22	19	0.39	0.11	0.41
(1,559)	1:596:A:PHE:HE1	1:604:A:THR:HG21	19	0.39	0.11	0.41
(1,559)	1:596:A:PHE:HE2	1:604:A:THR:HG23	19	0.39	0.11	0.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1369)	1:591:A:VAL:HG23	1:596:A:PHE:HB2	19	0.39	0.08	0.39
(1,1369)	1:591:A:VAL:HG22	1:596:A:PHE:HB2	19	0.39	0.08	0.39
(1,1369)	1:591:A:VAL:HG21	1:596:A:PHE:HB2	19	0.39	0.08	0.39
(1,1147)	1:565:A:LYS:HA	1:565:A:LYS:HD2	19	0.37	0.1	0.39
(1,1147)	1:565:A:LYS:HA	1:565:A:LYS:HD3	19	0.37	0.1	0.39
(1,1588)	1:583:A:LYS:H	1:581:A:GLU:HG2	19	0.35	0.13	0.34
(1,1588)	1:613:A:ALA:H	1:616:A:GLN:HG3	19	0.35	0.13	0.34
(1,1588)	1:613:A:ALA:H	1:611:A:MET:HB2	19	0.35	0.13	0.34
(1,2059)	1:615:A:GLU:HA	1:619:A:GLU:HG2	19	0.33	0.11	0.35
(1,1868)	1:569:A:GLU:HA	1:566:A:LEU:HA	19	0.32	0.09	0.32
(1,1868)	1:614:A:ALA:HA	1:615:A:GLU:HA	19	0.32	0.09	0.32
(1,1868)	1:612:A:ALA:HA	1:611:A:MET:HA	19	0.32	0.09	0.32
(1,1778)	1:612:A:ALA:HA	1:584:A:LEU:HD22	19	0.32	0.11	0.28
(1,1778)	1:612:A:ALA:HA	1:584:A:LEU:HD21	19	0.32	0.11	0.28
(1,1778)	1:612:A:ALA:HA	1:584:A:LEU:HD23	19	0.32	0.11	0.28
(1,1779)	1:614:A:ALA:HA	1:580:A:LEU:HD11	19	0.31	0.14	0.32
(1,1779)	1:614:A:ALA:HA	1:580:A:LEU:HD12	19	0.31	0.14	0.32
(1,1779)	1:614:A:ALA:HA	1:580:A:LEU:HD13	19	0.31	0.14	0.32
(1,1779)	1:614:A:ALA:HA	1:587:A:LEU:HD13	19	0.31	0.14	0.32
(1,1020)	1:604:A:THR:HG23	1:599:A:GLN:HG3	19	0.28	0.1	0.27
(1,1020)	1:604:A:THR:HG22	1:599:A:GLN:HG3	19	0.28	0.1	0.27
(1,1020)	1:604:A:THR:HG21	1:599:A:GLN:HG3	19	0.28	0.1	0.27
(1,1718)	1:604:A:THR:HG23	1:599:A:GLN:HG3	19	0.28	0.1	0.27
(1,1718)	1:604:A:THR:HG22	1:599:A:GLN:HG3	19	0.28	0.1	0.27
(1,1718)	1:604:A:THR:HG21	1:599:A:GLN:HG3	19	0.28	0.1	0.27
(1,1569)	1:607:A:VAL:H	1:587:A:LEU:HD23	19	0.27	0.12	0.28
(1,1569)	1:607:A:VAL:H	1:587:A:LEU:HD21	19	0.27	0.12	0.28
(1,1569)	1:607:A:VAL:H	1:608:A:LEU:HD21	19	0.27	0.12	0.28
(1,1569)	1:607:A:VAL:H	1:587:A:LEU:HD22	19	0.27	0.12	0.28
(1,1569)	1:607:A:VAL:H	1:608:A:LEU:HD22	19	0.27	0.12	0.28
(1,1569)	1:607:A:VAL:H	1:608:A:LEU:HD23	19	0.27	0.12	0.28
(1,554)	1:627:A:TYR:HE2	1:628:A:LEU:HD22	19	0.27	0.09	0.25
(1,554)	1:627:A:TYR:HE2	1:628:A:LEU:HD21	19	0.27	0.09	0.25
(1,554)	1:627:A:TYR:HE2	1:628:A:LEU:HD23	19	0.27	0.09	0.25
(1,1867)	1:564:A:TYR:HA	1:567:A:GLN:HA	19	0.26	0.07	0.26
(1,173)	1:612:A:ALA:H	1:611:A:MET:HB2	19	0.25	0.06	0.23
(1,1451)	1:599:A:GLN:H	1:600:A:PRO:HD3	19	0.25	0.11	0.25
(1,1451)	1:599:A:GLN:H	1:597:A:PHE:HB2	19	0.25	0.11	0.25
(1,1056)	1:622:A:PHE:HB2	1:577:A:LEU:HD23	19	0.25	0.06	0.26
(1,1056)	1:622:A:PHE:HB2	1:577:A:LEU:HD22	19	0.25	0.06	0.26
(1,1056)	1:622:A:PHE:HB2	1:577:A:LEU:HD21	19	0.25	0.06	0.26
(1,585)	1:596:A:PHE:HZ	1:607:A:VAL:HG13	19	0.23	0.06	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,585)	1:596:A:PHE:HZ	1:607:A:VAL:HG12	19	0.23	0.06	0.23
(1,585)	1:596:A:PHE:HZ	1:607:A:VAL:HG11	19	0.23	0.06	0.23
(1,1577)	1:609:A:ALA:H	1:608:A:LEU:HG	19	0.21	0.05	0.22
(1,162)	1:584:A:LEU:H	1:583:A:LYS:HG3	19	0.18	0.04	0.19
(1,810)	1:608:A:LEU:HA	1:608:A:LEU:HD13	19	0.16	0.02	0.16
(1,810)	1:608:A:LEU:HA	1:608:A:LEU:HD12	19	0.16	0.02	0.16
(1,810)	1:608:A:LEU:HA	1:608:A:LEU:HD11	19	0.16	0.02	0.16
(1,2110)	1:573:A:LEU:HD11	1:570:A:LEU:HB3	18	1.78	0.13	1.77
(1,2110)	1:573:A:LEU:HD13	1:570:A:LEU:HB3	18	1.78	0.13	1.77
(1,2110)	1:573:A:LEU:HD12	1:570:A:LEU:HB3	18	1.78	0.13	1.77
(1,1888)	1:568:A:ARG:HG3	1:571:A:GLU:HB3	18	0.89	0.26	0.94
(1,1888)	1:568:A:ARG:HG2	1:569:A:GLU:HB3	18	0.89	0.26	0.94
(1,1888)	1:568:A:ARG:HG2	1:571:A:GLU:HB3	18	0.89	0.26	0.94
(1,1888)	1:568:A:ARG:HG2	1:567:A:GLN:HB2	18	0.89	0.26	0.94
(1,1293)	1:577:A:LEU:HD11	1:573:A:LEU:HD12	18	0.86	0.16	0.88
(1,1293)	1:577:A:LEU:HD11	1:573:A:LEU:HD11	18	0.86	0.16	0.88
(1,1293)	1:577:A:LEU:HD11	1:573:A:LEU:HD13	18	0.86	0.16	0.88
(1,1293)	1:577:A:LEU:HD12	1:573:A:LEU:HD11	18	0.86	0.16	0.88
(1,1293)	1:577:A:LEU:HD12	1:573:A:LEU:HD13	18	0.86	0.16	0.88
(1,1293)	1:577:A:LEU:HD13	1:573:A:LEU:HD11	18	0.86	0.16	0.88
(1,1293)	1:577:A:LEU:HD12	1:573:A:LEU:HD12	18	0.86	0.16	0.88
(1,1293)	1:577:A:LEU:HD13	1:573:A:LEU:HD12	18	0.86	0.16	0.88
(1,1293)	1:577:A:LEU:HD13	1:573:A:LEU:HD13	18	0.86	0.16	0.88
(1,1729)	1:631:A:LEU:HD22	1:561:A:LYS:HA	18	0.67	0.19	0.73
(1,1729)	1:631:A:LEU:HD23	1:563:A:SER:HB2	18	0.67	0.19	0.73
(1,1729)	1:631:A:LEU:HD23	1:561:A:LYS:HA	18	0.67	0.19	0.73
(1,1729)	1:631:A:LEU:HD21	1:561:A:LYS:HA	18	0.67	0.19	0.73
(1,1729)	1:631:A:LEU:HD22	1:563:A:SER:HB2	18	0.67	0.19	0.73
(1,1326)	1:566:A:LEU:HD23	1:563:A:SER:HB3	18	0.58	0.32	0.54
(1,1326)	1:566:A:LEU:HD22	1:563:A:SER:HB3	18	0.58	0.32	0.54
(1,1326)	1:566:A:LEU:HD21	1:563:A:SER:HB3	18	0.58	0.32	0.54
(1,1120)	1:588:A:GLN:HA	1:611:A:MET:HE3	18	0.57	0.08	0.6
(1,1120)	1:588:A:GLN:HA	1:611:A:MET:HE2	18	0.57	0.08	0.6
(1,1120)	1:588:A:GLN:HA	1:611:A:MET:HE1	18	0.57	0.08	0.6
(1,956)	1:605:A:GLN:HB3	1:608:A:LEU:HD11	18	0.55	0.18	0.62
(1,956)	1:605:A:GLN:HB3	1:608:A:LEU:HD13	18	0.55	0.18	0.62
(1,956)	1:605:A:GLN:HB3	1:608:A:LEU:HD12	18	0.55	0.18	0.62
(1,1367)	1:570:A:LEU:HD22	1:628:A:LEU:HB3	18	0.52	0.18	0.6
(1,1367)	1:570:A:LEU:HD21	1:628:A:LEU:HB3	18	0.52	0.18	0.6
(1,1367)	1:570:A:LEU:HD23	1:628:A:LEU:HB3	18	0.52	0.18	0.6
(1,1924)	1:614:A:ALA:HB1	1:611:A:MET:HG2	18	0.49	0.06	0.5
(1,1924)	1:614:A:ALA:HB3	1:611:A:MET:HG2	18	0.49	0.06	0.5

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1924)	1:614:A:ALA:HB2	1:611:A:MET:HG2	18	0.49	0.06	0.5
(1,809)	1:605:A:GLN:HA	1:608:A:LEU:HD22	18	0.48	0.13	0.51
(1,809)	1:605:A:GLN:HA	1:608:A:LEU:HD21	18	0.48	0.13	0.51
(1,809)	1:605:A:GLN:HA	1:608:A:LEU:HD23	18	0.48	0.13	0.51
(1,2042)	1:573:A:LEU:HG	1:570:A:LEU:HA	18	0.47	0.12	0.49
(1,2042)	1:625:A:TRP:HA	1:573:A:LEU:HG	18	0.47	0.12	0.49
(1,1164)	1:601:A:HIS:HB3	1:605:A:GLN:HG2	18	0.46	0.12	0.48
(1,1164)	1:601:A:HIS:HB3	1:605:A:GLN:HG3	18	0.46	0.12	0.48
(1,2105)	1:566:A:LEU:HD23	1:628:A:LEU:HG	18	0.4	0.22	0.33
(1,2105)	1:566:A:LEU:HD22	1:628:A:LEU:HG	18	0.4	0.22	0.33
(1,2105)	1:566:A:LEU:HD23	1:569:A:GLU:HG3	18	0.4	0.22	0.33
(1,2105)	1:566:A:LEU:HD21	1:569:A:GLU:HG3	18	0.4	0.22	0.33
(1,2105)	1:566:A:LEU:HD21	1:628:A:LEU:HG	18	0.4	0.22	0.33
(1,2047)	1:608:A:LEU:HA	1:611:A:MET:HG2	18	0.36	0.05	0.37
(1,1402)	1:606:A:LYS:HB2	1:606:A:LYS:HE2	18	0.35	0.09	0.34
(1,1402)	1:606:A:LYS:HB2	1:606:A:LYS:HE3	18	0.35	0.09	0.34
(1,1683)	1:622:A:PHE:HE2	1:618:A:LEU:HD21	18	0.31	0.16	0.27
(1,1683)	1:622:A:PHE:HE2	1:618:A:LEU:HD22	18	0.31	0.16	0.27
(1,1683)	1:622:A:PHE:HE2	1:618:A:LEU:HD23	18	0.31	0.16	0.27
(1,1063)	1:610:A:ASP:HB2	1:587:A:LEU:HD12	18	0.26	0.07	0.29
(1,1063)	1:610:A:ASP:HB2	1:587:A:LEU:HD11	18	0.26	0.07	0.29
(1,1063)	1:610:A:ASP:HB2	1:587:A:LEU:HD13	18	0.26	0.07	0.29
(1,1706)	1:625:A:TRP:HD1	1:628:A:LEU:HB2	18	0.26	0.07	0.26
(1,1370)	1:604:A:THR:HG23	1:607:A:VAL:HB	18	0.26	0.08	0.26
(1,1370)	1:604:A:THR:HG21	1:607:A:VAL:HB	18	0.26	0.08	0.26
(1,1370)	1:604:A:THR:HG22	1:607:A:VAL:HB	18	0.26	0.08	0.26
(1,985)	1:591:A:VAL:HB	1:608:A:LEU:HD21	18	0.25	0.09	0.22
(1,985)	1:591:A:VAL:HB	1:608:A:LEU:HD22	18	0.25	0.09	0.22
(1,985)	1:591:A:VAL:HB	1:608:A:LEU:HD23	18	0.25	0.09	0.22
(1,820)	1:601:A:HIS:HA	1:605:A:GLN:HB2	18	0.2	0.03	0.2
(1,1509)	1:581:A:GLU:H	1:580:A:LEU:HG	18	0.18	0.03	0.18
(1,1509)	1:625:A:TRP:H	1:624:A:ARG:HG2	18	0.18	0.03	0.18
(1,774)	1:610:A:ASP:HA	1:587:A:LEU:HD12	18	0.18	0.03	0.18
(1,774)	1:610:A:ASP:HA	1:587:A:LEU:HD11	18	0.18	0.03	0.18
(1,774)	1:610:A:ASP:HA	1:587:A:LEU:HD13	18	0.18	0.03	0.18
(1,1307)	1:566:A:LEU:HD11	1:565:A:LYS:HA	17	1.38	1.46	0.37
(1,1307)	1:566:A:LEU:HD12	1:565:A:LYS:HA	17	1.38	1.46	0.37
(1,1307)	1:566:A:LEU:HD13	1:565:A:LYS:HA	17	1.38	1.46	0.37
(1,2118)	1:583:A:LYS:HE2	1:580:A:LEU:HD23	17	0.76	0.19	0.81
(1,2118)	1:583:A:LYS:HE2	1:580:A:LEU:HD22	17	0.76	0.19	0.81
(1,2118)	1:583:A:LYS:HE2	1:580:A:LEU:HD21	17	0.76	0.19	0.81
(1,2118)	1:583:A:LYS:HE3	1:580:A:LEU:HD23	17	0.76	0.19	0.81

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2118)	1:579:A:ASP:HB2	1:580:A:LEU:HD22	17	0.76	0.19	0.81
(1,2120)	1:573:A:LEU:HD23	1:624:A:ARG:HB2	17	0.72	0.27	0.7
(1,2120)	1:573:A:LEU:HD22	1:624:A:ARG:HB2	17	0.72	0.27	0.7
(1,2120)	1:573:A:LEU:HD21	1:624:A:ARG:HB2	17	0.72	0.27	0.7
(1,1333)	1:573:A:LEU:HD13	1:624:A:ARG:HD2	17	0.69	0.64	0.57
(1,1333)	1:573:A:LEU:HD12	1:624:A:ARG:HD2	17	0.69	0.64	0.57
(1,1333)	1:573:A:LEU:HD11	1:624:A:ARG:HD2	17	0.69	0.64	0.57
(1,2034)	1:618:A:LEU:HG	1:615:A:GLU:HA	17	0.44	0.09	0.47
(1,2034)	1:618:A:LEU:HG	1:581:A:GLU:HA	17	0.44	0.09	0.47
(1,1901)	1:613:A:ALA:HB1	1:616:A:GLN:HB2	17	0.43	0.14	0.43
(1,1901)	1:613:A:ALA:HB2	1:616:A:GLN:HB2	17	0.43	0.14	0.43
(1,1901)	1:613:A:ALA:HB3	1:616:A:GLN:HB2	17	0.43	0.14	0.43
(1,1901)	1:612:A:ALA:HB1	1:616:A:GLN:HB3	17	0.43	0.14	0.43
(1,1901)	1:612:A:ALA:HB2	1:616:A:GLN:HB3	17	0.43	0.14	0.43
(1,1901)	1:612:A:ALA:HB3	1:616:A:GLN:HB3	17	0.43	0.14	0.43
(1,1165)	1:601:A:HIS:HB2	1:605:A:GLN:HG2	17	0.39	0.13	0.39
(1,2124)	1:612:A:ALA:HA	1:611:A:MET:HE1	17	0.35	0.29	0.23
(1,2124)	1:612:A:ALA:HA	1:611:A:MET:HE3	17	0.35	0.29	0.23
(1,2124)	1:612:A:ALA:HA	1:611:A:MET:HE2	17	0.35	0.29	0.23
(1,634)	1:577:A:LEU:HD12	1:574:A:PRO:HA	17	0.34	0.09	0.35
(1,634)	1:577:A:LEU:HD13	1:574:A:PRO:HA	17	0.34	0.09	0.35
(1,634)	1:577:A:LEU:HD11	1:574:A:PRO:HA	17	0.34	0.09	0.35
(1,1708)	1:625:A:TRP:HD1	1:628:A:LEU:HD13	17	0.33	0.11	0.36
(1,1708)	1:625:A:TRP:HD1	1:628:A:LEU:HD11	17	0.33	0.11	0.36
(1,1708)	1:625:A:TRP:HD1	1:628:A:LEU:HD12	17	0.33	0.11	0.36
(1,1562)	1:604:A:THR:H	1:599:A:GLN:HB2	17	0.32	0.14	0.37
(1,1961)	1:610:A:ASP:HB3	1:587:A:LEU:HB3	17	0.32	0.11	0.33
(1,1431)	1:622:A:PHE:HE2	1:618:A:LEU:HD21	17	0.31	0.15	0.29
(1,1431)	1:622:A:PHE:HE2	1:618:A:LEU:HD22	17	0.31	0.15	0.29
(1,1431)	1:622:A:PHE:HE2	1:618:A:LEU:HD23	17	0.31	0.15	0.29
(1,1907)	1:591:A:VAL:HA	1:608:A:LEU:HD23	17	0.29	0.13	0.25
(1,1907)	1:591:A:VAL:HA	1:608:A:LEU:HD21	17	0.29	0.13	0.25
(1,1907)	1:591:A:VAL:HA	1:608:A:LEU:HD22	17	0.29	0.13	0.25
(1,1520)	1:577:A:LEU:H	1:574:A:PRO:HB2	17	0.27	0.06	0.27
(1,1520)	1:577:A:LEU:H	1:578:A:GLU:HG3	17	0.27	0.06	0.27
(1,717)	1:621:A:ALA:HB3	1:577:A:LEU:HD22	17	0.27	0.09	0.28
(1,717)	1:621:A:ALA:HB2	1:577:A:LEU:HD22	17	0.27	0.09	0.28
(1,717)	1:621:A:ALA:HB1	1:577:A:LEU:HD21	17	0.27	0.09	0.28
(1,717)	1:621:A:ALA:HB2	1:577:A:LEU:HD21	17	0.27	0.09	0.28
(1,717)	1:621:A:ALA:HB3	1:577:A:LEU:HD21	17	0.27	0.09	0.28
(1,717)	1:621:A:ALA:HB3	1:577:A:LEU:HD23	17	0.27	0.09	0.28
(1,717)	1:621:A:ALA:HB1	1:577:A:LEU:HD23	17	0.27	0.09	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1474)	1:589:A:THR:H	1:586:A:ALA:HA	17	0.24	0.08	0.24
(1,1963)	1:596:A:PHE:HB3	1:591:A:VAL:HG11	17	0.23	0.07	0.24
(1,1963)	1:596:A:PHE:HB3	1:591:A:VAL:HG12	17	0.23	0.07	0.24
(1,1963)	1:596:A:PHE:HB3	1:591:A:VAL:HG13	17	0.23	0.07	0.24
(1,1210)	1:606:A:LYS:HA	1:605:A:GLN:HB3	17	0.21	0.06	0.22
(1,1210)	1:606:A:LYS:HA	1:605:A:GLN:HB2	17	0.21	0.06	0.22
(1,1095)	1:565:A:LYS:HE3	1:566:A:LEU:HD13	16	1.35	0.83	1.0
(1,1095)	1:565:A:LYS:HE3	1:566:A:LEU:HD11	16	1.35	0.83	1.0
(1,1095)	1:565:A:LYS:HE2	1:566:A:LEU:HD13	16	1.35	0.83	1.0
(1,1095)	1:565:A:LYS:HE2	1:566:A:LEU:HD12	16	1.35	0.83	1.0
(1,1095)	1:565:A:LYS:HE3	1:566:A:LEU:HD12	16	1.35	0.83	1.0
(1,2166)	1:561:A:LYS:HG3	1:562:A:LEU:HD21	16	1.12	0.5	1.2
(1,2166)	1:561:A:LYS:HG3	1:562:A:LEU:HD23	16	1.12	0.5	1.2
(1,2166)	1:561:A:LYS:HG3	1:562:A:LEU:HD22	16	1.12	0.5	1.2
(1,2166)	1:562:A:LEU:HD13	1:561:A:LYS:HG3	16	1.12	0.5	1.2
(1,2166)	1:562:A:LEU:HD11	1:561:A:LYS:HG3	16	1.12	0.5	1.2
(1,2166)	1:562:A:LEU:HD12	1:561:A:LYS:HG3	16	1.12	0.5	1.2
(1,1871)	1:594:A:ALA:HB3	1:595:A:SER:HB2	16	0.88	0.26	0.9
(1,1871)	1:594:A:ALA:HB1	1:595:A:SER:HB2	16	0.88	0.26	0.9
(1,1871)	1:594:A:ALA:HB2	1:595:A:SER:HB2	16	0.88	0.26	0.9
(1,1871)	1:594:A:ALA:HB2	1:595:A:SER:HB3	16	0.88	0.26	0.9
(1,1760)	1:613:A:ALA:HB2	1:611:A:MET:HA	16	0.84	0.22	0.9
(1,1760)	1:594:A:ALA:HB3	1:595:A:SER:HB2	16	0.84	0.22	0.9
(1,1760)	1:594:A:ALA:HB1	1:595:A:SER:HB2	16	0.84	0.22	0.9
(1,1760)	1:613:A:ALA:HB3	1:611:A:MET:HA	16	0.84	0.22	0.9
(1,1760)	1:594:A:ALA:HB2	1:595:A:SER:HB2	16	0.84	0.22	0.9
(1,1760)	1:594:A:ALA:HB2	1:595:A:SER:HB3	16	0.84	0.22	0.9
(1,1592)	1:613:A:ALA:H	1:616:A:GLN:HB2	16	0.76	0.17	0.82
(1,1592)	1:583:A:LYS:H	1:581:A:GLU:HB2	16	0.76	0.17	0.82
(1,1592)	1:613:A:ALA:H	1:615:A:GLU:HG3	16	0.76	0.17	0.82
(1,1335)	1:566:A:LEU:HG	1:562:A:LEU:HD21	16	0.56	0.54	0.32
(1,1335)	1:566:A:LEU:HG	1:562:A:LEU:HD23	16	0.56	0.54	0.32
(1,1335)	1:566:A:LEU:HG	1:562:A:LEU:HD22	16	0.56	0.54	0.32
(1,1546)	1:568:A:ARG:H	1:567:A:GLN:HG3	16	0.22	0.1	0.2
(1,429)	1:618:A:LEU:H	1:617:A:GLU:HB2	16	0.21	0.09	0.18
(1,182)	1:581:A:GLU:H	1:580:A:LEU:HD12	16	0.17	0.04	0.16
(1,182)	1:581:A:GLU:H	1:580:A:LEU:HD13	16	0.17	0.04	0.16
(1,182)	1:581:A:GLU:H	1:580:A:LEU:HD11	16	0.17	0.04	0.16
(1,1340)	1:573:A:LEU:HA	1:576:A:LEU:HG	16	0.16	0.03	0.16
(1,1853)	1:554:A:THR:HB	1:555:A:VAL:HG21	15	0.55	0.16	0.55
(1,1853)	1:554:A:THR:HB	1:555:A:VAL:HG12	15	0.55	0.16	0.55
(1,1853)	1:554:A:THR:HB	1:555:A:VAL:HG13	15	0.55	0.16	0.55

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1853)	1:554:A:THR:HB	1:555:A:VAL:HG11	15	0.55	0.16	0.55
(1,1853)	1:554:A:THR:HB	1:555:A:VAL:HG23	15	0.55	0.16	0.55
(1,1853)	1:554:A:THR:HB	1:555:A:VAL:HG22	15	0.55	0.16	0.55
(1,110)	1:590:A:GLN:H	1:590:A:GLN:HG3	15	0.32	0.13	0.39
(1,602)	1:597:A:PHE:HZ	1:608:A:LEU:HD11	15	0.32	0.07	0.35
(1,602)	1:597:A:PHE:HZ	1:608:A:LEU:HD12	15	0.32	0.07	0.35
(1,602)	1:597:A:PHE:HZ	1:608:A:LEU:HD13	15	0.32	0.07	0.35
(1,603)	1:622:A:PHE:HD1	1:626:A:GLU:HG2	15	0.29	0.09	0.28
(1,1709)	1:625:A:TRP:HD1	1:573:A:LEU:HB2	15	0.29	0.13	0.24
(1,1709)	1:625:A:TRP:HD1	1:574:A:PRO:HG2	15	0.29	0.13	0.24
(1,1828)	1:601:A:HIS:HA	1:602:A:GLU:HG3	15	0.25	0.1	0.22
(1,1828)	1:601:A:HIS:HA	1:602:A:GLU:HG2	15	0.25	0.1	0.22
(1,1828)	1:601:A:HIS:HA	1:603:A:GLN:HG3	15	0.25	0.1	0.22
(1,1787)	1:621:A:ALA:HA	1:620:A:GLN:HB3	15	0.25	0.07	0.26
(1,1787)	1:621:A:ALA:HA	1:620:A:GLN:HB2	15	0.25	0.07	0.26
(1,1813)	1:588:A:GLN:HA	1:584:A:LEU:HD23	15	0.23	0.07	0.21
(1,1813)	1:588:A:GLN:HA	1:584:A:LEU:HD21	15	0.23	0.07	0.21
(1,1813)	1:588:A:GLN:HA	1:584:A:LEU:HD22	15	0.23	0.07	0.21
(1,1700)	1:622:A:PHE:HZ	1:618:A:LEU:HD13	15	0.22	0.1	0.22
(1,1700)	1:622:A:PHE:HZ	1:618:A:LEU:HD12	15	0.22	0.1	0.22
(1,1700)	1:622:A:PHE:HZ	1:618:A:LEU:HD11	15	0.22	0.1	0.22
(1,1700)	1:622:A:PHE:HZ	1:618:A:LEU:HD22	15	0.22	0.1	0.22
(1,928)	1:583:A:LYS:HG3	1:587:A:LEU:HD21	15	0.21	0.07	0.22
(1,928)	1:583:A:LYS:HG3	1:587:A:LEU:HD22	15	0.21	0.07	0.22
(1,928)	1:583:A:LYS:HG3	1:587:A:LEU:HD23	15	0.21	0.07	0.22
(1,1286)	1:566:A:LEU:HD23	1:569:A:GLU:HB2	14	1.6	0.13	1.57
(1,1286)	1:566:A:LEU:HD22	1:569:A:GLU:HB2	14	1.6	0.13	1.57
(1,1286)	1:566:A:LEU:HD21	1:569:A:GLU:HB2	14	1.6	0.13	1.57
(1,1918)	1:583:A:LYS:HD2	1:576:A:LEU:HD13	14	1.52	0.22	1.54
(1,1918)	1:565:A:LYS:HD3	1:566:A:LEU:HD23	14	1.52	0.22	1.54
(1,1918)	1:583:A:LYS:HD2	1:587:A:LEU:HD22	14	1.52	0.22	1.54
(1,1918)	1:565:A:LYS:HD3	1:566:A:LEU:HD21	14	1.52	0.22	1.54
(1,1918)	1:565:A:LYS:HD2	1:566:A:LEU:HD22	14	1.52	0.22	1.54
(1,1918)	1:565:A:LYS:HD3	1:566:A:LEU:HD22	14	1.52	0.22	1.54
(1,1918)	1:565:A:LYS:HD2	1:566:A:LEU:HD23	14	1.52	0.22	1.54
(1,1918)	1:583:A:LYS:HD2	1:587:A:LEU:HD23	14	1.52	0.22	1.54
(1,1917)	1:585:A:GLU:HB2	1:584:A:LEU:HD13	14	0.76	0.23	0.79
(1,1917)	1:585:A:GLU:HB2	1:584:A:LEU:HD11	14	0.76	0.23	0.79
(1,1917)	1:585:A:GLU:HB2	1:584:A:LEU:HD12	14	0.76	0.23	0.79
(1,1376)	1:566:A:LEU:HD22	1:563:A:SER:HB2	14	0.76	0.35	0.64
(1,1376)	1:566:A:LEU:HD21	1:563:A:SER:HB2	14	0.76	0.35	0.64
(1,1376)	1:566:A:LEU:HD23	1:563:A:SER:HB2	14	0.76	0.35	0.64

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1552)	1:567:A:GLN:H	1:568:A:ARG:HB2	14	0.71	0.07	0.7
(1,1552)	1:567:A:GLN:H	1:566:A:LEU:HG	14	0.71	0.07	0.7
(1,1552)	1:567:A:GLN:H	1:568:A:ARG:HB3	14	0.71	0.07	0.7
(1,300)	1:567:A:GLN:H	1:566:A:LEU:HD21	14	0.56	0.07	0.55
(1,300)	1:567:A:GLN:H	1:566:A:LEU:HD23	14	0.56	0.07	0.55
(1,300)	1:567:A:GLN:H	1:566:A:LEU:HD22	14	0.56	0.07	0.55
(1,2165)	1:606:A:LYS:HA	1:610:A:ASP:HB2	14	0.42	0.17	0.44
(1,2165)	1:606:A:LYS:HA	1:606:A:LYS:HE3	14	0.42	0.17	0.44
(1,2165)	1:606:A:LYS:HA	1:606:A:LYS:HE2	14	0.42	0.17	0.44
(1,1937)	1:616:A:GLN:HG3	1:612:A:ALA:HB3	14	0.36	0.14	0.36
(1,1937)	1:616:A:GLN:HG3	1:613:A:ALA:HB2	14	0.36	0.14	0.36
(1,1937)	1:616:A:GLN:HG3	1:613:A:ALA:HB1	14	0.36	0.14	0.36
(1,1937)	1:616:A:GLN:HG3	1:613:A:ALA:HB3	14	0.36	0.14	0.36
(1,321)	1:604:A:THR:H	1:596:A:PHE:HE1	14	0.33	0.07	0.34
(1,1515)	1:579:A:ASP:H	1:576:A:LEU:HD13	14	0.25	0.12	0.2
(1,1515)	1:579:A:ASP:H	1:576:A:LEU:HD12	14	0.25	0.12	0.2
(1,1515)	1:579:A:ASP:H	1:576:A:LEU:HD11	14	0.25	0.12	0.2
(1,1617)	1:617:A:GLU:H	1:580:A:LEU:HD21	14	0.24	0.1	0.19
(1,1617)	1:617:A:GLU:H	1:580:A:LEU:HD23	14	0.24	0.1	0.19
(1,1617)	1:617:A:GLU:H	1:580:A:LEU:HD22	14	0.24	0.1	0.19
(1,1669)	1:633:A:ASN:H	1:631:A:LEU:HB3	14	0.23	0.08	0.22
(1,1669)	1:633:A:ASN:H	1:632:A:LYS:HG3	14	0.23	0.08	0.22
(1,369)	1:609:A:ALA:H	1:608:A:LEU:HD13	14	0.19	0.06	0.2
(1,369)	1:609:A:ALA:H	1:608:A:LEU:HD11	14	0.19	0.06	0.2
(1,369)	1:609:A:ALA:H	1:608:A:LEU:HD12	14	0.19	0.06	0.2
(1,1933)	1:611:A:MET:HB2	1:584:A:LEU:HD23	14	0.19	0.06	0.16
(1,1933)	1:611:A:MET:HB2	1:608:A:LEU:HD22	14	0.19	0.06	0.16
(1,1933)	1:611:A:MET:HB2	1:608:A:LEU:HD23	14	0.19	0.06	0.16
(1,1933)	1:611:A:MET:HB2	1:584:A:LEU:HD21	14	0.19	0.06	0.16
(1,1933)	1:611:A:MET:HB2	1:608:A:LEU:HD21	14	0.19	0.06	0.16
(1,1363)	1:562:A:LEU:HD21	1:631:A:LEU:HB2	13	1.02	1.23	0.44
(1,1363)	1:562:A:LEU:HD23	1:631:A:LEU:HB2	13	1.02	1.23	0.44
(1,1363)	1:562:A:LEU:HD22	1:631:A:LEU:HB2	13	1.02	1.23	0.44
(1,1991)	1:562:A:LEU:HB3	1:566:A:LEU:HD13	13	0.94	0.18	1.01
(1,1991)	1:562:A:LEU:HB3	1:566:A:LEU:HD12	13	0.94	0.18	1.01
(1,1991)	1:562:A:LEU:HB3	1:566:A:LEU:HD11	13	0.94	0.18	1.01
(1,970)	1:632:A:LYS:HD3	1:570:A:LEU:HD11	13	0.71	0.54	0.64
(1,970)	1:632:A:LYS:HD3	1:570:A:LEU:HD12	13	0.71	0.54	0.64
(1,970)	1:632:A:LYS:HD3	1:570:A:LEU:HD13	13	0.71	0.54	0.64
(1,970)	1:632:A:LYS:HD2	1:570:A:LEU:HD12	13	0.71	0.54	0.64
(1,970)	1:632:A:LYS:HD2	1:570:A:LEU:HD11	13	0.71	0.54	0.64
(1,1960)	1:622:A:PHE:HB3	1:623:A:GLU:HB2	13	0.65	0.28	0.58

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1960)	1:622:A:PHE:HB3	1:619:A:GLU:HB2	13	0.65	0.28	0.58
(1,1960)	1:622:A:PHE:HB3	1:623:A:GLU:HG3	13	0.65	0.28	0.58
(1,1378)	1:624:A:ARG:HD3	1:573:A:LEU:HD13	13	0.63	0.69	0.36
(1,1378)	1:624:A:ARG:HD3	1:573:A:LEU:HD12	13	0.63	0.69	0.36
(1,1378)	1:624:A:ARG:HD3	1:573:A:LEU:HD11	13	0.63	0.69	0.36
(1,2025)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	13	0.54	0.14	0.55
(1,2025)	1:602:A:GLU:HG2	1:601:A:HIS:HB2	13	0.54	0.14	0.55
(1,2025)	1:622:A:PHE:HB3	1:623:A:GLU:HG3	13	0.54	0.14	0.55
(1,308)	1:566:A:LEU:H	1:566:A:LEU:HD21	13	0.52	0.08	0.56
(1,308)	1:566:A:LEU:H	1:566:A:LEU:HD23	13	0.52	0.08	0.56
(1,308)	1:566:A:LEU:H	1:566:A:LEU:HD22	13	0.52	0.08	0.56
(1,1939)	1:572:A:GLN:HG3	1:568:A:ARG:HG3	13	0.45	0.2	0.48
(1,1939)	1:572:A:GLN:HG3	1:573:A:LEU:HB3	13	0.45	0.2	0.48
(1,1939)	1:572:A:GLN:HG3	1:568:A:ARG:HG2	13	0.45	0.2	0.48
(1,1005)	1:603:A:GLN:HG3	1:604:A:THR:HG22	13	0.38	0.04	0.38
(1,1005)	1:603:A:GLN:HG3	1:604:A:THR:HG23	13	0.38	0.04	0.38
(1,1005)	1:603:A:GLN:HG3	1:604:A:THR:HG21	13	0.38	0.04	0.38
(1,1265)	1:593:A:ASP:HB3	1:595:A:SER:HB2	13	0.33	0.14	0.33
(1,1265)	1:593:A:ASP:HB3	1:595:A:SER:HB3	13	0.33	0.14	0.33
(1,1004)	1:604:A:THR:HG22	1:603:A:GLN:HG2	13	0.33	0.04	0.33
(1,1004)	1:604:A:THR:HG23	1:603:A:GLN:HG2	13	0.33	0.04	0.33
(1,1004)	1:604:A:THR:HG21	1:603:A:GLN:HG2	13	0.33	0.04	0.33
(1,1719)	1:604:A:THR:HG22	1:603:A:GLN:HG2	13	0.32	0.04	0.33
(1,1719)	1:604:A:THR:HG23	1:603:A:GLN:HG2	13	0.32	0.04	0.33
(1,1719)	1:604:A:THR:HG21	1:603:A:GLN:HG2	13	0.32	0.04	0.33
(1,1719)	1:604:A:THR:HG21	1:599:A:GLN:HG2	13	0.32	0.04	0.33
(1,664)	1:631:A:LEU:HD23	1:566:A:LEU:HB2	13	0.28	0.09	0.32
(1,664)	1:631:A:LEU:HD21	1:566:A:LEU:HB2	13	0.28	0.09	0.32
(1,664)	1:631:A:LEU:HD22	1:566:A:LEU:HB2	13	0.28	0.09	0.32
(1,507)	1:629:A:GLU:H	1:570:A:LEU:HD21	13	0.24	0.09	0.23
(1,507)	1:629:A:GLU:H	1:570:A:LEU:HD22	13	0.24	0.09	0.23
(1,507)	1:629:A:GLU:H	1:570:A:LEU:HD23	13	0.24	0.09	0.23
(1,1736)	1:607:A:VAL:HG13	1:611:A:MET:HE2	13	0.23	0.09	0.21
(1,1736)	1:607:A:VAL:HG11	1:608:A:LEU:HG	13	0.23	0.09	0.21
(1,1736)	1:607:A:VAL:HG13	1:608:A:LEU:HG	13	0.23	0.09	0.21
(1,1736)	1:607:A:VAL:HG12	1:608:A:LEU:HG	13	0.23	0.09	0.21
(1,1292)	1:577:A:LEU:HD22	1:573:A:LEU:HD13	13	0.18	0.07	0.15
(1,1292)	1:577:A:LEU:HD22	1:573:A:LEU:HD12	13	0.18	0.07	0.15
(1,1292)	1:577:A:LEU:HD21	1:573:A:LEU:HD11	13	0.18	0.07	0.15
(1,1292)	1:577:A:LEU:HD21	1:573:A:LEU:HD12	13	0.18	0.07	0.15
(1,1292)	1:577:A:LEU:HD23	1:573:A:LEU:HD11	13	0.18	0.07	0.15
(1,1292)	1:577:A:LEU:HD21	1:573:A:LEU:HD13	13	0.18	0.07	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1292)	1:577:A:LEU:HD22	1:573:A:LEU:HD11	13	0.18	0.07	0.15
(1,811)	1:618:A:LEU:HA	1:618:A:LEU:HD23	13	0.13	0.02	0.13
(1,811)	1:618:A:LEU:HA	1:618:A:LEU:HD21	13	0.13	0.02	0.13
(1,811)	1:618:A:LEU:HA	1:618:A:LEU:HD22	13	0.13	0.02	0.13
(1,1913)	1:585:A:GLU:HB3	1:586:A:ALA:HB3	12	0.7	0.14	0.74
(1,1913)	1:585:A:GLU:HB3	1:586:A:ALA:HB2	12	0.7	0.14	0.74
(1,1913)	1:585:A:GLU:HB3	1:586:A:ALA:HB1	12	0.7	0.14	0.74
(1,1913)	1:613:A:ALA:HB2	1:617:A:GLU:HB3	12	0.7	0.14	0.74
(1,2104)	1:566:A:LEU:HD22	1:562:A:LEU:HB2	12	0.7	0.3	0.64
(1,2104)	1:562:A:LEU:HG	1:566:A:LEU:HD23	12	0.7	0.3	0.64
(1,2104)	1:566:A:LEU:HD23	1:562:A:LEU:HB3	12	0.7	0.3	0.64
(1,2104)	1:566:A:LEU:HD23	1:562:A:LEU:HB2	12	0.7	0.3	0.64
(1,2104)	1:566:A:LEU:HD21	1:562:A:LEU:HB3	12	0.7	0.3	0.64
(1,2104)	1:566:A:LEU:HD21	1:562:A:LEU:HB2	12	0.7	0.3	0.64
(1,2104)	1:566:A:LEU:HD21	1:631:A:LEU:HB2	12	0.7	0.3	0.64
(1,2104)	1:566:A:LEU:HD23	1:631:A:LEU:HB2	12	0.7	0.3	0.64
(1,2104)	1:566:A:LEU:HD22	1:631:A:LEU:HB2	12	0.7	0.3	0.64
(1,838)	1:623:A:GLU:HA	1:626:A:GLU:HB3	12	0.63	0.21	0.66
(1,1111)	1:631:A:LEU:HD23	1:562:A:LEU:HB3	12	0.51	0.18	0.52
(1,1111)	1:631:A:LEU:HD21	1:562:A:LEU:HB3	12	0.51	0.18	0.52
(1,1111)	1:631:A:LEU:HD21	1:562:A:LEU:HB2	12	0.51	0.18	0.52
(1,1111)	1:631:A:LEU:HD22	1:562:A:LEU:HB2	12	0.51	0.18	0.52
(1,1111)	1:631:A:LEU:HD23	1:562:A:LEU:HB2	12	0.51	0.18	0.52
(1,1894)	1:576:A:LEU:HG	1:617:A:GLU:HG3	12	0.45	0.28	0.36
(1,1894)	1:562:A:LEU:HG	1:567:A:GLN:HG3	12	0.45	0.28	0.36
(1,1959)	1:622:A:PHE:HB2	1:619:A:GLU:HB2	12	0.44	0.25	0.4
(1,1633)	1:622:A:PHE:H	1:619:A:GLU:HB3	12	0.4	0.16	0.38
(1,1633)	1:622:A:PHE:H	1:620:A:GLN:HB2	12	0.4	0.16	0.38
(1,1633)	1:622:A:PHE:H	1:623:A:GLU:HB3	12	0.4	0.16	0.38
(1,584)	1:625:A:TRP:HD1	1:570:A:LEU:HD23	12	0.38	0.68	0.17
(1,584)	1:625:A:TRP:HD1	1:570:A:LEU:HD22	12	0.38	0.68	0.17
(1,584)	1:625:A:TRP:HD1	1:570:A:LEU:HD21	12	0.38	0.68	0.17
(1,2052)	1:603:A:GLN:HG3	1:599:A:GLN:HA	12	0.38	0.11	0.39
(1,2052)	1:603:A:GLN:HG3	1:600:A:PRO:HA	12	0.38	0.11	0.39
(1,2046)	1:626:A:GLU:HB3	1:627:A:TYR:HA	12	0.36	0.06	0.36
(1,2046)	1:623:A:GLU:HA	1:626:A:GLU:HB3	12	0.36	0.06	0.36
(1,1628)	1:621:A:ALA:H	1:620:A:GLN:HB2	12	0.35	0.04	0.35
(1,2051)	1:603:A:GLN:HG2	1:600:A:PRO:HA	12	0.32	0.11	0.34
(1,1731)	1:607:A:VAL:HG23	1:603:A:GLN:HB3	12	0.29	0.1	0.28
(1,1731)	1:607:A:VAL:HG21	1:603:A:GLN:HB3	12	0.29	0.1	0.28
(1,1731)	1:607:A:VAL:HG22	1:603:A:GLN:HB3	12	0.29	0.1	0.28
(1,1731)	1:607:A:VAL:HG21	1:603:A:GLN:HB2	12	0.29	0.1	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1731)	1:607:A:VAL:HG23	1:603:A:GLN:HB2	12	0.29	0.1	0.28
(1,1731)	1:607:A:VAL:HG22	1:603:A:GLN:HB2	12	0.29	0.1	0.28
(1,1437)	1:564:A:TYR:HD2	1:568:A:ARG:HG2	12	0.28	0.11	0.28
(1,1437)	1:564:A:TYR:HD2	1:568:A:ARG:HG3	12	0.28	0.11	0.28
(1,599)	1:601:A:HIS:HD2	1:602:A:GLU:HG2	12	0.26	0.1	0.26
(1,599)	1:601:A:HIS:HD2	1:602:A:GLU:HG3	12	0.26	0.1	0.26
(1,851)	1:604:A:THR:HA	1:608:A:LEU:HD11	12	0.26	0.14	0.22
(1,851)	1:604:A:THR:HA	1:608:A:LEU:HD12	12	0.26	0.14	0.22
(1,851)	1:604:A:THR:HA	1:608:A:LEU:HD13	12	0.26	0.14	0.22
(1,972)	1:629:A:GLU:HB2	1:570:A:LEU:HD13	12	0.24	0.05	0.26
(1,972)	1:629:A:GLU:HB2	1:570:A:LEU:HD11	12	0.24	0.05	0.26
(1,972)	1:629:A:GLU:HB2	1:570:A:LEU:HD12	12	0.24	0.05	0.26
(1,552)	1:596:A:PHE:HD1	1:607:A:VAL:HG23	12	0.21	0.05	0.23
(1,552)	1:596:A:PHE:HD1	1:607:A:VAL:HG22	12	0.21	0.05	0.23
(1,552)	1:596:A:PHE:HD1	1:607:A:VAL:HG21	12	0.21	0.05	0.23
(1,1568)	1:607:A:VAL:H	1:606:A:LYS:HG2	12	0.21	0.04	0.21
(1,1418)	1:596:A:PHE:HE2	1:591:A:VAL:HG23	12	0.17	0.05	0.17
(1,1418)	1:596:A:PHE:HE2	1:591:A:VAL:HG21	12	0.17	0.05	0.17
(1,1418)	1:596:A:PHE:HE2	1:591:A:VAL:HG22	12	0.17	0.05	0.17
(1,33)	1:598:A:SER:H	1:599:A:GLN:HG2	11	0.98	0.08	1.01
(1,2078)	1:562:A:LEU:HB3	1:566:A:LEU:HD13	11	0.92	0.19	1.01
(1,2078)	1:562:A:LEU:HB3	1:566:A:LEU:HD12	11	0.92	0.19	1.01
(1,2078)	1:562:A:LEU:HB3	1:566:A:LEU:HD11	11	0.92	0.19	1.01
(1,929)	1:565:A:LYS:HG2	1:566:A:LEU:HD13	11	0.87	0.82	0.62
(1,929)	1:565:A:LYS:HG2	1:566:A:LEU:HD11	11	0.87	0.82	0.62
(1,929)	1:565:A:LYS:HG2	1:566:A:LEU:HD12	11	0.87	0.82	0.62
(1,672)	1:607:A:VAL:HG22	1:606:A:LYS:HE2	11	0.65	0.34	0.68
(1,672)	1:607:A:VAL:HG21	1:606:A:LYS:HE2	11	0.65	0.34	0.68
(1,672)	1:607:A:VAL:HG22	1:606:A:LYS:HE3	11	0.65	0.34	0.68
(1,672)	1:607:A:VAL:HG21	1:606:A:LYS:HE3	11	0.65	0.34	0.68
(1,672)	1:607:A:VAL:HG23	1:606:A:LYS:HE3	11	0.65	0.34	0.68
(1,906)	1:596:A:PHE:HA	1:599:A:GLN:HG2	11	0.62	0.24	0.62
(1,2013)	1:565:A:LYS:HA	1:568:A:ARG:HB3	11	0.59	0.07	0.6
(1,24)	1:599:A:GLN:H	1:599:A:GLN:HG2	11	0.56	0.08	0.54
(1,1163)	1:599:A:GLN:HG3	1:600:A:PRO:HD3	11	0.52	0.26	0.46
(1,538)	1:635:A:GLY:H	1:631:A:LEU:HD11	11	0.44	0.12	0.47
(1,538)	1:635:A:GLY:H	1:631:A:LEU:HD13	11	0.44	0.12	0.47
(1,538)	1:635:A:GLY:H	1:631:A:LEU:HD12	11	0.44	0.12	0.47
(1,283)	1:569:A:GLU:H	1:568:A:ARG:HB3	11	0.34	0.04	0.35
(1,1694)	1:564:A:TYR:HD2	1:568:A:ARG:HG2	11	0.28	0.11	0.31
(1,1694)	1:564:A:TYR:HD2	1:568:A:ARG:HG3	11	0.28	0.11	0.31
(1,1694)	1:564:A:TYR:HD2	1:565:A:LYS:HG2	11	0.28	0.11	0.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1412)	1:584:A:LEU:HD22	1:615:A:GLU:HB2	11	0.27	0.13	0.21
(1,1412)	1:584:A:LEU:HD23	1:615:A:GLU:HB2	11	0.27	0.13	0.21
(1,1412)	1:584:A:LEU:HD21	1:615:A:GLU:HB2	11	0.27	0.13	0.21
(1,750)	1:604:A:THR:HG21	1:599:A:GLN:HA	11	0.27	0.07	0.27
(1,750)	1:604:A:THR:HG23	1:599:A:GLN:HA	11	0.27	0.07	0.27
(1,750)	1:604:A:THR:HG22	1:599:A:GLN:HA	11	0.27	0.07	0.27
(1,652)	1:591:A:VAL:HG13	1:608:A:LEU:HA	11	0.24	0.08	0.25
(1,652)	1:591:A:VAL:HG11	1:608:A:LEU:HA	11	0.24	0.08	0.25
(1,652)	1:591:A:VAL:HG12	1:608:A:LEU:HA	11	0.24	0.08	0.25
(1,1951)	1:615:A:GLU:HG2	1:584:A:LEU:HG	11	0.2	0.04	0.21
(1,2146)	1:615:A:GLU:HG2	1:584:A:LEU:HG	11	0.2	0.04	0.21
(1,2146)	1:588:A:GLN:HG2	1:584:A:LEU:HG	11	0.2	0.04	0.21
(1,642)	1:604:A:THR:HG21	1:596:A:PHE:HA	11	0.18	0.04	0.19
(1,642)	1:604:A:THR:HG23	1:596:A:PHE:HA	11	0.18	0.04	0.19
(1,642)	1:604:A:THR:HG22	1:596:A:PHE:HA	11	0.18	0.04	0.19
(1,1446)	1:568:A:ARG:HD3	1:564:A:TYR:HE2	11	0.14	0.03	0.14
(1,1446)	1:568:A:ARG:HD3	1:564:A:TYR:HE1	11	0.14	0.03	0.14
(1,1900)	1:567:A:GLN:HB2	1:562:A:LEU:HD12	10	1.33	0.85	0.99
(1,1900)	1:567:A:GLN:HB3	1:562:A:LEU:HD13	10	1.33	0.85	0.99
(1,1900)	1:567:A:GLN:HB2	1:562:A:LEU:HD11	10	1.33	0.85	0.99
(1,1900)	1:567:A:GLN:HB3	1:562:A:LEU:HD12	10	1.33	0.85	0.99
(1,1900)	1:567:A:GLN:HB2	1:562:A:LEU:HD13	10	1.33	0.85	0.99
(1,1278)	1:632:A:LYS:HG2	1:562:A:LEU:HD13	10	1.21	0.58	1.5
(1,1278)	1:632:A:LYS:HG2	1:562:A:LEU:HD12	10	1.21	0.58	1.5
(1,1278)	1:632:A:LYS:HG2	1:562:A:LEU:HD11	10	1.21	0.58	1.5
(1,964)	1:590:A:GLN:HB3	1:607:A:VAL:HG12	10	0.94	0.13	0.93
(1,964)	1:590:A:GLN:HB3	1:607:A:VAL:HG13	10	0.94	0.13	0.93
(1,1807)	1:587:A:LEU:HA	1:590:A:GLN:HB2	10	0.75	0.1	0.78
(1,1992)	1:562:A:LEU:HB2	1:632:A:LYS:HG2	10	0.5	0.24	0.4
(1,1992)	1:562:A:LEU:HB3	1:631:A:LEU:HG	10	0.5	0.24	0.4
(1,1992)	1:562:A:LEU:HB2	1:631:A:LEU:HG	10	0.5	0.24	0.4
(1,1534)	1:572:A:GLN:H	1:572:A:GLN:HB3	10	0.46	0.18	0.5
(1,1534)	1:572:A:GLN:H	1:571:A:GLU:HB3	10	0.46	0.18	0.5
(1,1021)	1:591:A:VAL:HG22	1:590:A:GLN:HG3	10	0.39	0.02	0.39
(1,1021)	1:591:A:VAL:HG23	1:590:A:GLN:HG3	10	0.39	0.02	0.39
(1,1946)	1:581:A:GLU:HG2	1:618:A:LEU:HD21	10	0.36	0.17	0.32
(1,1946)	1:581:A:GLU:HG2	1:618:A:LEU:HD23	10	0.36	0.17	0.32
(1,1946)	1:581:A:GLU:HG2	1:618:A:LEU:HD22	10	0.36	0.17	0.32
(1,1946)	1:581:A:GLU:HG2	1:584:A:LEU:HD12	10	0.36	0.17	0.32
(1,1484)	1:587:A:LEU:H	1:588:A:GLN:HG2	10	0.32	0.27	0.18
(1,1549)	1:567:A:GLN:H	1:563:A:SER:HB3	10	0.3	0.18	0.21
(1,1549)	1:567:A:GLN:H	1:568:A:ARG:HA	10	0.3	0.18	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1895)	1:618:A:LEU:HG	1:581:A:GLU:HB2	10	0.3	0.16	0.24
(1,1895)	1:570:A:LEU:HG	1:573:A:LEU:HB2	10	0.3	0.16	0.24
(1,1895)	1:618:A:LEU:HG	1:619:A:GLU:HB3	10	0.3	0.16	0.24
(1,1025)	1:590:A:GLN:HG2	1:591:A:VAL:HG22	10	0.28	0.03	0.28
(1,1025)	1:590:A:GLN:HG2	1:591:A:VAL:HG23	10	0.28	0.03	0.28
(1,1426)	1:627:A:TYR:HD2	1:628:A:LEU:HD22	10	0.25	0.08	0.25
(1,1426)	1:627:A:TYR:HD2	1:628:A:LEU:HD21	10	0.25	0.08	0.25
(1,1426)	1:627:A:TYR:HD2	1:628:A:LEU:HD23	10	0.25	0.08	0.25
(1,859)	1:604:A:THR:HB	1:608:A:LEU:HD23	10	0.24	0.1	0.24
(1,859)	1:604:A:THR:HB	1:608:A:LEU:HD22	10	0.24	0.1	0.24
(1,805)	1:629:A:GLU:HA	1:570:A:LEU:HD21	10	0.22	0.1	0.25
(1,805)	1:629:A:GLU:HA	1:570:A:LEU:HD22	10	0.22	0.1	0.25
(1,805)	1:629:A:GLU:HA	1:570:A:LEU:HD23	10	0.22	0.1	0.25
(1,1594)	1:614:A:ALA:H	1:615:A:GLU:HG3	10	0.22	0.08	0.21
(1,1594)	1:614:A:ALA:H	1:616:A:GLN:HB2	10	0.22	0.08	0.21
(1,1456)	1:597:A:PHE:H	1:595:A:SER:HA	10	0.18	0.08	0.14
(1,1445)	1:564:A:TYR:HE1	1:568:A:ARG:HD2	9	1.3	0.15	1.27
(1,1445)	1:564:A:TYR:HE2	1:568:A:ARG:HD2	9	1.3	0.15	1.27
(1,2162)	1:565:A:LYS:HA	1:564:A:TYR:HB2	9	1.21	0.36	1.33
(1,2162)	1:568:A:ARG:HD2	1:565:A:LYS:HA	9	1.21	0.36	1.33
(1,1447)	1:568:A:ARG:HD2	1:564:A:TYR:HD1	9	1.16	0.29	1.21
(1,1447)	1:568:A:ARG:HD2	1:564:A:TYR:HD2	9	1.16	0.29	1.21
(1,1986)	1:568:A:ARG:HD3	1:571:A:GLU:HB2	9	1.13	0.33	1.2
(1,1986)	1:568:A:ARG:HD3	1:567:A:GLN:HG3	9	1.13	0.33	1.2
(1,1174)	1:623:A:GLU:HG2	1:622:A:PHE:HB2	9	0.91	0.32	1.04
(1,2029)	1:568:A:ARG:HD3	1:565:A:LYS:HA	9	0.79	0.07	0.79
(1,2029)	1:568:A:ARG:HD3	1:567:A:GLN:HA	9	0.79	0.07	0.79
(1,1544)	1:569:A:GLU:H	1:566:A:LEU:HB3	9	0.67	0.03	0.67
(1,1264)	1:568:A:ARG:HD2	1:564:A:TYR:HA	9	0.62	0.21	0.63
(1,1790)	1:557:A:ARG:HA	1:555:A:VAL:HG22	9	0.45	0.27	0.46
(1,1790)	1:557:A:ARG:HA	1:555:A:VAL:HG21	9	0.45	0.27	0.46
(1,1790)	1:557:A:ARG:HA	1:555:A:VAL:HG12	9	0.45	0.27	0.46
(1,990)	1:591:A:VAL:HG23	1:611:A:MET:HG2	9	0.36	0.34	0.22
(1,990)	1:591:A:VAL:HG21	1:611:A:MET:HG2	9	0.36	0.34	0.22
(1,990)	1:591:A:VAL:HG22	1:611:A:MET:HG2	9	0.36	0.34	0.22
(1,1565)	1:607:A:VAL:H	1:610:A:ASP:HB2	9	0.35	0.08	0.38
(1,1565)	1:607:A:VAL:H	1:606:A:LYS:HE3	9	0.35	0.08	0.38
(1,1565)	1:607:A:VAL:H	1:606:A:LYS:HE2	9	0.35	0.08	0.38
(1,725)	1:600:A:PRO:HD3	1:599:A:GLN:HB2	9	0.34	0.08	0.31
(1,558)	1:564:A:TYR:HE2	1:568:A:ARG:HB2	9	0.28	0.07	0.29
(1,1756)	1:614:A:ALA:HB2	1:587:A:LEU:HB2	9	0.17	0.07	0.14
(1,1756)	1:614:A:ALA:HB3	1:587:A:LEU:HB2	9	0.17	0.07	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1756)	1:614:A:ALA:HB1	1:587:A:LEU:HB2	9	0.17	0.07	0.14
(1,1987)	1:614:A:ALA:HB2	1:587:A:LEU:HB2	9	0.17	0.07	0.14
(1,1987)	1:614:A:ALA:HB3	1:587:A:LEU:HB2	9	0.17	0.07	0.14
(1,1987)	1:614:A:ALA:HB1	1:587:A:LEU:HB2	9	0.17	0.07	0.14
(1,1710)	1:577:A:LEU:HD21	1:574:A:PRO:HG3	9	0.15	0.05	0.12
(1,1710)	1:577:A:LEU:HD23	1:574:A:PRO:HG3	9	0.15	0.05	0.12
(1,1710)	1:577:A:LEU:HD22	1:574:A:PRO:HG3	9	0.15	0.05	0.12
(1,1635)	1:623:A:GLU:H	1:622:A:PHE:HD1	9	0.15	0.04	0.13
(1,1266)	1:596:A:PHE:HA	1:593:A:ASP:HB3	9	0.15	0.04	0.14
(1,1266)	1:596:A:PHE:HA	1:593:A:ASP:HB2	9	0.15	0.04	0.14
(1,710)	1:594:A:ALA:HB3	1:595:A:SER:HA	9	0.14	0.02	0.14
(1,710)	1:594:A:ALA:HB1	1:595:A:SER:HA	9	0.14	0.02	0.14
(1,710)	1:594:A:ALA:HB2	1:595:A:SER:HA	9	0.14	0.02	0.14
(1,1586)	1:613:A:ALA:H	1:612:A:ALA:HA	9	0.11	0.01	0.11
(1,1912)	1:585:A:GLU:HB2	1:582:A:ALA:HB2	8	1.07	0.18	1.11
(1,1912)	1:585:A:GLU:HB2	1:582:A:ALA:HB1	8	1.07	0.18	1.11
(1,1912)	1:585:A:GLU:HB2	1:582:A:ALA:HB3	8	1.07	0.18	1.11
(1,1192)	1:568:A:ARG:HD2	1:565:A:LYS:HA	8	1.03	0.17	1.04
(1,1288)	1:566:A:LEU:HD22	1:562:A:LEU:HD21	8	0.82	0.56	0.63
(1,1288)	1:566:A:LEU:HD23	1:562:A:LEU:HD23	8	0.82	0.56	0.63
(1,1288)	1:566:A:LEU:HD23	1:562:A:LEU:HD22	8	0.82	0.56	0.63
(1,1288)	1:566:A:LEU:HD21	1:562:A:LEU:HD22	8	0.82	0.56	0.63
(1,1288)	1:566:A:LEU:HD22	1:562:A:LEU:HD23	8	0.82	0.56	0.63
(1,146)	1:586:A:ALA:H	1:585:A:GLU:HB2	8	0.58	0.05	0.6
(1,1365)	1:631:A:LEU:HD23	1:566:A:LEU:HD13	8	0.36	0.26	0.22
(1,1365)	1:631:A:LEU:HD21	1:566:A:LEU:HD13	8	0.36	0.26	0.22
(1,1365)	1:631:A:LEU:HD21	1:566:A:LEU:HD12	8	0.36	0.26	0.22
(1,1365)	1:631:A:LEU:HD22	1:566:A:LEU:HD12	8	0.36	0.26	0.22
(1,1365)	1:631:A:LEU:HD21	1:566:A:LEU:HD11	8	0.36	0.26	0.22
(1,1365)	1:631:A:LEU:HD23	1:566:A:LEU:HD11	8	0.36	0.26	0.22
(1,1390)	1:599:A:GLN:HG3	1:600:A:PRO:HD2	8	0.24	0.21	0.13
(1,2022)	1:599:A:GLN:HG3	1:600:A:PRO:HD2	8	0.24	0.21	0.13
(1,1789)	1:556:A:LYS:HA	1:555:A:VAL:HG11	8	0.23	0.1	0.24
(1,1789)	1:556:A:LYS:HA	1:555:A:VAL:HG13	8	0.23	0.1	0.24
(1,1789)	1:556:A:LYS:HA	1:555:A:VAL:HG22	8	0.23	0.1	0.24
(1,1789)	1:556:A:LYS:HA	1:555:A:VAL:HG12	8	0.23	0.1	0.24
(1,1401)	1:606:A:LYS:HB3	1:606:A:LYS:HE3	8	0.21	0.01	0.2
(1,1401)	1:606:A:LYS:HB3	1:606:A:LYS:HE2	8	0.21	0.01	0.2
(1,1377)	1:565:A:LYS:HD2	1:563:A:SER:HB2	8	0.18	0.06	0.16
(1,1377)	1:565:A:LYS:HD3	1:563:A:SER:HB2	8	0.18	0.06	0.16
(1,650)	1:591:A:VAL:HG13	1:588:A:GLN:HA	8	0.18	0.06	0.17
(1,650)	1:591:A:VAL:HG11	1:588:A:GLN:HA	8	0.18	0.06	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,650)	1:591:A:VAL:HG12	1:588:A:GLN:HA	8	0.18	0.06	0.17
(1,1374)	1:577:A:LEU:HD11	1:625:A:TRP:HB3	8	0.17	0.1	0.12
(1,1374)	1:577:A:LEU:HD12	1:625:A:TRP:HB3	8	0.17	0.1	0.12
(1,1374)	1:577:A:LEU:HD13	1:625:A:TRP:HB3	8	0.17	0.1	0.12
(1,1487)	1:587:A:LEU:H	1:587:A:LEU:HD22	8	0.16	0.04	0.18
(1,1487)	1:587:A:LEU:H	1:587:A:LEU:HD23	8	0.16	0.04	0.18
(1,1487)	1:587:A:LEU:H	1:587:A:LEU:HD21	8	0.16	0.04	0.18
(1,600)	1:601:A:HIS:HD2	1:602:A:GLU:HB3	8	0.15	0.03	0.15
(1,1244)	1:569:A:GLU:HG3	1:566:A:LEU:HA	8	0.14	0.03	0.14
(1,135)	1:588:A:GLN:H	1:591:A:VAL:HG21	8	0.14	0.02	0.15
(1,135)	1:588:A:GLN:H	1:591:A:VAL:HG22	8	0.14	0.02	0.15
(1,135)	1:588:A:GLN:H	1:591:A:VAL:HG23	8	0.14	0.02	0.15
(1,858)	1:604:A:THR:HB	1:607:A:VAL:HB	8	0.13	0.03	0.12
(1,938)	1:631:A:LEU:HG	1:562:A:LEU:HD23	7	1.32	1.16	0.49
(1,938)	1:631:A:LEU:HG	1:562:A:LEU:HD22	7	1.32	1.16	0.49
(1,1452)	1:599:A:GLN:H	1:600:A:PRO:HG2	7	1.29	0.27	1.39
(1,1154)	1:603:A:GLN:HG2	1:600:A:PRO:HB3	7	0.93	0.32	0.82
(1,1995)	1:557:A:ARG:HD3	1:555:A:VAL:HG21	7	0.69	0.3	0.73
(1,1995)	1:557:A:ARG:HD2	1:555:A:VAL:HG12	7	0.69	0.3	0.73
(1,1995)	1:557:A:ARG:HD2	1:555:A:VAL:HG11	7	0.69	0.3	0.73
(1,1995)	1:557:A:ARG:HD2	1:555:A:VAL:HG22	7	0.69	0.3	0.73
(1,1396)	1:632:A:LYS:HG3	1:562:A:LEU:HB2	7	0.65	0.36	0.56
(1,1396)	1:632:A:LYS:HG3	1:562:A:LEU:HB3	7	0.65	0.36	0.56
(1,968)	1:604:A:THR:HG23	1:603:A:GLN:HB3	7	0.65	0.08	0.64
(1,968)	1:604:A:THR:HG22	1:603:A:GLN:HB3	7	0.65	0.08	0.64
(1,968)	1:604:A:THR:HG21	1:603:A:GLN:HB3	7	0.65	0.08	0.64
(1,149)	1:586:A:ALA:H	1:589:A:THR:HG23	7	0.45	0.32	0.27
(1,149)	1:586:A:ALA:H	1:589:A:THR:HG21	7	0.45	0.32	0.27
(1,149)	1:586:A:ALA:H	1:589:A:THR:HG22	7	0.45	0.32	0.27
(1,1717)	1:604:A:THR:HG21	1:608:A:LEU:HG	7	0.45	0.08	0.47
(1,1717)	1:604:A:THR:HG23	1:608:A:LEU:HG	7	0.45	0.08	0.47
(1,1717)	1:604:A:THR:HG22	1:608:A:LEU:HG	7	0.45	0.08	0.47
(1,1717)	1:604:A:THR:HG22	1:603:A:GLN:HB3	7	0.45	0.08	0.47
(1,1220)	1:551:A:LYS:HD2	1:551:A:LYS:HA	7	0.37	0.1	0.4
(1,1220)	1:551:A:LYS:HD3	1:551:A:LYS:HA	7	0.37	0.1	0.4
(1,1874)	1:632:A:LYS:HG2	1:562:A:LEU:HD21	7	0.36	0.19	0.23
(1,1874)	1:632:A:LYS:HG2	1:562:A:LEU:HD22	7	0.36	0.19	0.23
(1,1874)	1:632:A:LYS:HG2	1:562:A:LEU:HD23	7	0.36	0.19	0.23
(1,327)	1:604:A:THR:H	1:603:A:GLN:HB3	7	0.31	0.03	0.3
(1,1689)	1:596:A:PHE:HD1	1:607:A:VAL:HB	7	0.25	0.06	0.24
(1,1689)	1:596:A:PHE:HD1	1:599:A:GLN:HG3	7	0.25	0.06	0.24
(1,1940)	1:620:A:GLN:HG2	1:621:A:ALA:HB1	7	0.24	0.07	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1940)	1:620:A:GLN:HG2	1:621:A:ALA:HB2	7	0.24	0.07	0.23
(1,1940)	1:572:A:GLN:HG2	1:568:A:ARG:HG3	7	0.24	0.07	0.23
(1,1940)	1:572:A:GLN:HG2	1:568:A:ARG:HG2	7	0.24	0.07	0.23
(1,262)	1:571:A:GLU:H	1:571:A:GLU:HG2	7	0.24	0.14	0.17
(1,1023)	1:590:A:GLN:HG3	1:587:A:LEU:HD23	7	0.22	0.07	0.21
(1,1023)	1:590:A:GLN:HG3	1:587:A:LEU:HD22	7	0.22	0.07	0.21
(1,1023)	1:590:A:GLN:HG3	1:587:A:LEU:HD21	7	0.22	0.07	0.21
(1,1328)	1:573:A:LEU:HD11	1:574:A:PRO:HD3	7	0.21	0.06	0.2
(1,1328)	1:573:A:LEU:HD13	1:574:A:PRO:HD3	7	0.21	0.06	0.2
(1,1328)	1:573:A:LEU:HD12	1:574:A:PRO:HD3	7	0.21	0.06	0.2
(1,1682)	1:622:A:PHE:HD2	1:577:A:LEU:HD13	7	0.2	0.06	0.2
(1,1682)	1:622:A:PHE:HD2	1:577:A:LEU:HD11	7	0.2	0.06	0.2
(1,1682)	1:622:A:PHE:HD2	1:577:A:LEU:HD12	7	0.2	0.06	0.2
(1,274)	1:570:A:LEU:H	1:569:A:GLU:HG2	7	0.2	0.07	0.16
(1,1957)	1:622:A:PHE:HB2	1:619:A:GLU:HB2	7	0.19	0.02	0.19
(1,1957)	1:622:A:PHE:HB2	1:619:A:GLU:HB3	7	0.19	0.02	0.19
(1,621)	1:577:A:LEU:HD21	1:573:A:LEU:HA	7	0.18	0.04	0.16
(1,621)	1:577:A:LEU:HD23	1:573:A:LEU:HA	7	0.18	0.04	0.16
(1,621)	1:577:A:LEU:HD22	1:573:A:LEU:HA	7	0.18	0.04	0.16
(1,1530)	1:573:A:LEU:H	1:572:A:GLN:HB3	7	0.18	0.07	0.16
(1,1040)	1:629:A:GLU:HG3	1:570:A:LEU:HD13	7	0.17	0.04	0.19
(1,1040)	1:629:A:GLU:HG3	1:570:A:LEU:HD11	7	0.17	0.04	0.19
(1,1040)	1:629:A:GLU:HG3	1:570:A:LEU:HD12	7	0.17	0.04	0.19
(1,1889)	1:568:A:ARG:HG2	1:569:A:GLU:HB2	7	0.17	0.08	0.16
(1,1889)	1:568:A:ARG:HG3	1:571:A:GLU:HB2	7	0.17	0.08	0.16
(1,1698)	1:564:A:TYR:HD2	1:567:A:GLN:HB2	7	0.16	0.04	0.16
(1,1698)	1:564:A:TYR:HD1	1:567:A:GLN:HB2	7	0.16	0.04	0.16
(1,1488)	1:586:A:ALA:H	1:583:A:LYS:HA	7	0.14	0.03	0.12
(1,1488)	1:586:A:ALA:H	1:585:A:GLU:HA	7	0.14	0.03	0.12
(1,708)	1:592:A:ALA:HB3	1:593:A:ASP:HA	7	0.13	0.02	0.13
(1,708)	1:592:A:ALA:HB1	1:593:A:ASP:HA	7	0.13	0.02	0.13
(1,708)	1:592:A:ALA:HB2	1:593:A:ASP:HA	7	0.13	0.02	0.13
(1,749)	1:562:A:LEU:HA	1:566:A:LEU:HD22	6	2.49	0.63	2.82
(1,749)	1:562:A:LEU:HA	1:566:A:LEU:HD23	6	2.49	0.63	2.82
(1,749)	1:562:A:LEU:HA	1:566:A:LEU:HD21	6	2.49	0.63	2.82
(1,1000)	1:565:A:LYS:HB2	1:566:A:LEU:HD13	6	1.95	0.69	2.13
(1,1000)	1:565:A:LYS:HB2	1:566:A:LEU:HD11	6	1.95	0.69	2.13
(1,1000)	1:565:A:LYS:HB2	1:566:A:LEU:HD12	6	1.95	0.69	2.13
(1,1331)	1:566:A:LEU:HD22	1:628:A:LEU:HA	6	1.08	0.28	1.16
(1,1331)	1:566:A:LEU:HD23	1:628:A:LEU:HA	6	1.08	0.28	1.16
(1,1331)	1:566:A:LEU:HD21	1:628:A:LEU:HA	6	1.08	0.28	1.16
(1,1287)	1:566:A:LEU:HD22	1:631:A:LEU:HD23	6	0.8	0.26	0.76

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1287)	1:566:A:LEU:HD23	1:631:A:LEU:HD22	6	0.8	0.26	0.76
(1,1287)	1:566:A:LEU:HD21	1:631:A:LEU:HD21	6	0.8	0.26	0.76
(1,1287)	1:566:A:LEU:HD22	1:631:A:LEU:HD22	6	0.8	0.26	0.76
(1,1287)	1:566:A:LEU:HD21	1:631:A:LEU:HD22	6	0.8	0.26	0.76
(1,438)	1:619:A:GLU:H	1:619:A:GLU:HB3	6	0.7	0.01	0.71
(1,1303)	1:581:A:GLU:HG3	1:618:A:LEU:HD13	6	0.67	0.39	0.5
(1,1303)	1:581:A:GLU:HG3	1:618:A:LEU:HD12	6	0.67	0.39	0.5
(1,2114)	1:615:A:GLU:HB2	1:584:A:LEU:HD12	6	0.61	0.32	0.5
(1,2114)	1:581:A:GLU:HG3	1:618:A:LEU:HD12	6	0.61	0.32	0.5
(1,2114)	1:581:A:GLU:HG3	1:618:A:LEU:HD13	6	0.61	0.32	0.5
(1,317)	1:563:A:SER:H	1:566:A:LEU:HD23	6	0.59	0.25	0.6
(1,317)	1:563:A:SER:H	1:566:A:LEU:HD21	6	0.59	0.25	0.6
(1,317)	1:563:A:SER:H	1:566:A:LEU:HD22	6	0.59	0.25	0.6
(1,2056)	1:572:A:GLN:HG3	1:569:A:GLU:HA	6	0.49	0.25	0.44
(1,2056)	1:599:A:GLN:HG2	1:598:A:SER:HB3	6	0.49	0.25	0.44
(1,299)	1:567:A:GLN:H	1:566:A:LEU:HD12	6	0.41	0.09	0.42
(1,299)	1:567:A:GLN:H	1:566:A:LEU:HD13	6	0.41	0.09	0.42
(1,299)	1:567:A:GLN:H	1:566:A:LEU:HD11	6	0.41	0.09	0.42
(1,870)	1:556:A:LYS:HA	1:556:A:LYS:HE2	6	0.39	0.17	0.38
(1,870)	1:556:A:LYS:HA	1:556:A:LYS:HE3	6	0.39	0.17	0.38
(1,1730)	1:607:A:VAL:HG23	1:587:A:LEU:HD23	6	0.36	0.17	0.38
(1,1730)	1:607:A:VAL:HG21	1:587:A:LEU:HD23	6	0.36	0.17	0.38
(1,1730)	1:607:A:VAL:HG22	1:587:A:LEU:HD21	6	0.36	0.17	0.38
(1,1730)	1:607:A:VAL:HG21	1:587:A:LEU:HD22	6	0.36	0.17	0.38
(1,473)	1:623:A:GLU:H	1:623:A:GLU:HB2	6	0.35	0.01	0.35
(1,2121)	1:581:A:GLU:HG2	1:618:A:LEU:HD21	6	0.35	0.25	0.27
(1,2121)	1:581:A:GLU:HG2	1:618:A:LEU:HD23	6	0.35	0.25	0.27
(1,2121)	1:581:A:GLU:HG2	1:618:A:LEU:HD22	6	0.35	0.25	0.27
(1,307)	1:566:A:LEU:H	1:566:A:LEU:HD12	6	0.28	0.11	0.29
(1,307)	1:566:A:LEU:H	1:566:A:LEU:HD13	6	0.28	0.11	0.29
(1,307)	1:566:A:LEU:H	1:566:A:LEU:HD11	6	0.28	0.11	0.29
(1,2036)	1:556:A:LYS:HD3	1:556:A:LYS:HA	6	0.26	0.11	0.3
(1,2036)	1:556:A:LYS:HD2	1:556:A:LYS:HA	6	0.26	0.11	0.3
(1,2036)	1:561:A:LYS:HD3	1:561:A:LYS:HA	6	0.26	0.11	0.3
(1,2036)	1:561:A:LYS:HD2	1:561:A:LYS:HA	6	0.26	0.11	0.3
(1,581)	1:601:A:HIS:HD2	1:605:A:GLN:HG3	6	0.26	0.07	0.28
(1,581)	1:601:A:HIS:HD2	1:605:A:GLN:HG2	6	0.26	0.07	0.28
(1,2088)	1:576:A:LEU:HD12	1:617:A:GLU:HG3	6	0.25	0.1	0.29
(1,2088)	1:576:A:LEU:HD11	1:617:A:GLU:HG3	6	0.25	0.1	0.29
(1,2169)	1:576:A:LEU:HD12	1:617:A:GLU:HG3	6	0.25	0.1	0.29
(1,2169)	1:576:A:LEU:HD11	1:617:A:GLU:HG3	6	0.25	0.1	0.29
(1,1563)	1:605:A:GLN:H	1:605:A:GLN:HE22	6	0.24	0.1	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,248)	1:573:A:LEU:H	1:572:A:GLN:HB2	6	0.24	0.15	0.21
(1,745)	1:562:A:LEU:HA	1:562:A:LEU:HD23	6	0.21	0.02	0.22
(1,745)	1:562:A:LEU:HA	1:562:A:LEU:HD21	6	0.21	0.02	0.22
(1,745)	1:562:A:LEU:HA	1:562:A:LEU:HD22	6	0.21	0.02	0.22
(1,1849)	1:604:A:THR:HA	1:599:A:GLN:HB2	6	0.21	0.05	0.21
(1,2167)	1:606:A:LYS:HB3	1:606:A:LYS:HE3	6	0.21	0.01	0.2
(1,1920)	1:613:A:ALA:HB2	1:617:A:GLU:HB2	6	0.21	0.05	0.21
(1,1920)	1:613:A:ALA:HB3	1:617:A:GLU:HB2	6	0.21	0.05	0.21
(1,1920)	1:613:A:ALA:HB1	1:617:A:GLU:HB2	6	0.21	0.05	0.21
(1,1670)	1:633:A:ASN:H	1:631:A:LEU:HB2	6	0.21	0.05	0.22
(1,18)	1:599:A:GLN:H	1:596:A:PHE:HD1	6	0.19	0.07	0.18
(1,18)	1:599:A:GLN:H	1:596:A:PHE:HD2	6	0.19	0.07	0.18
(1,1398)	1:587:A:LEU:HD22	1:583:A:LYS:HG2	6	0.17	0.05	0.15
(1,1398)	1:587:A:LEU:HD21	1:583:A:LYS:HG2	6	0.17	0.05	0.15
(1,1110)	1:628:A:LEU:HB2	1:570:A:LEU:HD21	6	0.15	0.03	0.15
(1,1110)	1:628:A:LEU:HB2	1:570:A:LEU:HD22	6	0.15	0.03	0.15
(1,1110)	1:628:A:LEU:HB2	1:570:A:LEU:HD23	6	0.15	0.03	0.15
(1,920)	1:604:A:THR:HB	1:601:A:HIS:HA	6	0.13	0.02	0.12
(1,1845)	1:554:A:THR:HA	1:555:A:VAL:HG23	5	0.52	0.16	0.58
(1,1845)	1:554:A:THR:HA	1:555:A:VAL:HG11	5	0.52	0.16	0.58
(1,1014)	1:605:A:GLN:HG3	1:608:A:LEU:HD12	5	0.45	0.26	0.29
(1,1014)	1:605:A:GLN:HG2	1:608:A:LEU:HD13	5	0.45	0.26	0.29
(1,1014)	1:605:A:GLN:HG2	1:608:A:LEU:HD11	5	0.45	0.26	0.29
(1,564)	1:597:A:PHE:HE2	1:591:A:VAL:HG11	5	0.24	0.1	0.18
(1,564)	1:597:A:PHE:HE2	1:591:A:VAL:HG12	5	0.24	0.1	0.18
(1,564)	1:597:A:PHE:HE2	1:591:A:VAL:HG13	5	0.24	0.1	0.18
(1,730)	1:600:A:PRO:HD3	1:603:A:GLN:HG2	5	0.23	0.08	0.25
(1,1749)	1:613:A:ALA:HB2	1:617:A:GLU:HB2	5	0.22	0.05	0.22
(1,1749)	1:613:A:ALA:HB1	1:617:A:GLU:HB2	5	0.22	0.05	0.22
(1,1749)	1:613:A:ALA:HB3	1:617:A:GLU:HB2	5	0.22	0.05	0.22
(1,601)	1:601:A:HIS:HD2	1:605:A:GLN:HB3	5	0.2	0.09	0.14
(1,601)	1:601:A:HIS:HD2	1:605:A:GLN:HB2	5	0.2	0.09	0.14
(1,1745)	1:614:A:ALA:HB2	1:580:A:LEU:HD22	5	0.18	0.07	0.15
(1,1745)	1:614:A:ALA:HB3	1:580:A:LEU:HD22	5	0.18	0.07	0.15
(1,1745)	1:614:A:ALA:HB2	1:580:A:LEU:HD23	5	0.18	0.07	0.15
(1,1745)	1:614:A:ALA:HB3	1:580:A:LEU:HD23	5	0.18	0.07	0.15
(1,1745)	1:614:A:ALA:HB1	1:580:A:LEU:HD23	5	0.18	0.07	0.15
(1,1324)	1:628:A:LEU:HA	1:628:A:LEU:HD12	5	0.14	0.03	0.13
(1,1324)	1:628:A:LEU:HA	1:628:A:LEU:HD13	5	0.14	0.03	0.13
(1,123)	1:589:A:THR:H	1:592:A:ALA:HB3	5	0.13	0.03	0.11
(1,123)	1:589:A:THR:H	1:592:A:ALA:HB1	5	0.13	0.03	0.11
(1,123)	1:589:A:THR:H	1:592:A:ALA:HB2	5	0.13	0.03	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,782)	1:579:A:ASP:HA	1:578:A:GLU:HB2	5	0.13	0.01	0.13
(1,1414)	1:596:A:PHE:HD2	1:591:A:VAL:HG11	5	0.11	0.0	0.11
(1,1414)	1:596:A:PHE:HD2	1:591:A:VAL:HG13	5	0.11	0.0	0.11
(1,1414)	1:596:A:PHE:HD2	1:591:A:VAL:HG12	5	0.11	0.0	0.11
(1,2136)	1:573:A:LEU:HA	1:573:A:LEU:HD13	5	0.11	0.01	0.1
(1,2136)	1:573:A:LEU:HA	1:573:A:LEU:HD11	5	0.11	0.01	0.1
(1,2136)	1:573:A:LEU:HA	1:573:A:LEU:HD12	5	0.11	0.01	0.1
(1,1006)	1:567:A:GLN:HG3	1:562:A:LEU:HD11	4	0.98	0.53	1.08
(1,1006)	1:567:A:GLN:HG3	1:562:A:LEU:HD12	4	0.98	0.53	1.08
(1,1006)	1:567:A:GLN:HG3	1:562:A:LEU:HD13	4	0.98	0.53	1.08
(1,1034)	1:569:A:GLU:HG2	1:573:A:LEU:HD12	4	0.94	0.76	0.78
(1,1034)	1:569:A:GLU:HG2	1:573:A:LEU:HD13	4	0.94	0.76	0.78
(1,1923)	1:614:A:ALA:HB3	1:611:A:MET:HG3	4	0.44	0.27	0.44
(1,1923)	1:614:A:ALA:HB2	1:611:A:MET:HG3	4	0.44	0.27	0.44
(1,1923)	1:614:A:ALA:HB1	1:611:A:MET:HG3	4	0.44	0.27	0.44
(1,1763)	1:621:A:ALA:HB1	1:617:A:GLU:HG2	4	0.39	0.13	0.4
(1,1763)	1:621:A:ALA:HB2	1:617:A:GLU:HG2	4	0.39	0.13	0.4
(1,1763)	1:621:A:ALA:HB3	1:617:A:GLU:HG2	4	0.39	0.13	0.4
(1,1553)	1:566:A:LEU:H	1:565:A:LYS:HB3	4	0.34	0.19	0.34
(1,1553)	1:566:A:LEU:H	1:566:A:LEU:HG	4	0.34	0.19	0.34
(1,1190)	1:562:A:LEU:HB3	1:632:A:LYS:HA	4	0.33	0.16	0.3
(1,1190)	1:562:A:LEU:HB2	1:632:A:LYS:HA	4	0.33	0.16	0.3
(1,1061)	1:610:A:ASP:HB3	1:607:A:VAL:HG11	4	0.24	0.12	0.2
(1,1061)	1:610:A:ASP:HB3	1:607:A:VAL:HG13	4	0.24	0.12	0.2
(1,1061)	1:610:A:ASP:HB3	1:607:A:VAL:HG12	4	0.24	0.12	0.2
(1,1978)	1:583:A:LYS:HE2	1:587:A:LEU:HD21	4	0.24	0.14	0.18
(1,1978)	1:583:A:LYS:HE3	1:587:A:LEU:HD22	4	0.24	0.14	0.18
(1,1978)	1:632:A:LYS:HE2	1:570:A:LEU:HD21	4	0.24	0.14	0.18
(1,922)	1:612:A:ALA:HB3	1:611:A:MET:HE2	4	0.23	0.13	0.18
(1,922)	1:612:A:ALA:HB3	1:611:A:MET:HE3	4	0.23	0.13	0.18
(1,922)	1:612:A:ALA:HB1	1:611:A:MET:HE3	4	0.23	0.13	0.18
(1,922)	1:612:A:ALA:HB3	1:611:A:MET:HE1	4	0.23	0.13	0.18
(1,1950)	1:615:A:GLU:HG3	1:612:A:ALA:HB3	4	0.2	0.04	0.2
(1,1950)	1:615:A:GLU:HG3	1:612:A:ALA:HB1	4	0.2	0.04	0.2
(1,1950)	1:576:A:LEU:HG	1:617:A:GLU:HG3	4	0.2	0.04	0.2
(1,2081)	1:608:A:LEU:HD21	1:607:A:VAL:HB	4	0.18	0.01	0.18
(1,2081)	1:608:A:LEU:HD23	1:607:A:VAL:HB	4	0.18	0.01	0.18
(1,64)	1:595:A:SER:H	1:596:A:PHE:HB2	4	0.17	0.07	0.14
(1,1911)	1:581:A:GLU:HB3	1:618:A:LEU:HD11	4	0.17	0.04	0.18
(1,1911)	1:581:A:GLU:HB3	1:618:A:LEU:HD13	4	0.17	0.04	0.18
(1,1660)	1:631:A:LEU:H	1:631:A:LEU:HD11	4	0.12	0.01	0.12
(1,1660)	1:631:A:LEU:H	1:631:A:LEU:HD13	4	0.12	0.01	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1425)	1:596:A:PHE:HE1	1:607:A:VAL:HG13	4	0.12	0.02	0.12
(1,1425)	1:596:A:PHE:HE1	1:607:A:VAL:HG11	4	0.12	0.02	0.12
(1,1425)	1:596:A:PHE:HE1	1:607:A:VAL:HG12	4	0.12	0.02	0.12
(1,776)	1:628:A:LEU:HA	1:562:A:LEU:HD23	3	1.7	0.5	1.77
(1,776)	1:628:A:LEU:HA	1:562:A:LEU:HD22	3	1.7	0.5	1.77
(1,1362)	1:631:A:LEU:HB3	1:562:A:LEU:HD22	3	1.52	0.39	1.66
(1,1011)	1:567:A:GLN:HG2	1:562:A:LEU:HD11	3	1.28	0.24	1.39
(1,1011)	1:567:A:GLN:HG2	1:562:A:LEU:HD12	3	1.28	0.24	1.39
(1,1011)	1:567:A:GLN:HG2	1:562:A:LEU:HD13	3	1.28	0.24	1.39
(1,156)	1:585:A:GLU:H	1:581:A:GLU:HG2	3	1.23	0.8	1.76
(1,609)	1:625:A:TRP:HD1	1:573:A:LEU:HD12	3	1.13	0.72	1.58
(1,609)	1:625:A:TRP:HD1	1:573:A:LEU:HD13	3	1.13	0.72	1.58
(1,925)	1:565:A:LYS:HG3	1:566:A:LEU:HD12	3	1.01	0.93	0.36
(1,925)	1:565:A:LYS:HG3	1:566:A:LEU:HD11	3	1.01	0.93	0.36
(1,579)	1:627:A:TYR:HD2	1:624:A:ARG:HD3	3	0.99	0.08	1.03
(1,896)	1:617:A:GLU:HA	1:620:A:GLN:HG2	3	0.9	0.18	0.8
(1,1381)	1:573:A:LEU:HD12	1:624:A:ARG:HB2	3	0.83	0.53	0.96
(1,1381)	1:573:A:LEU:HD13	1:624:A:ARG:HB2	3	0.83	0.53	0.96
(1,1671)	1:633:A:ASN:H	1:562:A:LEU:HD22	3	0.74	0.07	0.74
(1,1671)	1:633:A:ASN:H	1:570:A:LEU:HD11	3	0.74	0.07	0.74
(1,1665)	1:632:A:LYS:H	1:562:A:LEU:HD22	3	0.7	0.19	0.58
(1,1665)	1:632:A:LYS:H	1:570:A:LEU:HD13	3	0.7	0.19	0.58
(1,1319)	1:567:A:GLN:HA	1:562:A:LEU:HD11	3	0.43	0.31	0.32
(1,1319)	1:567:A:GLN:HA	1:562:A:LEU:HD12	3	0.43	0.31	0.32
(1,1319)	1:567:A:GLN:HA	1:562:A:LEU:HD13	3	0.43	0.31	0.32
(1,869)	1:557:A:ARG:HA	1:557:A:ARG:HD2	3	0.4	0.01	0.4
(1,869)	1:557:A:ARG:HA	1:557:A:ARG:HD3	3	0.4	0.01	0.4
(1,2092)	1:567:A:GLN:HB3	1:562:A:LEU:HD12	3	0.37	0.22	0.22
(1,2092)	1:562:A:LEU:HD12	1:570:A:LEU:HB2	3	0.37	0.22	0.22
(1,2092)	1:562:A:LEU:HD11	1:570:A:LEU:HB2	3	0.37	0.22	0.22
(1,1668)	1:633:A:ASN:H	1:629:A:GLU:HA	3	0.35	0.2	0.3
(1,1752)	1:614:A:ALA:HB3	1:611:A:MET:HG3	3	0.35	0.25	0.19
(1,1752)	1:614:A:ALA:HB2	1:611:A:MET:HG3	3	0.35	0.25	0.19
(1,542)	1:625:A:TRP:HE1	1:629:A:GLU:HG3	3	0.29	0.05	0.27
(1,1170)	1:629:A:GLU:HG2	1:626:A:GLU:HA	3	0.28	0.07	0.26
(1,264)	1:571:A:GLU:H	1:571:A:GLU:HG3	3	0.28	0.02	0.28
(1,1759)	1:609:A:ALA:HB3	1:605:A:GLN:HA	3	0.27	0.1	0.23
(1,1759)	1:609:A:ALA:HB2	1:605:A:GLN:HA	3	0.27	0.1	0.23
(1,544)	1:625:A:TRP:HE1	1:570:A:LEU:HD13	3	0.24	0.05	0.22
(1,544)	1:625:A:TRP:HE1	1:570:A:LEU:HD12	3	0.24	0.05	0.22
(1,1382)	1:573:A:LEU:HD13	1:624:A:ARG:HG2	3	0.23	0.09	0.22
(1,1382)	1:573:A:LEU:HD12	1:624:A:ARG:HG2	3	0.23	0.09	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,819)	1:604:A:THR:HG22	1:601:A:HIS:HA	3	0.19	0.08	0.14
(1,819)	1:604:A:THR:HG21	1:601:A:HIS:HA	3	0.19	0.08	0.14
(1,1364)	1:628:A:LEU:HD23	1:631:A:LEU:HB2	3	0.19	0.01	0.19
(1,1364)	1:628:A:LEU:HD21	1:631:A:LEU:HB2	3	0.19	0.01	0.19
(1,1740)	1:628:A:LEU:HD23	1:631:A:LEU:HB2	3	0.19	0.01	0.19
(1,1740)	1:628:A:LEU:HD21	1:631:A:LEU:HB2	3	0.19	0.01	0.19
(1,596)	1:564:A:TYR:HD2	1:564:A:TYR:HA	3	0.18	0.04	0.16
(1,1114)	1:567:A:GLN:HG2	1:562:A:LEU:HB3	3	0.17	0.03	0.15
(1,1114)	1:567:A:GLN:HG2	1:562:A:LEU:HB2	3	0.17	0.03	0.15
(1,273)	1:570:A:LEU:H	1:569:A:GLU:HB2	3	0.16	0.04	0.16
(1,1632)	1:622:A:PHE:H	1:619:A:GLU:HB2	3	0.14	0.02	0.14
(1,2175)	1:597:A:PHE:HD1	1:604:A:THR:HB	3	0.14	0.02	0.14
(1,881)	1:568:A:ARG:HA	1:568:A:ARG:HD2	3	0.13	0.03	0.13
(1,446)	1:620:A:GLN:H	1:619:A:GLU:HG3	3	0.13	0.03	0.12
(1,966)	1:591:A:VAL:HA	1:608:A:LEU:HD22	3	0.12	0.01	0.11
(1,966)	1:591:A:VAL:HA	1:608:A:LEU:HD21	3	0.12	0.01	0.11
(1,1781)	1:609:A:ALA:HA	1:608:A:LEU:HB2	3	0.11	0.0	0.11
(1,276)	1:570:A:LEU:H	1:570:A:LEU:HD23	3	0.1	0.0	0.1
(1,276)	1:570:A:LEU:H	1:570:A:LEU:HD22	3	0.1	0.0	0.1
(1,231)	1:576:A:LEU:H	1:573:A:LEU:HD23	2	2.02	0.1	2.02
(1,231)	1:576:A:LEU:H	1:573:A:LEU:HD22	2	2.02	0.1	2.02
(1,2094)	1:573:A:LEU:HD21	1:577:A:LEU:HG	2	1.92	0.03	1.92
(1,2094)	1:573:A:LEU:HD23	1:577:A:LEU:HG	2	1.92	0.03	1.92
(1,1219)	1:606:A:LYS:HD2	1:607:A:VAL:HA	2	1.55	0.01	1.55
(1,2123)	1:573:A:LEU:HD12	1:624:A:ARG:HB2	2	1.18	0.22	1.18
(1,1080)	1:576:A:LEU:HB3	1:573:A:LEU:HD23	2	1.17	0.17	1.17
(1,1080)	1:576:A:LEU:HB3	1:573:A:LEU:HD22	2	1.17	0.17	1.17
(1,223)	1:577:A:LEU:H	1:573:A:LEU:HD21	2	1.14	0.05	1.14
(1,223)	1:577:A:LEU:H	1:573:A:LEU:HD23	2	1.14	0.05	1.14
(1,1294)	1:573:A:LEU:HD13	1:628:A:LEU:HD13	2	1.04	0.09	1.04
(1,866)	1:582:A:ALA:HA	1:581:A:GLU:HG2	2	0.86	0.15	0.86
(1,1885)	1:624:A:ARG:HG2	1:628:A:LEU:HD11	2	0.8	0.18	0.8
(1,1885)	1:628:A:LEU:HD22	1:624:A:ARG:HG2	2	0.8	0.18	0.8
(1,1177)	1:623:A:GLU:HG2	1:622:A:PHE:HB3	2	0.56	0.05	0.56
(1,1886)	1:624:A:ARG:HG3	1:628:A:LEU:HD11	2	0.53	0.04	0.53
(1,1886)	1:624:A:ARG:HG3	1:628:A:LEU:HD12	2	0.53	0.04	0.53
(1,625)	1:577:A:LEU:HD11	1:573:A:LEU:HD21	2	0.4	0.07	0.4
(1,625)	1:577:A:LEU:HD13	1:573:A:LEU:HD23	2	0.4	0.07	0.4
(1,1405)	1:606:A:LYS:HD2	1:607:A:VAL:HG21	2	0.4	0.16	0.4
(1,124)	1:589:A:THR:H	1:589:A:THR:HG22	2	0.38	0.08	0.38
(1,1533)	1:572:A:GLN:H	1:571:A:GLU:HB2	2	0.37	0.17	0.37
(1,1533)	1:572:A:GLN:H	1:572:A:GLN:HB2	2	0.37	0.17	0.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1158)	1:600:A:PRO:HD2	1:603:A:GLN:HG2	2	0.36	0.1	0.36
(1,1320)	1:562:A:LEU:HA	1:562:A:LEU:HD13	2	0.35	0.0	0.35
(1,1155)	1:603:A:GLN:HG3	1:600:A:PRO:HD3	2	0.32	0.08	0.32
(1,2098)	1:581:A:GLU:HG3	1:618:A:LEU:HD21	2	0.32	0.08	0.32
(1,2098)	1:581:A:GLU:HG3	1:618:A:LEU:HD22	2	0.32	0.08	0.32
(1,969)	1:573:A:LEU:HG	1:576:A:LEU:HD23	2	0.32	0.02	0.32
(1,1604)	1:628:A:LEU:H	1:570:A:LEU:HG	2	0.32	0.12	0.32
(1,1943)	1:590:A:GLN:HG2	1:589:A:THR:HG22	2	0.31	0.03	0.31
(1,1941)	1:616:A:GLN:HG2	1:613:A:ALA:HB2	2	0.3	0.2	0.3
(1,1941)	1:616:A:GLN:HG2	1:613:A:ALA:HB1	2	0.3	0.2	0.3
(1,1152)	1:565:A:LYS:HB2	1:565:A:LYS:HE3	2	0.27	0.04	0.27
(1,1295)	1:573:A:LEU:HD13	1:624:A:ARG:HG3	2	0.27	0.02	0.27
(1,668)	1:631:A:LEU:HD13	1:635:A:GLY:HA2	2	0.26	0.15	0.26
(1,668)	1:631:A:LEU:HD12	1:635:A:GLY:HA3	2	0.26	0.15	0.26
(1,691)	1:628:A:LEU:HD13	1:569:A:GLU:HB2	2	0.26	0.01	0.26
(1,991)	1:611:A:MET:HG3	1:587:A:LEU:HD12	2	0.24	0.01	0.24
(1,1776)	1:600:A:PRO:HG2	1:599:A:GLN:HA	2	0.24	0.05	0.24
(1,1094)	1:632:A:LYS:HE3	1:570:A:LEU:HD11	2	0.22	0.04	0.22
(1,1094)	1:632:A:LYS:HE2	1:570:A:LEU:HD13	2	0.22	0.04	0.22
(1,1461)	1:593:A:ASP:H	1:591:A:VAL:H	2	0.22	0.01	0.22
(1,2048)	1:611:A:MET:HG3	1:584:A:LEU:HA	2	0.21	0.03	0.21
(1,1218)	1:606:A:LYS:HD3	1:606:A:LYS:HA	2	0.2	0.03	0.2
(1,1216)	1:606:A:LYS:HD2	1:606:A:LYS:HA	2	0.2	0.01	0.2
(1,848)	1:622:A:PHE:HA	1:573:A:LEU:HD21	2	0.19	0.02	0.19
(1,848)	1:622:A:PHE:HA	1:573:A:LEU:HD23	2	0.19	0.02	0.19
(1,1009)	1:603:A:GLN:HG2	1:599:A:GLN:HB3	2	0.19	0.05	0.19
(1,249)	1:573:A:LEU:H	1:573:A:LEU:HG	2	0.18	0.04	0.18
(1,1391)	1:614:A:ALA:HA	1:583:A:LYS:HE3	2	0.18	0.04	0.18
(1,1391)	1:614:A:ALA:HA	1:583:A:LYS:HE2	2	0.18	0.04	0.18
(1,258)	1:572:A:GLN:H	1:572:A:GLN:HG3	2	0.18	0.0	0.18
(1,2151)	1:628:A:LEU:HB3	1:625:A:TRP:HA	2	0.17	0.06	0.17
(1,471)	1:623:A:GLU:H	1:623:A:GLU:HG3	2	0.17	0.01	0.17
(1,1460)	1:606:A:LYS:H	1:608:A:LEU:H	2	0.16	0.0	0.16
(1,1935)	1:567:A:GLN:HG2	1:562:A:LEU:HG	2	0.16	0.01	0.16
(1,1935)	1:567:A:GLN:HG2	1:562:A:LEU:HB2	2	0.16	0.01	0.16
(1,636)	1:577:A:LEU:HD11	1:621:A:ALA:HA	2	0.14	0.02	0.14
(1,636)	1:577:A:LEU:HD12	1:621:A:ALA:HA	2	0.14	0.02	0.14
(1,1721)	1:604:A:THR:HG22	1:601:A:HIS:HA	2	0.14	0.01	0.14
(1,1721)	1:604:A:THR:HG21	1:601:A:HIS:HA	2	0.14	0.01	0.14
(1,1584)	1:611:A:MET:H	1:587:A:LEU:HD21	2	0.13	0.0	0.13
(1,1584)	1:611:A:MET:H	1:587:A:LEU:HD22	2	0.13	0.0	0.13
(1,78)	1:593:A:ASP:H	1:589:A:THR:HA	2	0.12	0.02	0.12

Continued on next page...

Continued from previous page...

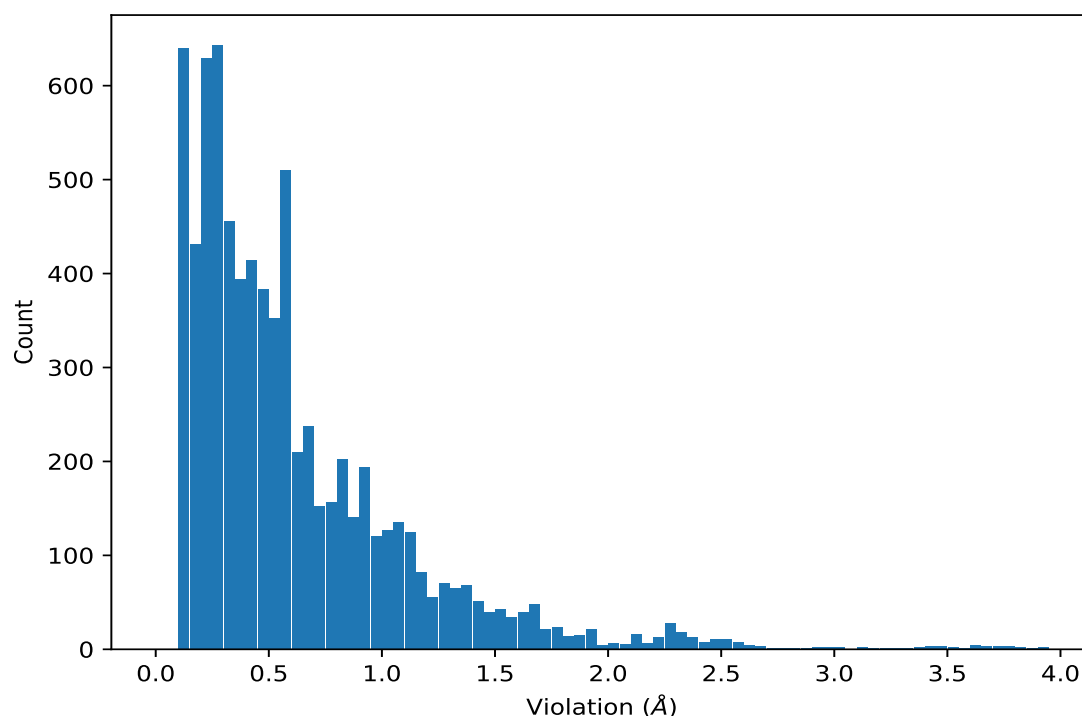
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,314)	1:565:A:LYS:H	1:565:A:LYS:HG3	2	0.12	0.0	0.12
(1,1246)	1:582:A:ALA:HA	1:585:A:GLU:HG3	2	0.12	0.0	0.12
(2,2)	1:577:A:LEU:N	1:573:A:LEU:O	2	0.12	0.0	0.12
(2,12)	1:583:A:LYS:N	1:579:A:ASP:O	2	0.11	0.01	0.11
(1,2028)	1:564:A:TYR:HB2	1:567:A:GLN:HB2	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1274)	1:618:A:LEU:HD23	1:577:A:LEU:HD23	13	3.95
(1,1274)	1:618:A:LEU:HD23	1:577:A:LEU:HD21	11	3.91
(1,1274)	1:618:A:LEU:HD23	1:577:A:LEU:HD23	15	3.85
(1,1280)	1:573:A:LEU:HD23	1:580:A:LEU:HD11	10	3.83
(1,1274)	1:618:A:LEU:HD22	1:577:A:LEU:HD22	17	3.81
(1,1274)	1:618:A:LEU:HD21	1:577:A:LEU:HD21	1	3.76
(1,1274)	1:618:A:LEU:HD21	1:577:A:LEU:HD23	2	3.76
(1,1274)	1:618:A:LEU:HD22	1:577:A:LEU:HD22	7	3.75
(1,1274)	1:618:A:LEU:HD23	1:577:A:LEU:HD22	5	3.74
(1,1366)	1:566:A:LEU:HD22	1:631:A:LEU:HD13	11	3.72
(1,1274)	1:618:A:LEU:HD23	1:577:A:LEU:HD23	9	3.7
(1,1274)	1:618:A:LEU:HD22	1:577:A:LEU:HD23	10	3.68
(1,1274)	1:618:A:LEU:HD23	1:577:A:LEU:HD22	20	3.68
(1,1274)	1:618:A:LEU:HD23	1:577:A:LEU:HD22	12	3.67
(1,1363)	1:562:A:LEU:HD22	1:631:A:LEU:HB2	14	3.65
(1,1274)	1:618:A:LEU:HD21	1:577:A:LEU:HD22	4	3.64
(1,1274)	1:618:A:LEU:HD21	1:577:A:LEU:HD21	8	3.62
(1,1274)	1:618:A:LEU:HD22	1:577:A:LEU:HD23	3	3.6
(1,1366)	1:566:A:LEU:HD23	1:631:A:LEU:HD11	5	3.58
(1,1274)	1:618:A:LEU:HD23	1:577:A:LEU:HD23	19	3.54
(1,1274)	1:618:A:LEU:HD21	1:577:A:LEU:HD22	16	3.52
(1,1307)	1:566:A:LEU:HD13	1:565:A:LYS:HA	7	3.47
(1,1307)	1:566:A:LEU:HD11	1:565:A:LYS:HA	5	3.46
(1,1274)	1:618:A:LEU:HD21	1:577:A:LEU:HD22	18	3.46
(1,1274)	1:618:A:LEU:HD22	1:577:A:LEU:HD22	6	3.43
(1,1280)	1:573:A:LEU:HD21	1:580:A:LEU:HD12	1	3.42
(1,1307)	1:566:A:LEU:HD12	1:565:A:LYS:HA	15	3.41
(1,1366)	1:566:A:LEU:HD22	1:631:A:LEU:HD13	2	3.4
(1,1307)	1:566:A:LEU:HD11	1:565:A:LYS:HA	11	3.39
(1,1363)	1:562:A:LEU:HD22	1:631:A:LEU:HB2	5	3.33
(1,929)	1:565:A:LYS:HG2	1:566:A:LEU:HD11	10	3.3
(1,1307)	1:566:A:LEU:HD12	1:565:A:LYS:HA	2	3.24
(1,1095)	1:565:A:LYS:HE3	1:566:A:LEU:HD11	10	3.17
(1,1366)	1:566:A:LEU:HD22	1:631:A:LEU:HD13	10	3.15
(1,1307)	1:566:A:LEU:HD11	1:565:A:LYS:HA	10	3.14
(1,938)	1:631:A:LEU:HG	1:562:A:LEU:HD22	5	3.02
(1,749)	1:562:A:LEU:HA	1:566:A:LEU:HD22	10	3.02
(1,1366)	1:566:A:LEU:HD21	1:631:A:LEU:HD13	15	2.99
(1,1309)	1:573:A:LEU:HD22	1:576:A:LEU:HB2	10	2.99
(1,749)	1:562:A:LEU:HA	1:566:A:LEU:HD22	2	2.94
(1,749)	1:562:A:LEU:HA	1:566:A:LEU:HD21	15	2.94
(1,1930)	1:565:A:LYS:HB3	1:569:A:GLU:HB3	17	2.85
(1,1900)	1:567:A:GLN:HB2	1:562:A:LEU:HD11	19	2.83

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,938)	1:631:A:LEU:HG	1:562:A:LEU:HD22	14	2.8
(1,749)	1:562:A:LEU:HA	1:566:A:LEU:HD21	7	2.7
(1,1366)	1:566:A:LEU:HD21	1:631:A:LEU:HD11	7	2.69
(1,1930)	1:565:A:LYS:HB3	1:569:A:GLU:HB3	8	2.67
(1,1363)	1:562:A:LEU:HD23	1:631:A:LEU:HB2	19	2.66
(1,584)	1:625:A:TRP:HD1	1:570:A:LEU:HD22	19	2.63
(1,1748)	1:613:A:ALA:HB2	1:580:A:LEU:HD23	17	2.6
(1,1747)	1:613:A:ALA:HB2	1:580:A:LEU:HD23	17	2.6
(1,1746)	1:612:A:ALA:HB3	1:584:A:LEU:HD22	4	2.6
(1,1748)	1:613:A:ALA:HB3	1:580:A:LEU:HD21	7	2.59
(1,1748)	1:613:A:ALA:HB2	1:580:A:LEU:HD23	14	2.59
(1,1747)	1:613:A:ALA:HB3	1:580:A:LEU:HD21	7	2.59
(1,1747)	1:613:A:ALA:HB2	1:580:A:LEU:HD23	14	2.59
(1,1309)	1:573:A:LEU:HD23	1:576:A:LEU:HB2	1	2.58
(1,1748)	1:613:A:ALA:HB2	1:580:A:LEU:HD23	15	2.57
(1,1747)	1:613:A:ALA:HB2	1:580:A:LEU:HD23	15	2.57
(1,1333)	1:573:A:LEU:HD13	1:624:A:ARG:HD2	1	2.57
(1,1936)	1:588:A:GLN:HG3	1:591:A:VAL:HG23	12	2.55
(1,1746)	1:612:A:ALA:HB1	1:584:A:LEU:HD22	8	2.53
(1,1936)	1:588:A:GLN:HG3	1:591:A:VAL:HG11	15	2.52
(1,1936)	1:588:A:GLN:HG3	1:591:A:VAL:HG21	19	2.52
(1,1748)	1:613:A:ALA:HB1	1:580:A:LEU:HD22	9	2.52
(1,1747)	1:613:A:ALA:HB1	1:580:A:LEU:HD22	9	2.52
(1,1746)	1:612:A:ALA:HB2	1:584:A:LEU:HD21	6	2.52
(1,1936)	1:588:A:GLN:HG3	1:591:A:VAL:HG21	20	2.51
(1,1746)	1:612:A:ALA:HB3	1:584:A:LEU:HD22	2	2.51
(1,1095)	1:565:A:LYS:HE3	1:566:A:LEU:HD13	7	2.51
(1,1930)	1:556:A:LYS:HB3	1:555:A:VAL:HB	1	2.5
(1,1936)	1:588:A:GLN:HG3	1:591:A:VAL:HG23	2	2.49
(1,1936)	1:588:A:GLN:HG3	1:591:A:VAL:HG13	5	2.48
(1,1936)	1:588:A:GLN:HG3	1:591:A:VAL:HG21	7	2.48
(1,1936)	1:588:A:GLN:HG3	1:591:A:VAL:HG23	9	2.47
(1,1900)	1:567:A:GLN:HB2	1:562:A:LEU:HD13	14	2.47
(1,1746)	1:612:A:ALA:HB3	1:584:A:LEU:HD21	17	2.47
(1,1746)	1:612:A:ALA:HB3	1:584:A:LEU:HD22	18	2.46
(1,1000)	1:565:A:LYS:HB2	1:566:A:LEU:HD13	2	2.46
(1,1969)	1:579:A:ASP:HB3	1:578:A:GLU:HB2	19	2.45
(1,1936)	1:588:A:GLN:HG3	1:591:A:VAL:HG22	16	2.45
(1,1746)	1:612:A:ALA:HB3	1:584:A:LEU:HD23	9	2.45
(1,1936)	1:588:A:GLN:HG3	1:591:A:VAL:HG21	11	2.44
(1,1846)	1:622:A:PHE:HA	1:576:A:LEU:HD22	9	2.44
(1,1746)	1:612:A:ALA:HB1	1:584:A:LEU:HD22	15	2.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1936)	1:588:A:GLN:HG3	1:591:A:VAL:HG21	1	2.43
(1,1746)	1:612:A:ALA:HB2	1:584:A:LEU:HD23	12	2.42
(1,1746)	1:612:A:ALA:HB1	1:584:A:LEU:HD21	13	2.42
(1,1095)	1:565:A:LYS:HE2	1:566:A:LEU:HD12	15	2.42
(1,1000)	1:565:A:LYS:HB2	1:566:A:LEU:HD11	5	2.42
(1,1936)	1:588:A:GLN:HG3	1:591:A:VAL:HG12	10	2.4
(1,1900)	1:567:A:GLN:HB2	1:562:A:LEU:HD12	5	2.4
(1,1969)	1:579:A:ASP:HB3	1:578:A:GLU:HB2	12	2.39
(1,1969)	1:579:A:ASP:HB3	1:578:A:GLU:HB2	13	2.39
(1,1936)	1:588:A:GLN:HG3	1:591:A:VAL:HG22	17	2.38
(1,1846)	1:622:A:PHE:HA	1:576:A:LEU:HD21	12	2.38
(1,1746)	1:612:A:ALA:HB2	1:584:A:LEU:HD23	20	2.38
(1,1846)	1:622:A:PHE:HA	1:576:A:LEU:HD23	3	2.37
(1,1936)	1:588:A:GLN:HG3	1:591:A:VAL:HG21	6	2.36
(1,1846)	1:622:A:PHE:HA	1:576:A:LEU:HD22	18	2.36
(1,1969)	1:579:A:ASP:HB3	1:578:A:GLU:HB2	5	2.35
(1,1969)	1:579:A:ASP:HB3	1:578:A:GLU:HB2	9	2.35
(1,1969)	1:579:A:ASP:HB3	1:578:A:GLU:HB2	16	2.35
(1,1969)	1:579:A:ASP:HB3	1:578:A:GLU:HB2	8	2.34
(1,1969)	1:579:A:ASP:HB3	1:578:A:GLU:HB2	18	2.34
(1,1969)	1:579:A:ASP:HB3	1:578:A:GLU:HB2	20	2.34
(1,1936)	1:588:A:GLN:HG3	1:591:A:VAL:HG22	18	2.34
(1,1846)	1:622:A:PHE:HA	1:576:A:LEU:HD22	16	2.34
(1,1969)	1:579:A:ASP:HB3	1:578:A:GLU:HB2	3	2.33
(1,1748)	1:613:A:ALA:HB1	1:580:A:LEU:HD21	11	2.33
(1,1747)	1:613:A:ALA:HB1	1:580:A:LEU:HD21	11	2.33
(1,1746)	1:612:A:ALA:HB3	1:584:A:LEU:HD22	11	2.33
(1,1936)	1:588:A:GLN:HG3	1:591:A:VAL:HG22	4	2.32
(1,1846)	1:622:A:PHE:HA	1:576:A:LEU:HD21	2	2.32
(1,1378)	1:624:A:ARG:HD3	1:573:A:LEU:HD13	1	2.32
(1,925)	1:565:A:LYS:HG3	1:566:A:LEU:HD11	10	2.32
(1,1969)	1:579:A:ASP:HB3	1:578:A:GLU:HB2	17	2.31
(1,1936)	1:588:A:GLN:HG3	1:591:A:VAL:HG13	3	2.31
(1,1930)	1:556:A:LYS:HB3	1:555:A:VAL:HB	5	2.31
(1,1746)	1:612:A:ALA:HB1	1:584:A:LEU:HD22	16	2.31
(1,1746)	1:612:A:ALA:HB2	1:584:A:LEU:HD22	19	2.31
(1,1969)	1:579:A:ASP:HB3	1:578:A:GLU:HB2	1	2.3
(1,1969)	1:579:A:ASP:HB3	1:578:A:GLU:HB2	11	2.3
(1,1936)	1:588:A:GLN:HG3	1:591:A:VAL:HG22	13	2.3
(1,1930)	1:556:A:LYS:HB3	1:555:A:VAL:HB	6	2.3
(1,1748)	1:613:A:ALA:HB2	1:580:A:LEU:HD22	4	2.3
(1,1747)	1:613:A:ALA:HB2	1:580:A:LEU:HD22	4	2.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1969)	1:579:A:ASP:HB3	1:575:A:GLN:HB2	2	2.29
(1,1969)	1:579:A:ASP:HB3	1:578:A:GLU:HB2	4	2.29
(1,1930)	1:556:A:LYS:HB3	1:555:A:VAL:HB	13	2.29
(1,1846)	1:622:A:PHE:HA	1:576:A:LEU:HD21	8	2.29
(1,1748)	1:613:A:ALA:HB3	1:580:A:LEU:HD23	13	2.29
(1,1747)	1:613:A:ALA:HB3	1:580:A:LEU:HD23	13	2.29
(1,1936)	1:588:A:GLN:HG3	1:591:A:VAL:HG22	8	2.28
(1,1846)	1:622:A:PHE:HA	1:576:A:LEU:HD21	7	2.28
(1,1748)	1:613:A:ALA:HB2	1:580:A:LEU:HD22	19	2.28
(1,1747)	1:613:A:ALA:HB2	1:580:A:LEU:HD22	19	2.28
(1,1746)	1:612:A:ALA:HB1	1:584:A:LEU:HD22	5	2.28
(1,1748)	1:613:A:ALA:HB1	1:580:A:LEU:HD23	10	2.27
(1,1747)	1:613:A:ALA:HB1	1:580:A:LEU:HD23	10	2.27
(1,776)	1:628:A:LEU:HA	1:562:A:LEU:HD23	14	2.27
(1,1748)	1:613:A:ALA:HB1	1:580:A:LEU:HD23	8	2.26
(1,1747)	1:613:A:ALA:HB1	1:580:A:LEU:HD23	8	2.26
(1,1746)	1:612:A:ALA:HB3	1:584:A:LEU:HD21	14	2.26
(1,1969)	1:579:A:ASP:HB3	1:578:A:GLU:HB2	7	2.25
(1,1969)	1:579:A:ASP:HB3	1:578:A:GLU:HB2	14	2.25
(1,1846)	1:622:A:PHE:HA	1:576:A:LEU:HD22	13	2.25
(1,1746)	1:612:A:ALA:HB3	1:584:A:LEU:HD21	10	2.25
(1,1095)	1:565:A:LYS:HE3	1:566:A:LEU:HD13	2	2.25
(1,1746)	1:612:A:ALA:HB2	1:584:A:LEU:HD22	1	2.24
(1,1746)	1:612:A:ALA:HB2	1:584:A:LEU:HD23	7	2.24
(1,1969)	1:579:A:ASP:HB3	1:578:A:GLU:HB2	15	2.23
(1,1095)	1:565:A:LYS:HE3	1:566:A:LEU:HD11	5	2.23
(1,1930)	1:556:A:LYS:HB3	1:555:A:VAL:HB	15	2.22
(1,1748)	1:613:A:ALA:HB1	1:580:A:LEU:HD21	1	2.22
(1,1748)	1:613:A:ALA:HB3	1:580:A:LEU:HD23	3	2.22
(1,1748)	1:613:A:ALA:HB1	1:580:A:LEU:HD23	12	2.22
(1,1747)	1:613:A:ALA:HB1	1:580:A:LEU:HD21	1	2.22
(1,1747)	1:613:A:ALA:HB3	1:580:A:LEU:HD23	3	2.22
(1,1747)	1:613:A:ALA:HB1	1:580:A:LEU:HD23	12	2.22
(1,1053)	1:577:A:LEU:HD13	1:617:A:GLU:HG3	19	2.22
(1,1288)	1:566:A:LEU:HD23	1:562:A:LEU:HD23	5	2.2
(1,2139)	1:566:A:LEU:HD22	1:632:A:LYS:HA	18	2.19
(1,1333)	1:573:A:LEU:HD13	1:624:A:ARG:HD2	10	2.17
(1,1846)	1:622:A:PHE:HA	1:576:A:LEU:HD21	6	2.16
(1,1753)	1:614:A:ALA:HB3	1:616:A:GLN:HB2	2	2.16
(1,1748)	1:613:A:ALA:HB2	1:580:A:LEU:HD23	18	2.15
(1,1747)	1:613:A:ALA:HB2	1:580:A:LEU:HD23	18	2.15
(1,1378)	1:624:A:ARG:HD3	1:573:A:LEU:HD13	10	2.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1846)	1:622:A:PHE:HA	1:576:A:LEU:HD22	17	2.14
(1,1000)	1:565:A:LYS:HB2	1:566:A:LEU:HD13	7	2.14
(1,1969)	1:579:A:ASP:HB3	1:575:A:GLN:HB2	6	2.13
(1,1846)	1:622:A:PHE:HA	1:576:A:LEU:HD23	20	2.13
(1,1748)	1:613:A:ALA:HB2	1:580:A:LEU:HD23	20	2.13
(1,1747)	1:613:A:ALA:HB2	1:580:A:LEU:HD23	20	2.13
(1,1000)	1:565:A:LYS:HB2	1:566:A:LEU:HD12	11	2.13
(1,1000)	1:565:A:LYS:HB2	1:566:A:LEU:HD12	15	2.13
(1,1936)	1:588:A:GLN:HG3	1:591:A:VAL:HG22	14	2.12
(1,1846)	1:622:A:PHE:HA	1:576:A:LEU:HD23	4	2.12
(1,1278)	1:632:A:LYS:HG2	1:562:A:LEU:HD13	4	2.12
(1,231)	1:576:A:LEU:H	1:573:A:LEU:HD22	10	2.12
(1,1746)	1:612:A:ALA:HB1	1:584:A:LEU:HD23	3	2.11
(1,970)	1:632:A:LYS:HD2	1:570:A:LEU:HD11	19	2.11
(1,1748)	1:613:A:ALA:HB1	1:580:A:LEU:HD22	5	2.1
(1,1747)	1:613:A:ALA:HB1	1:580:A:LEU:HD22	5	2.1
(1,2166)	1:561:A:LYS:HG3	1:562:A:LEU:HD23	3	2.09
(1,1748)	1:613:A:ALA:HB2	1:580:A:LEU:HD21	2	2.09
(1,1747)	1:613:A:ALA:HB2	1:580:A:LEU:HD21	2	2.09
(1,1846)	1:622:A:PHE:HA	1:576:A:LEU:HD22	11	2.06
(1,1753)	1:614:A:ALA:HB2	1:617:A:GLU:HB2	15	2.06
(1,1846)	1:622:A:PHE:HA	1:576:A:LEU:HD22	5	2.05
(1,1034)	1:569:A:GLU:HG2	1:573:A:LEU:HD13	1	2.05
(1,938)	1:631:A:LEU:HG	1:562:A:LEU:HD22	19	2.05
(1,749)	1:562:A:LEU:HA	1:566:A:LEU:HD23	11	2.03
(1,1846)	1:622:A:PHE:HA	1:576:A:LEU:HD23	1	2.0
(1,1846)	1:622:A:PHE:HA	1:576:A:LEU:HD23	15	2.0
(1,1318)	1:570:A:LEU:HD23	1:574:A:PRO:HD3	19	1.98
(1,2166)	1:561:A:LYS:HG3	1:562:A:LEU:HD23	12	1.97
(1,1930)	1:556:A:LYS:HB3	1:555:A:VAL:HB	20	1.97
(1,1969)	1:579:A:ASP:HB3	1:575:A:GLN:HB2	10	1.96
(1,2110)	1:573:A:LEU:HD12	1:570:A:LEU:HB3	4	1.95
(1,2094)	1:573:A:LEU:HD21	1:577:A:LEU:HG	1	1.95
(1,1753)	1:614:A:ALA:HB2	1:617:A:GLU:HB2	19	1.95
(1,1748)	1:613:A:ALA:HB1	1:580:A:LEU:HD23	6	1.95
(1,1748)	1:613:A:ALA:HB3	1:580:A:LEU:HD23	16	1.95
(1,1747)	1:613:A:ALA:HB1	1:580:A:LEU:HD23	6	1.95
(1,1747)	1:613:A:ALA:HB3	1:580:A:LEU:HD23	16	1.95
(1,1902)	1:609:A:ALA:HB3	1:608:A:LEU:HG	9	1.94
(1,1902)	1:567:A:GLN:HB2	1:562:A:LEU:HB3	13	1.94
(1,2110)	1:573:A:LEU:HD13	1:570:A:LEU:HB3	9	1.93
(1,2110)	1:573:A:LEU:HD13	1:570:A:LEU:HB3	14	1.93

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1902)	1:567:A:GLN:HB2	1:570:A:LEU:HB3	8	1.93
(1,1902)	1:567:A:GLN:HB2	1:562:A:LEU:HB3	20	1.93
(1,231)	1:576:A:LEU:H	1:573:A:LEU:HD23	1	1.93
(1,1930)	1:556:A:LYS:HB3	1:555:A:VAL:HB	12	1.92
(1,1846)	1:622:A:PHE:HA	1:576:A:LEU:HD23	10	1.92
(1,2139)	1:566:A:LEU:HD21	1:632:A:LYS:HA	6	1.91
(1,2110)	1:573:A:LEU:HD12	1:570:A:LEU:HB3	7	1.91
(1,1362)	1:631:A:LEU:HB3	1:562:A:LEU:HD22	14	1.91
(1,1335)	1:566:A:LEU:HG	1:562:A:LEU:HD23	14	1.91
(1,1286)	1:566:A:LEU:HD23	1:569:A:GLU:HB2	6	1.91
(1,2139)	1:566:A:LEU:HD23	1:632:A:LYS:HA	3	1.9
(1,1753)	1:614:A:ALA:HB1	1:617:A:GLU:HB2	12	1.9
(1,2139)	1:566:A:LEU:HD22	1:632:A:LYS:HA	19	1.89
(1,2110)	1:573:A:LEU:HD13	1:570:A:LEU:HB3	3	1.89
(1,2094)	1:573:A:LEU:HD23	1:577:A:LEU:HG	10	1.89
(1,1928)	1:583:A:LYS:HB3	1:584:A:LEU:HD21	14	1.89
(1,1753)	1:614:A:ALA:HB1	1:616:A:GLN:HB3	5	1.88
(1,2110)	1:573:A:LEU:HD11	1:570:A:LEU:HB3	15	1.87
(1,2110)	1:573:A:LEU:HD12	1:570:A:LEU:HB3	19	1.87
(1,2155)	1:628:A:LEU:HD12	1:624:A:ARG:HB2	15	1.86
(1,2110)	1:573:A:LEU:HD13	1:570:A:LEU:HB3	11	1.86
(1,1902)	1:567:A:GLN:HB2	1:562:A:LEU:HB3	12	1.86
(1,1753)	1:614:A:ALA:HB3	1:617:A:GLU:HB2	13	1.86
(1,1753)	1:614:A:ALA:HB3	1:617:A:GLU:HB2	16	1.86
(1,1918)	1:583:A:LYS:HD2	1:587:A:LEU:HD22	6	1.85
(1,1069)	1:579:A:ASP:HB2	1:583:A:LYS:HB2	17	1.84
(1,1955)	1:622:A:PHE:HB3	1:618:A:LEU:HD12	20	1.83
(1,1753)	1:614:A:ALA:HB3	1:617:A:GLU:HB2	6	1.83
(1,1753)	1:614:A:ALA:HB3	1:617:A:GLU:HB2	18	1.83
(1,1069)	1:579:A:ASP:HB2	1:583:A:LYS:HB2	9	1.83
(1,1069)	1:579:A:ASP:HB2	1:583:A:LYS:HB2	19	1.83
(1,156)	1:585:A:GLU:H	1:581:A:GLU:HG2	2	1.83
(1,2033)	1:577:A:LEU:HG	1:578:A:GLU:HA	11	1.81
(1,1753)	1:614:A:ALA:HB1	1:616:A:GLN:HB3	7	1.81
(1,965)	1:574:A:PRO:HG3	1:570:A:LEU:HD22	19	1.81
(1,1928)	1:583:A:LYS:HB3	1:584:A:LEU:HD22	16	1.8
(1,1753)	1:614:A:ALA:HB3	1:616:A:GLN:HB3	20	1.8
(1,1715)	1:577:A:LEU:HD12	1:620:A:GLN:HG3	6	1.8
(1,1069)	1:579:A:ASP:HB2	1:583:A:LYS:HB2	20	1.8
(1,2033)	1:577:A:LEU:HG	1:578:A:GLU:HA	16	1.79
(1,1846)	1:622:A:PHE:HA	1:576:A:LEU:HD22	19	1.79
(1,2110)	1:573:A:LEU:HD11	1:570:A:LEU:HB3	2	1.78

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1955)	1:622:A:PHE:HB3	1:618:A:LEU:HD11	7	1.78
(1,1918)	1:565:A:LYS:HD2	1:566:A:LEU:HD22	9	1.78
(1,1069)	1:579:A:ASP:HB2	1:583:A:LYS:HB2	14	1.78
(1,2138)	1:618:A:LEU:HD11	1:614:A:ALA:HA	18	1.77
(1,1928)	1:583:A:LYS:HB3	1:584:A:LEU:HD23	7	1.77
(1,1286)	1:566:A:LEU:HD22	1:569:A:GLU:HB2	3	1.77
(1,776)	1:628:A:LEU:HA	1:562:A:LEU:HD22	5	1.77
(1,2110)	1:573:A:LEU:HD12	1:570:A:LEU:HB3	20	1.76
(1,2033)	1:577:A:LEU:HG	1:578:A:GLU:HA	13	1.76
(1,2033)	1:577:A:LEU:HG	1:578:A:GLU:HA	15	1.76
(1,2033)	1:577:A:LEU:HG	1:578:A:GLU:HA	17	1.76
(1,1955)	1:622:A:PHE:HB3	1:618:A:LEU:HD11	1	1.76
(1,1955)	1:622:A:PHE:HB3	1:618:A:LEU:HD13	13	1.76
(1,1069)	1:579:A:ASP:HB2	1:583:A:LYS:HB2	8	1.76
(1,1069)	1:579:A:ASP:HB2	1:583:A:LYS:HB2	18	1.76
(1,156)	1:585:A:GLU:H	1:581:A:GLU:HG2	7	1.76
(1,2033)	1:577:A:LEU:HG	1:578:A:GLU:HA	10	1.75
(1,1928)	1:583:A:LYS:HB3	1:584:A:LEU:HD21	17	1.75
(1,1753)	1:614:A:ALA:HB3	1:617:A:GLU:HB2	9	1.75
(1,1278)	1:632:A:LYS:HG2	1:562:A:LEU:HD13	17	1.75
(1,1069)	1:579:A:ASP:HB2	1:583:A:LYS:HB2	12	1.75
(1,2110)	1:573:A:LEU:HD12	1:570:A:LEU:HB3	17	1.74
(1,1955)	1:622:A:PHE:HB3	1:618:A:LEU:HD12	19	1.74
(1,1918)	1:583:A:LYS:HD2	1:576:A:LEU:HD13	1	1.74
(1,1902)	1:567:A:GLN:HB3	1:562:A:LEU:HB3	4	1.74
(1,1286)	1:566:A:LEU:HD21	1:569:A:GLU:HB2	16	1.74
(1,2139)	1:566:A:LEU:HD21	1:632:A:LYS:HA	16	1.73
(1,2110)	1:573:A:LEU:HD12	1:570:A:LEU:HB3	18	1.73
(1,2033)	1:577:A:LEU:HG	1:578:A:GLU:HA	6	1.73
(1,1955)	1:622:A:PHE:HB3	1:618:A:LEU:HD13	15	1.73
(1,1955)	1:622:A:PHE:HB3	1:618:A:LEU:HD12	17	1.73
(1,1753)	1:614:A:ALA:HB1	1:617:A:GLU:HB2	17	1.73
(1,1069)	1:579:A:ASP:HB2	1:583:A:LYS:HB2	5	1.73
(1,2110)	1:573:A:LEU:HD11	1:570:A:LEU:HB3	16	1.72
(1,2033)	1:577:A:LEU:HG	1:578:A:GLU:HA	3	1.72
(1,1069)	1:579:A:ASP:HB2	1:583:A:LYS:HB2	11	1.72
(1,2139)	1:566:A:LEU:HD23	1:632:A:LYS:HA	1	1.71
(1,2033)	1:577:A:LEU:HG	1:578:A:GLU:HA	12	1.71
(1,1928)	1:583:A:LYS:HB3	1:584:A:LEU:HD23	3	1.71
(1,1753)	1:614:A:ALA:HB2	1:617:A:GLU:HB2	1	1.71
(1,1069)	1:579:A:ASP:HB2	1:583:A:LYS:HB2	2	1.71
(1,1069)	1:579:A:ASP:HB2	1:583:A:LYS:HB2	13	1.71

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2033)	1:577:A:LEU:HG	1:578:A:GLU:HA	1	1.7
(1,2033)	1:577:A:LEU:HG	1:578:A:GLU:HA	18	1.7
(1,2033)	1:577:A:LEU:HG	1:578:A:GLU:HA	20	1.7
(1,1955)	1:622:A:PHE:HB3	1:618:A:LEU:HD11	3	1.7
(1,1955)	1:622:A:PHE:HB3	1:618:A:LEU:HD11	5	1.7
(1,1955)	1:622:A:PHE:HB3	1:618:A:LEU:HD12	8	1.7
(1,1928)	1:583:A:LYS:HB3	1:584:A:LEU:HD22	5	1.7
(1,1928)	1:583:A:LYS:HB3	1:584:A:LEU:HD22	11	1.7
(1,1928)	1:583:A:LYS:HB3	1:584:A:LEU:HD23	12	1.7
(1,1753)	1:614:A:ALA:HB2	1:617:A:GLU:HB2	10	1.7
(1,1715)	1:577:A:LEU:HD13	1:619:A:GLU:HG2	1	1.7
(1,1385)	1:622:A:PHE:HB2	1:625:A:TRP:HB2	13	1.7
(1,1069)	1:579:A:ASP:HB2	1:583:A:LYS:HB2	3	1.7
(1,609)	1:625:A:TRP:HD1	1:573:A:LEU:HD12	1	1.7
(1,2110)	1:573:A:LEU:HD11	1:570:A:LEU:HB3	12	1.69
(1,2033)	1:577:A:LEU:HG	1:578:A:GLU:HA	2	1.69
(1,2033)	1:577:A:LEU:HG	1:578:A:GLU:HA	4	1.69
(1,2033)	1:577:A:LEU:HG	1:578:A:GLU:HA	8	1.69
(1,1955)	1:622:A:PHE:HB3	1:618:A:LEU:HD11	6	1.69
(1,1928)	1:583:A:LYS:HB3	1:584:A:LEU:HD22	8	1.69
(1,1928)	1:583:A:LYS:HB3	1:584:A:LEU:HD22	15	1.69
(1,1928)	1:583:A:LYS:HB3	1:584:A:LEU:HD22	19	1.69
(1,2138)	1:584:A:LEU:HD13	1:589:A:THR:HB	6	1.68
(1,2110)	1:573:A:LEU:HD12	1:570:A:LEU:HB3	5	1.68
(1,2110)	1:573:A:LEU:HD11	1:570:A:LEU:HB3	13	1.68
(1,1955)	1:622:A:PHE:HB3	1:618:A:LEU:HD11	9	1.68
(1,1945)	1:585:A:GLU:HG2	1:582:A:ALA:HB2	6	1.68
(1,1928)	1:583:A:LYS:HB3	1:584:A:LEU:HD22	1	1.68
(1,1928)	1:583:A:LYS:HB3	1:584:A:LEU:HD22	4	1.68
(1,1928)	1:583:A:LYS:HB3	1:584:A:LEU:HD23	20	1.68
(1,1918)	1:565:A:LYS:HD3	1:566:A:LEU:HD21	20	1.68
(1,1385)	1:622:A:PHE:HB2	1:625:A:TRP:HB2	17	1.68
(1,1286)	1:566:A:LEU:HD21	1:569:A:GLU:HB2	4	1.68
(1,1069)	1:579:A:ASP:HB2	1:583:A:LYS:HB2	16	1.68
(1,2033)	1:577:A:LEU:HG	1:578:A:GLU:HA	7	1.67
(1,2033)	1:577:A:LEU:HG	1:578:A:GLU:HA	9	1.67
(1,1955)	1:622:A:PHE:HB3	1:618:A:LEU:HD13	10	1.67
(1,2149)	1:628:A:LEU:HD23	1:631:A:LEU:HD12	9	1.66
(1,1928)	1:583:A:LYS:HB3	1:584:A:LEU:HD21	10	1.66
(1,1928)	1:583:A:LYS:HB3	1:584:A:LEU:HD21	13	1.66
(1,1794)	1:566:A:LEU:HA	1:570:A:LEU:HB3	3	1.66
(1,1794)	1:566:A:LEU:HA	1:570:A:LEU:HB3	15	1.66

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1362)	1:631:A:LEU:HB3	1:562:A:LEU:HD22	5	1.66
(1,1335)	1:566:A:LEU:HG	1:562:A:LEU:HD23	5	1.66
(1,1286)	1:566:A:LEU:HD22	1:569:A:GLU:HB2	17	1.66
(1,1069)	1:579:A:ASP:HB2	1:583:A:LYS:HB2	7	1.66
(1,1069)	1:579:A:ASP:HB2	1:583:A:LYS:HB2	10	1.66
(1,1069)	1:579:A:ASP:HB2	1:583:A:LYS:HB2	15	1.66
(1,2110)	1:573:A:LEU:HD12	1:570:A:LEU:HB3	8	1.65
(1,1955)	1:622:A:PHE:HB3	1:618:A:LEU:HD11	4	1.65
(1,1753)	1:614:A:ALA:HB2	1:617:A:GLU:HB2	11	1.65
(1,1393)	1:630:A:ALA:HB3	1:626:A:GLU:HB2	15	1.65
(1,1955)	1:622:A:PHE:HB3	1:618:A:LEU:HD12	11	1.64
(1,1955)	1:622:A:PHE:HB3	1:618:A:LEU:HD12	18	1.64
(1,1918)	1:565:A:LYS:HD2	1:566:A:LEU:HD23	14	1.64
(1,1393)	1:630:A:ALA:HB2	1:626:A:GLU:HB2	16	1.64
(1,1024)	1:590:A:GLN:HG3	1:589:A:THR:HG22	5	1.64
(1,2074)	1:576:A:LEU:HB2	1:574:A:PRO:HA	19	1.63
(1,1930)	1:565:A:LYS:HB3	1:569:A:GLU:HB3	3	1.63
(1,1918)	1:583:A:LYS:HD2	1:587:A:LEU:HD23	16	1.63
(1,1753)	1:614:A:ALA:HB1	1:617:A:GLU:HB2	3	1.63
(1,1715)	1:577:A:LEU:HD11	1:617:A:GLU:HG2	11	1.63
(1,1385)	1:622:A:PHE:HB2	1:625:A:TRP:HB2	20	1.63
(1,1376)	1:566:A:LEU:HD23	1:563:A:SER:HB2	11	1.63
(1,1286)	1:566:A:LEU:HD21	1:569:A:GLU:HB2	14	1.63
(1,1279)	1:618:A:LEU:HD21	1:580:A:LEU:HD13	17	1.63
(1,2155)	1:628:A:LEU:HD12	1:624:A:ARG:HB2	16	1.62
(1,2033)	1:562:A:LEU:HG	1:563:A:SER:HB3	5	1.62
(1,1902)	1:567:A:GLN:HB2	1:562:A:LEU:HB3	17	1.62
(1,1794)	1:566:A:LEU:HA	1:570:A:LEU:HB3	10	1.62
(1,1753)	1:614:A:ALA:HB2	1:617:A:GLU:HB2	14	1.62
(1,1715)	1:577:A:LEU:HD12	1:617:A:GLU:HG2	2	1.62
(1,1715)	1:577:A:LEU:HD13	1:620:A:GLN:HG3	13	1.62
(1,1069)	1:579:A:ASP:HB2	1:583:A:LYS:HB2	4	1.62
(1,611)	1:625:A:TRP:HH2	1:626:A:GLU:HG3	11	1.62
(1,2139)	1:566:A:LEU:HD21	1:632:A:LYS:HA	13	1.61
(1,2139)	1:566:A:LEU:HD23	1:632:A:LYS:HA	20	1.61
(1,1955)	1:622:A:PHE:HB3	1:618:A:LEU:HD12	12	1.61
(1,1928)	1:583:A:LYS:HB3	1:584:A:LEU:HD22	2	1.61
(1,1794)	1:566:A:LEU:HA	1:570:A:LEU:HB3	17	1.61
(1,1518)	1:578:A:GLU:H	1:576:A:LEU:HD13	10	1.61
(1,1053)	1:577:A:LEU:HD12	1:617:A:GLU:HG3	7	1.61
(1,1006)	1:567:A:GLN:HG3	1:562:A:LEU:HD12	5	1.61
(1,1794)	1:566:A:LEU:HA	1:570:A:LEU:HB3	16	1.6

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1715)	1:577:A:LEU:HD12	1:617:A:GLU:HG2	10	1.6
(1,1385)	1:622:A:PHE:HB2	1:625:A:TRP:HB2	9	1.6
(1,1069)	1:579:A:ASP:HB2	1:583:A:LYS:HB2	1	1.6
(1,1930)	1:556:A:LYS:HB3	1:555:A:VAL:HB	2	1.59
(1,1928)	1:583:A:LYS:HB3	1:584:A:LEU:HD21	6	1.59
(1,1794)	1:566:A:LEU:HA	1:570:A:LEU:HB3	7	1.59
(1,1634)	1:622:A:PHE:H	1:576:A:LEU:HD22	9	1.59
(1,1279)	1:618:A:LEU:HD22	1:580:A:LEU:HD11	11	1.59
(1,2138)	1:584:A:LEU:HD12	1:582:A:ALA:HA	9	1.58
(1,1928)	1:583:A:LYS:HB3	1:584:A:LEU:HD21	9	1.58
(1,1794)	1:566:A:LEU:HA	1:570:A:LEU:HB3	13	1.58
(1,1715)	1:577:A:LEU:HD11	1:620:A:GLN:HG3	3	1.58
(1,1286)	1:566:A:LEU:HD23	1:569:A:GLU:HB2	1	1.58
(1,611)	1:625:A:TRP:HH2	1:626:A:GLU:HG3	6	1.58
(1,609)	1:625:A:TRP:HD1	1:573:A:LEU:HD12	10	1.58
(1,2163)	1:588:A:GLN:HA	1:607:A:VAL:HG11	19	1.57
(1,2138)	1:584:A:LEU:HD13	1:582:A:ALA:HA	15	1.57
(1,1955)	1:622:A:PHE:HB3	1:618:A:LEU:HD12	2	1.57
(1,1902)	1:567:A:GLN:HB2	1:562:A:LEU:HB2	2	1.57
(1,1873)	1:613:A:ALA:HB3	1:587:A:LEU:HD11	20	1.57
(1,1715)	1:577:A:LEU:HD11	1:619:A:GLU:HG2	12	1.57
(1,1715)	1:577:A:LEU:HD11	1:620:A:GLN:HG3	18	1.57
(1,1385)	1:622:A:PHE:HB2	1:625:A:TRP:HB2	15	1.57
(1,1069)	1:579:A:ASP:HB2	1:583:A:LYS:HB2	6	1.57
(1,2074)	1:576:A:LEU:HB2	1:574:A:PRO:HA	9	1.56
(1,1715)	1:577:A:LEU:HD11	1:617:A:GLU:HG2	16	1.56
(1,1715)	1:577:A:LEU:HD12	1:620:A:GLN:HG3	20	1.56
(1,1385)	1:622:A:PHE:HB2	1:625:A:TRP:HB2	12	1.56
(1,1286)	1:566:A:LEU:HD22	1:569:A:GLU:HB2	8	1.56
(1,1286)	1:566:A:LEU:HD21	1:569:A:GLU:HB2	18	1.56
(1,1219)	1:606:A:LYS:HD2	1:607:A:VAL:HA	11	1.56
(1,2074)	1:576:A:LEU:HB2	1:574:A:PRO:HA	10	1.55
(1,1918)	1:565:A:LYS:HD2	1:566:A:LEU:HD23	19	1.55
(1,1850)	1:589:A:THR:HA	1:590:A:GLN:HG3	5	1.55
(1,1794)	1:566:A:LEU:HA	1:570:A:LEU:HB3	20	1.55
(1,1722)	1:591:A:VAL:HG13	1:611:A:MET:HB2	14	1.55
(1,1286)	1:566:A:LEU:HD21	1:569:A:GLU:HB2	19	1.55
(1,2140)	1:628:A:LEU:HD13	1:625:A:TRP:HB3	5	1.54
(1,2138)	1:584:A:LEU:HD13	1:582:A:ALA:HA	13	1.54
(1,1344)	1:577:A:LEU:HB3	1:618:A:LEU:HD23	13	1.54
(1,1279)	1:618:A:LEU:HD23	1:580:A:LEU:HD13	4	1.54
(1,1278)	1:632:A:LYS:HG2	1:562:A:LEU:HD12	13	1.54

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1219)	1:606:A:LYS:HD2	1:607:A:VAL:HA	5	1.54
(1,611)	1:625:A:TRP:HH2	1:626:A:GLU:HG3	1	1.54
(1,2138)	1:584:A:LEU:HD11	1:582:A:ALA:HA	3	1.53
(1,2138)	1:584:A:LEU:HD13	1:582:A:ALA:HA	8	1.53
(1,2074)	1:576:A:LEU:HB2	1:574:A:PRO:HA	1	1.53
(1,1385)	1:622:A:PHE:HB2	1:625:A:TRP:HB2	4	1.53
(1,1385)	1:622:A:PHE:HB2	1:625:A:TRP:HB2	7	1.53
(1,1053)	1:577:A:LEU:HD12	1:617:A:GLU:HG3	15	1.53
(1,611)	1:625:A:TRP:HH2	1:626:A:GLU:HG3	3	1.53
(1,611)	1:625:A:TRP:HH2	1:626:A:GLU:HG3	10	1.53
(1,2140)	1:628:A:LEU:HD12	1:625:A:TRP:HB3	14	1.52
(1,2138)	1:584:A:LEU:HD11	1:582:A:ALA:HA	4	1.52
(1,2138)	1:584:A:LEU:HD11	1:582:A:ALA:HA	20	1.52
(1,2074)	1:576:A:LEU:HB2	1:574:A:PRO:HA	4	1.52
(1,1918)	1:565:A:LYS:HD3	1:566:A:LEU:HD23	4	1.52
(1,1873)	1:613:A:ALA:HB2	1:587:A:LEU:HD12	5	1.52
(1,1715)	1:577:A:LEU:HD11	1:620:A:GLN:HG3	4	1.52
(1,1715)	1:577:A:LEU:HD11	1:620:A:GLN:HG3	5	1.52
(1,1445)	1:564:A:TYR:HE1	1:568:A:ARG:HD2	20	1.52
(1,1385)	1:622:A:PHE:HB2	1:625:A:TRP:HB2	8	1.52
(1,1385)	1:622:A:PHE:HB2	1:625:A:TRP:HB2	16	1.52
(1,1024)	1:590:A:GLN:HG3	1:589:A:THR:HG22	15	1.52
(1,2149)	1:628:A:LEU:HD21	1:631:A:LEU:HD12	4	1.51
(1,2138)	1:584:A:LEU:HD11	1:582:A:ALA:HA	1	1.51
(1,2138)	1:618:A:LEU:HD13	1:614:A:ALA:HA	5	1.51
(1,1393)	1:630:A:ALA:HB2	1:626:A:GLU:HB2	13	1.51
(1,1385)	1:622:A:PHE:HB2	1:625:A:TRP:HB2	14	1.51
(1,1279)	1:618:A:LEU:HD22	1:580:A:LEU:HD12	5	1.51
(1,1279)	1:618:A:LEU:HD22	1:580:A:LEU:HD11	19	1.51
(1,1278)	1:632:A:LYS:HG2	1:562:A:LEU:HD13	8	1.51
(1,1278)	1:632:A:LYS:HG2	1:562:A:LEU:HD12	12	1.51
(1,1011)	1:567:A:GLN:HG2	1:562:A:LEU:HD12	5	1.51
(1,2138)	1:584:A:LEU:HD13	1:582:A:ALA:HA	12	1.5
(1,2074)	1:576:A:LEU:HB2	1:574:A:PRO:HA	12	1.5
(1,1928)	1:583:A:LYS:HB3	1:584:A:LEU:HD23	18	1.5
(1,1753)	1:614:A:ALA:HB2	1:617:A:GLU:HB2	4	1.5
(1,1445)	1:564:A:TYR:HE1	1:568:A:ARG:HD2	6	1.5
(1,1278)	1:632:A:LYS:HG2	1:562:A:LEU:HD11	20	1.5
(1,2074)	1:576:A:LEU:HB2	1:574:A:PRO:HA	15	1.49
(1,1955)	1:622:A:PHE:HB3	1:618:A:LEU:HD11	16	1.49
(1,1850)	1:589:A:THR:HA	1:590:A:GLN:HG3	10	1.49
(1,1794)	1:566:A:LEU:HA	1:570:A:LEU:HB3	11	1.49

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1794)	1:566:A:LEU:HA	1:570:A:LEU:HB3	12	1.49
(1,1715)	1:577:A:LEU:HD12	1:620:A:GLN:HG3	8	1.49
(1,1385)	1:622:A:PHE:HB2	1:625:A:TRP:HB2	3	1.49
(1,1385)	1:622:A:PHE:HB2	1:625:A:TRP:HB2	11	1.49
(1,1286)	1:566:A:LEU:HD23	1:569:A:GLU:HB2	9	1.49
(1,2155)	1:628:A:LEU:HD11	1:624:A:ARG:HB2	5	1.48
(1,2139)	1:566:A:LEU:HD23	1:632:A:LYS:HA	17	1.48
(1,2074)	1:576:A:LEU:HB2	1:574:A:PRO:HA	14	1.48
(1,2074)	1:576:A:LEU:HB2	1:574:A:PRO:HA	17	1.48
(1,1918)	1:565:A:LYS:HD2	1:566:A:LEU:HD23	18	1.48
(1,1794)	1:566:A:LEU:HA	1:570:A:LEU:HB3	9	1.48
(1,1753)	1:614:A:ALA:HB1	1:617:A:GLU:HB2	8	1.48
(1,1713)	1:577:A:LEU:HD11	1:617:A:GLU:HG3	6	1.48
(1,1634)	1:622:A:PHE:H	1:576:A:LEU:HD22	16	1.48
(1,1385)	1:622:A:PHE:HB2	1:625:A:TRP:HB2	5	1.48
(1,1385)	1:622:A:PHE:HB2	1:625:A:TRP:HB2	18	1.48
(1,1286)	1:566:A:LEU:HD23	1:569:A:GLU:HB2	13	1.48
(1,1286)	1:566:A:LEU:HD22	1:569:A:GLU:HB2	20	1.48
(1,975)	1:615:A:GLU:HB2	1:584:A:LEU:HD11	7	1.48
(1,611)	1:625:A:TRP:HH2	1:626:A:GLU:HG3	7	1.48
(1,2149)	1:628:A:LEU:HD21	1:631:A:LEU:HD12	3	1.47
(1,2138)	1:584:A:LEU:HD13	1:589:A:THR:HB	2	1.47
(1,2119)	1:569:A:GLU:HB3	1:566:A:LEU:HD13	17	1.47
(1,2074)	1:576:A:LEU:HB2	1:574:A:PRO:HA	7	1.47
(1,1396)	1:632:A:LYS:HG3	1:562:A:LEU:HB3	11	1.47
(1,1385)	1:622:A:PHE:HB2	1:625:A:TRP:HB2	19	1.47
(1,1279)	1:618:A:LEU:HD23	1:580:A:LEU:HD13	16	1.47
(1,611)	1:625:A:TRP:HH2	1:626:A:GLU:HG3	2	1.47
(1,2166)	1:562:A:LEU:HD11	1:561:A:LYS:HG3	14	1.46
(1,2138)	1:584:A:LEU:HD13	1:582:A:ALA:HA	10	1.46
(1,2074)	1:576:A:LEU:HB2	1:574:A:PRO:HA	3	1.46
(1,2074)	1:576:A:LEU:HB2	1:574:A:PRO:HA	16	1.46
(1,2074)	1:576:A:LEU:HB2	1:574:A:PRO:HA	18	1.46
(1,1715)	1:577:A:LEU:HD13	1:620:A:GLN:HG3	9	1.46
(1,1393)	1:630:A:ALA:HB3	1:626:A:GLU:HB2	12	1.46
(1,2156)	1:634:A:GLY:HA2	1:633:A:ASN:HB2	14	1.45
(1,1945)	1:585:A:GLU:HG2	1:582:A:ALA:HB1	18	1.45
(1,1850)	1:589:A:THR:HA	1:590:A:GLN:HG3	20	1.45
(1,1393)	1:630:A:ALA:HB3	1:626:A:GLU:HB2	18	1.45
(1,1344)	1:577:A:LEU:HB3	1:618:A:LEU:HD21	2	1.45
(1,1154)	1:603:A:GLN:HG2	1:600:A:PRO:HB3	16	1.45
(1,611)	1:625:A:TRP:HH2	1:626:A:GLU:HG3	5	1.45

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2156)	1:634:A:GLY:HA3	1:633:A:ASN:HB2	10	1.44
(1,2074)	1:576:A:LEU:HB2	1:574:A:PRO:HA	2	1.44
(1,1850)	1:589:A:THR:HA	1:590:A:GLN:HG3	15	1.44
(1,1684)	1:625:A:TRP:HE3	1:573:A:LEU:HD21	1	1.44
(1,1634)	1:622:A:PHE:H	1:576:A:LEU:HD22	18	1.44
(1,1518)	1:578:A:GLU:H	1:576:A:LEU:HD13	1	1.44
(1,1447)	1:568:A:ARG:HD2	1:564:A:TYR:HD1	6	1.44
(1,2166)	1:561:A:LYS:HG3	1:562:A:LEU:HD21	8	1.43
(1,2166)	1:561:A:LYS:HG3	1:562:A:LEU:HD22	17	1.43
(1,2156)	1:634:A:GLY:HA2	1:633:A:ASN:HB2	19	1.43
(1,2074)	1:576:A:LEU:HB2	1:574:A:PRO:HA	13	1.43
(1,1945)	1:585:A:GLU:HG2	1:582:A:ALA:HB3	3	1.43
(1,1918)	1:565:A:LYS:HD3	1:566:A:LEU:HD22	13	1.43
(1,1873)	1:613:A:ALA:HB2	1:587:A:LEU:HD12	10	1.43
(1,1850)	1:589:A:THR:HA	1:590:A:GLN:HG3	9	1.43
(1,1850)	1:589:A:THR:HA	1:590:A:GLN:HG3	13	1.43
(1,1518)	1:578:A:GLU:H	1:576:A:LEU:HD13	19	1.43
(1,1452)	1:599:A:GLN:H	1:600:A:PRO:HG2	10	1.43
(1,1452)	1:599:A:GLN:H	1:600:A:PRO:HG2	14	1.43
(1,1279)	1:618:A:LEU:HD22	1:580:A:LEU:HD12	9	1.43
(1,1279)	1:618:A:LEU:HD22	1:580:A:LEU:HD13	13	1.43
(1,611)	1:625:A:TRP:HH2	1:626:A:GLU:HG3	8	1.43
(1,611)	1:625:A:TRP:HH2	1:626:A:GLU:HG3	15	1.43
(1,2166)	1:561:A:LYS:HG3	1:562:A:LEU:HD21	1	1.42
(1,2156)	1:634:A:GLY:HA3	1:633:A:ASN:HB2	20	1.42
(1,2139)	1:566:A:LEU:HD22	1:632:A:LYS:HA	14	1.42
(1,2138)	1:584:A:LEU:HD12	1:582:A:ALA:HA	11	1.42
(1,2074)	1:576:A:LEU:HB2	1:574:A:PRO:HA	6	1.42
(1,1850)	1:589:A:THR:HA	1:590:A:GLN:HG3	12	1.42
(1,1794)	1:566:A:LEU:HA	1:570:A:LEU:HB3	1	1.42
(1,1634)	1:622:A:PHE:H	1:576:A:LEU:HD22	13	1.42
(1,1630)	1:621:A:ALA:H	1:576:A:LEU:HD21	9	1.42
(1,1612)	1:616:A:GLN:H	1:618:A:LEU:HD22	4	1.42
(1,1445)	1:564:A:TYR:HE2	1:568:A:ARG:HD2	10	1.42
(1,1344)	1:577:A:LEU:HB3	1:618:A:LEU:HD22	7	1.42
(1,2140)	1:628:A:LEU:HD13	1:625:A:TRP:HB3	6	1.41
(1,2140)	1:628:A:LEU:HD11	1:625:A:TRP:HB3	15	1.41
(1,2123)	1:573:A:LEU:HD12	1:624:A:ARG:HB2	1	1.41
(1,1947)	1:581:A:GLU:HG2	1:584:A:LEU:HD11	6	1.41
(1,1850)	1:589:A:THR:HA	1:590:A:GLN:HG3	19	1.41
(1,1447)	1:568:A:ARG:HD2	1:564:A:TYR:HD1	20	1.41
(1,1381)	1:573:A:LEU:HD12	1:624:A:ARG:HB2	1	1.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1344)	1:577:A:LEU:HB3	1:618:A:LEU:HD23	15	1.41
(1,1024)	1:590:A:GLN:HG3	1:589:A:THR:HG23	10	1.41
(1,2162)	1:565:A:LYS:HA	1:564:A:TYR:HB2	10	1.4
(1,2156)	1:634:A:GLY:HA3	1:633:A:ASN:HB2	15	1.4
(1,2140)	1:628:A:LEU:HD11	1:625:A:TRP:HB3	16	1.4
(1,2139)	1:566:A:LEU:HD21	1:632:A:LYS:HA	9	1.4
(1,2110)	1:573:A:LEU:HD13	1:570:A:LEU:HB3	6	1.4
(1,2074)	1:576:A:LEU:HB2	1:574:A:PRO:HA	20	1.4
(1,1850)	1:589:A:THR:HA	1:590:A:GLN:HG3	2	1.4
(1,1715)	1:577:A:LEU:HD13	1:620:A:GLN:HG3	17	1.4
(1,1452)	1:599:A:GLN:H	1:600:A:PRO:HG2	16	1.4
(1,611)	1:625:A:TRP:HH2	1:626:A:GLU:HG3	14	1.4
(1,2156)	1:634:A:GLY:HA3	1:633:A:ASN:HB2	8	1.39
(1,2156)	1:634:A:GLY:HA3	1:633:A:ASN:HB2	16	1.39
(1,1918)	1:565:A:LYS:HD3	1:566:A:LEU:HD21	17	1.39
(1,1518)	1:578:A:GLU:H	1:576:A:LEU:HD11	11	1.39
(1,1452)	1:599:A:GLN:H	1:600:A:PRO:HG2	5	1.39
(1,1452)	1:599:A:GLN:H	1:600:A:PRO:HG2	13	1.39
(1,1393)	1:630:A:ALA:HB3	1:626:A:GLU:HB2	10	1.39
(1,1385)	1:622:A:PHE:HB2	1:625:A:TRP:HB2	2	1.39
(1,1331)	1:566:A:LEU:HD23	1:628:A:LEU:HA	5	1.39
(1,1326)	1:566:A:LEU:HD23	1:563:A:SER:HB3	2	1.39
(1,1279)	1:618:A:LEU:HD23	1:580:A:LEU:HD12	1	1.39
(1,1279)	1:618:A:LEU:HD22	1:580:A:LEU:HD11	15	1.39
(1,1024)	1:590:A:GLN:HG3	1:589:A:THR:HG22	12	1.39
(1,1011)	1:567:A:GLN:HG2	1:562:A:LEU:HD11	19	1.39
(1,2166)	1:561:A:LYS:HG3	1:562:A:LEU:HD23	4	1.38
(1,2156)	1:634:A:GLY:HA3	1:633:A:ASN:HB2	3	1.38
(1,2156)	1:634:A:GLY:HA3	1:633:A:ASN:HB2	11	1.38
(1,2156)	1:634:A:GLY:HA3	1:633:A:ASN:HB2	17	1.38
(1,2138)	1:584:A:LEU:HD13	1:582:A:ALA:HA	16	1.38
(1,2138)	1:584:A:LEU:HD11	1:582:A:ALA:HA	19	1.38
(1,1986)	1:568:A:ARG:HD3	1:567:A:GLN:HG3	20	1.38
(1,1634)	1:622:A:PHE:H	1:576:A:LEU:HD23	1	1.38
(1,1634)	1:622:A:PHE:H	1:576:A:LEU:HD21	2	1.38
(1,611)	1:625:A:TRP:HH2	1:626:A:GLU:HG3	19	1.38
(1,2156)	1:634:A:GLY:HA3	1:633:A:ASN:HB2	6	1.37
(1,2119)	1:569:A:GLU:HB3	1:566:A:LEU:HD13	9	1.37
(1,2074)	1:576:A:LEU:HB2	1:574:A:PRO:HA	5	1.37
(1,2074)	1:576:A:LEU:HB2	1:574:A:PRO:HA	8	1.37
(1,1956)	1:627:A:TYR:HB3	1:630:A:ALA:HB2	15	1.37
(1,1945)	1:585:A:GLU:HG2	1:582:A:ALA:HB1	9	1.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1918)	1:565:A:LYS:HD3	1:566:A:LEU:HD23	3	1.37
(1,1873)	1:613:A:ALA:HB1	1:587:A:LEU:HD12	13	1.37
(1,1518)	1:578:A:GLU:H	1:576:A:LEU:HD11	6	1.37
(1,1393)	1:630:A:ALA:HB2	1:626:A:GLU:HB2	6	1.37
(1,1393)	1:630:A:ALA:HB1	1:626:A:GLU:HB2	11	1.37
(1,1286)	1:566:A:LEU:HD21	1:569:A:GLU:HB2	12	1.37
(1,1192)	1:568:A:ARG:HD2	1:565:A:LYS:HA	18	1.37
(1,611)	1:625:A:TRP:HH2	1:626:A:GLU:HG3	17	1.37
(1,2162)	1:565:A:LYS:HA	1:564:A:TYR:HB2	6	1.36
(1,2156)	1:634:A:GLY:HA3	1:633:A:ASN:HB2	4	1.36
(1,2156)	1:634:A:GLY:HA3	1:633:A:ASN:HB2	12	1.36
(1,2139)	1:566:A:LEU:HD23	1:632:A:LYS:HA	8	1.36
(1,1930)	1:565:A:LYS:HB3	1:569:A:GLU:HB3	4	1.36
(1,1452)	1:599:A:GLN:H	1:600:A:PRO:HG2	6	1.36
(1,1393)	1:630:A:ALA:HB3	1:626:A:GLU:HB2	2	1.36
(1,1385)	1:622:A:PHE:HB2	1:625:A:TRP:HB2	1	1.36
(1,1279)	1:618:A:LEU:HD22	1:580:A:LEU:HD12	12	1.36
(1,975)	1:615:A:GLU:HB2	1:584:A:LEU:HD12	16	1.36
(1,611)	1:625:A:TRP:HH2	1:626:A:GLU:HG3	18	1.36
(1,2156)	1:634:A:GLY:HA3	1:633:A:ASN:HB2	2	1.35
(1,2074)	1:576:A:LEU:HB2	1:574:A:PRO:HA	11	1.35
(1,1986)	1:568:A:ARG:HD3	1:567:A:GLN:HG3	10	1.35
(1,1956)	1:627:A:TYR:HB3	1:630:A:ALA:HB2	2	1.35
(1,1794)	1:566:A:LEU:HA	1:570:A:LEU:HB3	2	1.35
(1,1344)	1:577:A:LEU:HB3	1:618:A:LEU:HD22	17	1.35
(1,1274)	1:618:A:LEU:HD21	1:577:A:LEU:HD23	14	1.35
(1,796)	1:577:A:LEU:HA	1:618:A:LEU:HD23	11	1.35
(1,611)	1:625:A:TRP:HH2	1:626:A:GLU:HG3	16	1.35
(1,2162)	1:565:A:LYS:HA	1:564:A:TYR:HB2	1	1.34
(1,2149)	1:628:A:LEU:HD21	1:631:A:LEU:HD13	14	1.34
(1,2140)	1:628:A:LEU:HD12	1:625:A:TRP:HB3	11	1.34
(1,1930)	1:565:A:LYS:HB3	1:569:A:GLU:HB3	19	1.34
(1,1898)	1:628:A:LEU:HG	1:631:A:LEU:HB2	4	1.34
(1,1713)	1:577:A:LEU:HD11	1:581:A:GLU:HB2	14	1.34
(1,1634)	1:622:A:PHE:H	1:576:A:LEU:HD23	3	1.34
(1,1634)	1:622:A:PHE:H	1:576:A:LEU:HD23	4	1.34
(1,1634)	1:622:A:PHE:H	1:576:A:LEU:HD21	12	1.34
(1,1518)	1:578:A:GLU:H	1:576:A:LEU:HD13	5	1.34
(1,1344)	1:577:A:LEU:HB3	1:618:A:LEU:HD23	20	1.34
(1,1331)	1:566:A:LEU:HD21	1:628:A:LEU:HA	10	1.34
(1,1279)	1:618:A:LEU:HD23	1:580:A:LEU:HD12	2	1.34
(1,1279)	1:618:A:LEU:HD21	1:580:A:LEU:HD11	10	1.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1080)	1:576:A:LEU:HB3	1:573:A:LEU:HD22	10	1.34
(1,611)	1:625:A:TRP:HH2	1:626:A:GLU:HG3	9	1.34
(1,2162)	1:565:A:LYS:HA	1:564:A:TYR:HB2	12	1.33
(1,2162)	1:565:A:LYS:HA	1:564:A:TYR:HB2	18	1.33
(1,2162)	1:565:A:LYS:HA	1:564:A:TYR:HB2	20	1.33
(1,2156)	1:634:A:GLY:HA3	1:633:A:ASN:HB2	5	1.33
(1,2156)	1:634:A:GLY:HA2	1:633:A:ASN:HB2	9	1.33
(1,2156)	1:634:A:GLY:HA3	1:633:A:ASN:HB2	13	1.33
(1,2120)	1:573:A:LEU:HD21	1:624:A:ARG:HB2	4	1.33
(1,1956)	1:627:A:TYR:HB3	1:630:A:ALA:HB2	18	1.33
(1,1518)	1:578:A:GLU:H	1:576:A:LEU:HD12	4	1.33
(1,1385)	1:622:A:PHE:HB2	1:625:A:TRP:HB2	6	1.33
(1,1344)	1:577:A:LEU:HB3	1:618:A:LEU:HD21	8	1.33
(1,1279)	1:618:A:LEU:HD23	1:580:A:LEU:HD11	8	1.33
(1,796)	1:577:A:LEU:HA	1:618:A:LEU:HD23	13	1.33
(1,2149)	1:628:A:LEU:HD21	1:631:A:LEU:HD13	17	1.32
(1,2140)	1:628:A:LEU:HD11	1:625:A:TRP:HB3	17	1.32
(1,2138)	1:584:A:LEU:HD12	1:582:A:ALA:HA	17	1.32
(1,1986)	1:568:A:ARG:HD3	1:567:A:GLN:HG3	5	1.32
(1,1956)	1:627:A:TYR:HB3	1:630:A:ALA:HB2	12	1.32
(1,1794)	1:566:A:LEU:HA	1:570:A:LEU:HB3	18	1.32
(1,1713)	1:577:A:LEU:HD13	1:581:A:GLU:HB2	18	1.32
(1,1684)	1:625:A:TRP:HE3	1:573:A:LEU:HD23	10	1.32
(1,1518)	1:578:A:GLU:H	1:576:A:LEU:HD12	17	1.32
(1,1445)	1:564:A:TYR:HE1	1:568:A:ARG:HD2	12	1.32
(1,2139)	1:566:A:LEU:HD22	1:632:A:LYS:HA	12	1.31
(1,2138)	1:584:A:LEU:HD12	1:589:A:THR:HB	7	1.31
(1,1956)	1:627:A:TYR:HB3	1:630:A:ALA:HB3	1	1.31
(1,1956)	1:627:A:TYR:HB3	1:630:A:ALA:HB2	5	1.31
(1,1956)	1:627:A:TYR:HB3	1:630:A:ALA:HB1	8	1.31
(1,1956)	1:627:A:TYR:HB3	1:630:A:ALA:HB3	11	1.31
(1,1956)	1:627:A:TYR:HB3	1:630:A:ALA:HB1	16	1.31
(1,1898)	1:628:A:LEU:HG	1:631:A:LEU:HB2	9	1.31
(1,1873)	1:613:A:ALA:HB1	1:587:A:LEU:HD11	7	1.31
(1,1634)	1:622:A:PHE:H	1:576:A:LEU:HD21	7	1.31
(1,1376)	1:566:A:LEU:HD21	1:563:A:SER:HB2	7	1.31
(1,1344)	1:577:A:LEU:HB3	1:618:A:LEU:HD22	10	1.31
(1,1344)	1:577:A:LEU:HB3	1:618:A:LEU:HD23	11	1.31
(1,1335)	1:566:A:LEU:HG	1:562:A:LEU:HD23	19	1.31
(1,1287)	1:566:A:LEU:HD22	1:631:A:LEU:HD23	11	1.31
(1,2162)	1:565:A:LYS:HA	1:564:A:TYR:HB2	8	1.3
(1,2162)	1:565:A:LYS:HA	1:564:A:TYR:HB2	13	1.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2161)	1:628:A:LEU:HA	1:630:A:ALA:HB2	18	1.3
(1,1956)	1:627:A:TYR:HB3	1:630:A:ALA:HB2	10	1.3
(1,1871)	1:594:A:ALA:HB1	1:595:A:SER:HB2	19	1.3
(1,1634)	1:622:A:PHE:H	1:576:A:LEU:HD23	20	1.3
(1,1630)	1:621:A:ALA:H	1:576:A:LEU:HD23	3	1.3
(1,1630)	1:621:A:ALA:H	1:576:A:LEU:HD23	8	1.3
(1,1630)	1:621:A:ALA:H	1:576:A:LEU:HD21	18	1.3
(1,1279)	1:618:A:LEU:HD21	1:580:A:LEU:HD13	3	1.3
(1,749)	1:562:A:LEU:HA	1:566:A:LEU:HD23	5	1.3
(1,2149)	1:628:A:LEU:HD22	1:631:A:LEU:HD11	20	1.29
(1,1960)	1:622:A:PHE:HB3	1:623:A:GLU:HB2	1	1.29
(1,1958)	1:622:A:PHE:HB3	1:623:A:GLU:HB2	1	1.29
(1,1947)	1:581:A:GLU:HG2	1:584:A:LEU:HD13	12	1.29
(1,1945)	1:585:A:GLU:HG2	1:582:A:ALA:HB2	2	1.29
(1,1930)	1:565:A:LYS:HB3	1:569:A:GLU:HB3	10	1.29
(1,1794)	1:566:A:LEU:HA	1:570:A:LEU:HB3	6	1.29
(1,1634)	1:622:A:PHE:H	1:576:A:LEU:HD21	8	1.29
(1,1612)	1:616:A:GLN:H	1:618:A:LEU:HD21	13	1.29
(1,1612)	1:616:A:GLN:H	1:618:A:LEU:HD11	14	1.29
(1,1590)	1:583:A:LYS:H	1:618:A:LEU:HD22	20	1.29
(1,1447)	1:568:A:ARG:HD2	1:564:A:TYR:HD2	10	1.29
(1,1331)	1:566:A:LEU:HD22	1:628:A:LEU:HA	11	1.29
(1,1024)	1:590:A:GLN:HG3	1:589:A:THR:HG21	2	1.29
(1,1024)	1:590:A:GLN:HG3	1:589:A:THR:HG23	9	1.29
(1,1024)	1:590:A:GLN:HG3	1:589:A:THR:HG23	20	1.29
(1,796)	1:577:A:LEU:HA	1:618:A:LEU:HD21	7	1.29
(1,796)	1:577:A:LEU:HA	1:618:A:LEU:HD22	15	1.29
(1,2166)	1:561:A:LYS:HG3	1:562:A:LEU:HD23	20	1.28
(1,2156)	1:634:A:GLY:HA3	1:633:A:ASN:HB2	7	1.28
(1,2140)	1:628:A:LEU:HD11	1:625:A:TRP:HB3	2	1.28
(1,1956)	1:627:A:TYR:HB3	1:630:A:ALA:HB1	13	1.28
(1,1873)	1:613:A:ALA:HB3	1:587:A:LEU:HD13	17	1.28
(1,1518)	1:578:A:GLU:H	1:576:A:LEU:HD13	20	1.28
(1,1393)	1:630:A:ALA:HB3	1:626:A:GLU:HB2	5	1.28
(1,1344)	1:577:A:LEU:HB3	1:618:A:LEU:HD23	5	1.28
(1,1279)	1:618:A:LEU:HD21	1:580:A:LEU:HD12	7	1.28
(1,611)	1:625:A:TRP:HH2	1:626:A:GLU:HG3	20	1.28
(1,2140)	1:628:A:LEU:HD12	1:625:A:TRP:HB3	18	1.27
(1,2140)	1:628:A:LEU:HD13	1:625:A:TRP:HB3	19	1.27
(1,2119)	1:569:A:GLU:HB3	1:566:A:LEU:HD11	4	1.27
(1,1630)	1:621:A:ALA:H	1:576:A:LEU:HD22	4	1.27
(1,1445)	1:564:A:TYR:HE1	1:568:A:ARG:HD2	18	1.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1393)	1:630:A:ALA:HB3	1:626:A:GLU:HB2	17	1.27
(1,1279)	1:618:A:LEU:HD23	1:580:A:LEU:HD11	18	1.27
(1,1250)	1:626:A:GLU:HG2	1:623:A:GLU:HA	6	1.27
(1,975)	1:615:A:GLU:HB2	1:584:A:LEU:HD12	20	1.27
(1,929)	1:565:A:LYS:HG2	1:566:A:LEU:HD13	7	1.27
(1,796)	1:577:A:LEU:HA	1:618:A:LEU:HD22	17	1.27
(1,611)	1:625:A:TRP:HH2	1:626:A:GLU:HG3	4	1.27
(1,2172)	1:625:A:TRP:HE3	1:573:A:LEU:HD21	1	1.26
(1,2149)	1:628:A:LEU:HD21	1:631:A:LEU:HD13	19	1.26
(1,1930)	1:565:A:LYS:HB3	1:569:A:GLU:HB3	16	1.26
(1,1898)	1:628:A:LEU:HG	1:631:A:LEU:HB2	3	1.26
(1,1873)	1:613:A:ALA:HB2	1:587:A:LEU:HD13	8	1.26
(1,1873)	1:613:A:ALA:HB2	1:587:A:LEU:HD13	11	1.26
(1,1715)	1:577:A:LEU:HD12	1:620:A:GLN:HG3	14	1.26
(1,1713)	1:577:A:LEU:HD13	1:581:A:GLU:HB2	3	1.26
(1,1630)	1:621:A:ALA:H	1:576:A:LEU:HD21	13	1.26
(1,1518)	1:578:A:GLU:H	1:576:A:LEU:HD11	3	1.26
(1,1447)	1:568:A:ARG:HD2	1:564:A:TYR:HD1	18	1.26
(1,1392)	1:621:A:ALA:HB2	1:625:A:TRP:HB3	10	1.26
(1,1385)	1:622:A:PHE:HB2	1:625:A:TRP:HB2	10	1.26
(1,1154)	1:603:A:GLN:HG2	1:600:A:PRO:HB3	13	1.26
(1,1024)	1:590:A:GLN:HG3	1:589:A:THR:HG23	19	1.26
(1,964)	1:590:A:GLN:HB3	1:607:A:VAL:HG13	13	1.26
(1,796)	1:577:A:LEU:HA	1:618:A:LEU:HD23	5	1.26
(1,2140)	1:628:A:LEU:HD13	1:625:A:TRP:HB3	10	1.25
(1,2140)	1:628:A:LEU:HD12	1:625:A:TRP:HB3	20	1.25
(1,1947)	1:615:A:GLU:HG2	1:584:A:LEU:HD11	18	1.25
(1,1873)	1:613:A:ALA:HB3	1:587:A:LEU:HD11	2	1.25
(1,1873)	1:613:A:ALA:HB3	1:587:A:LEU:HD11	14	1.25
(1,1873)	1:613:A:ALA:HB3	1:587:A:LEU:HD13	19	1.25
(1,1794)	1:566:A:LEU:HA	1:570:A:LEU:HB3	4	1.25
(1,1713)	1:577:A:LEU:HD11	1:581:A:GLU:HB2	12	1.25
(1,1634)	1:622:A:PHE:H	1:576:A:LEU:HD22	17	1.25
(1,1518)	1:578:A:GLU:H	1:576:A:LEU:HD11	7	1.25
(1,1393)	1:630:A:ALA:HB2	1:626:A:GLU:HB2	8	1.25
(1,1344)	1:577:A:LEU:HB3	1:618:A:LEU:HD22	6	1.25
(1,1174)	1:623:A:GLU:HG2	1:622:A:PHE:HB2	14	1.25
(1,2140)	1:628:A:LEU:HD13	1:625:A:TRP:HB3	8	1.24
(1,2125)	1:580:A:LEU:HD22	1:617:A:GLU:HA	5	1.24
(1,1995)	1:557:A:ARG:HD2	1:555:A:VAL:HG22	11	1.24
(1,1956)	1:627:A:TYR:HB3	1:630:A:ALA:HB1	6	1.24
(1,1944)	1:582:A:ALA:HB1	1:578:A:GLU:HG3	8	1.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1918)	1:565:A:LYS:HD3	1:566:A:LEU:HD21	8	1.24
(1,1912)	1:585:A:GLU:HB2	1:582:A:ALA:HB1	13	1.24
(1,1912)	1:585:A:GLU:HB2	1:582:A:ALA:HB2	20	1.24
(1,1873)	1:613:A:ALA:HB3	1:587:A:LEU:HD11	4	1.24
(1,1873)	1:613:A:ALA:HB3	1:587:A:LEU:HD13	18	1.24
(1,1630)	1:621:A:ALA:H	1:576:A:LEU:HD21	16	1.24
(1,1590)	1:583:A:LYS:H	1:618:A:LEU:HD22	15	1.24
(1,1518)	1:578:A:GLU:H	1:576:A:LEU:HD13	13	1.24
(1,1393)	1:630:A:ALA:HB2	1:626:A:GLU:HB2	7	1.24
(1,1344)	1:577:A:LEU:HB3	1:618:A:LEU:HD23	12	1.24
(1,796)	1:577:A:LEU:HA	1:618:A:LEU:HD21	4	1.24
(1,1958)	1:622:A:PHE:HB3	1:623:A:GLU:HB2	9	1.23
(1,1930)	1:565:A:LYS:HB3	1:569:A:GLU:HB3	14	1.23
(1,1902)	1:567:A:GLN:HB2	1:562:A:LEU:HB3	18	1.23
(1,1888)	1:568:A:ARG:HG2	1:569:A:GLU:HB3	3	1.23
(1,1713)	1:577:A:LEU:HD11	1:581:A:GLU:HB2	20	1.23
(1,1518)	1:578:A:GLU:H	1:576:A:LEU:HD12	2	1.23
(1,1445)	1:564:A:TYR:HE1	1:568:A:ARG:HD2	1	1.23
(1,1445)	1:564:A:TYR:HE1	1:568:A:ARG:HD2	8	1.23
(1,1393)	1:630:A:ALA:HB1	1:626:A:GLU:HB2	4	1.23
(1,1034)	1:569:A:GLU:HG2	1:573:A:LEU:HD13	10	1.23
(1,2149)	1:628:A:LEU:HD21	1:631:A:LEU:HD13	6	1.22
(1,2149)	1:628:A:LEU:HD23	1:631:A:LEU:HD13	13	1.22
(1,2125)	1:580:A:LEU:HD21	1:617:A:GLU:HA	2	1.22
(1,1590)	1:583:A:LYS:H	1:618:A:LEU:HD23	8	1.22
(1,1518)	1:578:A:GLU:H	1:576:A:LEU:HD11	15	1.22
(1,1393)	1:630:A:ALA:HB1	1:626:A:GLU:HB2	20	1.22
(1,1392)	1:621:A:ALA:HB3	1:625:A:TRP:HB3	14	1.22
(1,1344)	1:577:A:LEU:HB3	1:618:A:LEU:HD21	4	1.22
(1,1303)	1:581:A:GLU:HG3	1:618:A:LEU:HD13	2	1.22
(1,1250)	1:626:A:GLU:HG2	1:623:A:GLU:HA	8	1.22
(1,2149)	1:628:A:LEU:HD21	1:631:A:LEU:HD13	18	1.21
(1,2125)	1:580:A:LEU:HD23	1:617:A:GLU:HA	10	1.21
(1,2119)	1:569:A:GLU:HB3	1:566:A:LEU:HD12	12	1.21
(1,1986)	1:568:A:ARG:HD3	1:571:A:GLU:HB2	13	1.21
(1,1743)	1:628:A:LEU:HD22	1:570:A:LEU:HA	5	1.21
(1,1741)	1:628:A:LEU:HD21	1:627:A:TYR:HA	5	1.21
(1,1722)	1:591:A:VAL:HG12	1:611:A:MET:HB2	13	1.21
(1,1713)	1:577:A:LEU:HD13	1:581:A:GLU:HB2	7	1.21
(1,1590)	1:583:A:LYS:H	1:618:A:LEU:HD13	7	1.21
(1,1590)	1:583:A:LYS:H	1:618:A:LEU:HD22	9	1.21
(1,1518)	1:578:A:GLU:H	1:576:A:LEU:HD12	9	1.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1518)	1:578:A:GLU:H	1:576:A:LEU:HD12	18	1.21
(1,1447)	1:568:A:ARG:HD2	1:564:A:TYR:HD1	1	1.21
(1,1393)	1:630:A:ALA:HB1	1:626:A:GLU:HB2	1	1.21
(1,1366)	1:566:A:LEU:HD21	1:631:A:LEU:HD11	20	1.21
(1,1344)	1:577:A:LEU:HB3	1:618:A:LEU:HD22	3	1.21
(1,1344)	1:577:A:LEU:HB3	1:618:A:LEU:HD23	9	1.21
(1,1344)	1:577:A:LEU:HB3	1:618:A:LEU:HD21	18	1.21
(1,1024)	1:590:A:GLN:HG3	1:589:A:THR:HG23	13	1.21
(1,649)	1:591:A:VAL:HG11	1:596:A:PHE:HB2	4	1.21
(1,2125)	1:580:A:LEU:HD23	1:617:A:GLU:HA	3	1.2
(1,2125)	1:607:A:VAL:HG11	1:590:A:GLN:HA	6	1.2
(1,1986)	1:568:A:ARG:HD3	1:571:A:GLU:HB2	12	1.2
(1,1733)	1:607:A:VAL:HG21	1:610:A:ASP:HB3	8	1.2
(1,1612)	1:616:A:GLN:H	1:618:A:LEU:HD22	8	1.2
(1,1590)	1:583:A:LYS:H	1:618:A:LEU:HD21	10	1.2
(1,1518)	1:578:A:GLU:H	1:576:A:LEU:HD13	8	1.2
(1,1393)	1:630:A:ALA:HB1	1:626:A:GLU:HB2	9	1.2
(1,1393)	1:630:A:ALA:HB1	1:626:A:GLU:HB2	14	1.2
(1,1376)	1:566:A:LEU:HD21	1:563:A:SER:HB2	15	1.2
(1,1279)	1:618:A:LEU:HD22	1:580:A:LEU:HD13	20	1.2
(1,796)	1:577:A:LEU:HA	1:618:A:LEU:HD23	9	1.2
(1,2125)	1:580:A:LEU:HD23	1:617:A:GLU:HA	13	1.19
(1,2124)	1:612:A:ALA:HA	1:611:A:MET:HE2	14	1.19
(1,2114)	1:581:A:GLU:HG3	1:618:A:LEU:HD13	7	1.19
(1,1986)	1:568:A:ARG:HD3	1:571:A:GLU:HB2	8	1.19
(1,1888)	1:568:A:ARG:HG2	1:569:A:GLU:HB3	16	1.19
(1,1871)	1:594:A:ALA:HB3	1:595:A:SER:HB2	1	1.19
(1,1713)	1:577:A:LEU:HD12	1:581:A:GLU:HB2	9	1.19
(1,1634)	1:622:A:PHE:H	1:576:A:LEU:HD22	11	1.19
(1,1630)	1:621:A:ALA:H	1:576:A:LEU:HD23	2	1.19
(1,1612)	1:616:A:GLN:H	1:618:A:LEU:HD23	3	1.19
(1,1590)	1:583:A:LYS:H	1:618:A:LEU:HD21	3	1.19
(1,1590)	1:583:A:LYS:H	1:618:A:LEU:HD11	19	1.19
(1,1447)	1:568:A:ARG:HD2	1:564:A:TYR:HD1	12	1.19
(1,1445)	1:564:A:TYR:HE1	1:568:A:ARG:HD2	13	1.19
(1,1392)	1:621:A:ALA:HB2	1:625:A:TRP:HB3	18	1.19
(1,1344)	1:577:A:LEU:HB3	1:618:A:LEU:HD21	1	1.19
(1,1303)	1:581:A:GLU:HG3	1:618:A:LEU:HD13	7	1.19
(1,1250)	1:626:A:GLU:HG2	1:623:A:GLU:HA	18	1.19
(1,1015)	1:609:A:ALA:HB3	1:605:A:GLN:HG3	9	1.19
(1,796)	1:577:A:LEU:HA	1:618:A:LEU:HD23	2	1.19
(1,796)	1:577:A:LEU:HA	1:618:A:LEU:HD23	8	1.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,623)	1:577:A:LEU:HD13	1:618:A:LEU:HD21	2	1.19
(1,623)	1:577:A:LEU:HD11	1:618:A:LEU:HD21	16	1.19
(1,611)	1:625:A:TRP:HH2	1:626:A:GLU:HG3	12	1.19
(1,223)	1:577:A:LEU:H	1:573:A:LEU:HD23	10	1.19
(1,1986)	1:568:A:ARG:HD3	1:567:A:GLN:HG3	6	1.18
(1,1956)	1:627:A:TYR:HB3	1:630:A:ALA:HB3	20	1.18
(1,1945)	1:585:A:GLU:HG2	1:582:A:ALA:HB1	10	1.18
(1,1912)	1:585:A:GLU:HB2	1:582:A:ALA:HB1	11	1.18
(1,1900)	1:567:A:GLN:HB3	1:562:A:LEU:HD12	7	1.18
(1,1713)	1:577:A:LEU:HD13	1:581:A:GLU:HB2	15	1.18
(1,1634)	1:622:A:PHE:H	1:576:A:LEU:HD22	5	1.18
(1,1634)	1:622:A:PHE:H	1:576:A:LEU:HD23	15	1.18
(1,1630)	1:621:A:ALA:H	1:576:A:LEU:HD21	17	1.18
(1,1393)	1:630:A:ALA:HB2	1:626:A:GLU:HB2	3	1.18
(1,796)	1:577:A:LEU:HA	1:618:A:LEU:HD22	19	1.18
(1,2140)	1:628:A:LEU:HD13	1:625:A:TRP:HB3	3	1.17
(1,2125)	1:580:A:LEU:HD22	1:617:A:GLU:HA	19	1.17
(1,1947)	1:615:A:GLU:HG2	1:584:A:LEU:HD12	15	1.17
(1,1888)	1:568:A:ARG:HG2	1:569:A:GLU:HB3	14	1.17
(1,1873)	1:613:A:ALA:HB2	1:587:A:LEU:HD12	1	1.17
(1,1850)	1:589:A:THR:HA	1:590:A:GLN:HG3	3	1.17
(1,1743)	1:628:A:LEU:HD23	1:570:A:LEU:HA	2	1.17
(1,1713)	1:577:A:LEU:HD13	1:581:A:GLU:HB2	1	1.17
(1,1684)	1:625:A:TRP:HE3	1:573:A:LEU:HD22	20	1.17
(1,1612)	1:616:A:GLN:H	1:618:A:LEU:HD21	9	1.17
(1,1612)	1:616:A:GLN:H	1:618:A:LEU:HD21	11	1.17
(1,1590)	1:583:A:LYS:H	1:618:A:LEU:HD23	1	1.17
(1,1590)	1:583:A:LYS:H	1:618:A:LEU:HD13	5	1.17
(1,1583)	1:611:A:MET:H	1:609:A:ALA:HB2	10	1.17
(1,1392)	1:621:A:ALA:HB2	1:625:A:TRP:HB3	6	1.17
(1,1392)	1:621:A:ALA:HB3	1:625:A:TRP:HB3	8	1.17
(1,649)	1:591:A:VAL:HG11	1:596:A:PHE:HB2	7	1.17
(1,623)	1:577:A:LEU:HD12	1:618:A:LEU:HD22	10	1.17
(1,2139)	1:566:A:LEU:HD22	1:632:A:LYS:HA	4	1.16
(1,2125)	1:580:A:LEU:HD23	1:617:A:GLU:HA	12	1.16
(1,2125)	1:580:A:LEU:HD23	1:617:A:GLU:HA	15	1.16
(1,1956)	1:627:A:TYR:HB3	1:630:A:ALA:HB3	9	1.16
(1,1945)	1:585:A:GLU:HG2	1:582:A:ALA:HB3	5	1.16
(1,1945)	1:585:A:GLU:HG2	1:582:A:ALA:HB3	14	1.16
(1,1873)	1:613:A:ALA:HB2	1:587:A:LEU:HD13	6	1.16
(1,1794)	1:566:A:LEU:HA	1:570:A:LEU:HB3	8	1.16
(1,1684)	1:625:A:TRP:HE3	1:573:A:LEU:HD21	16	1.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1630)	1:621:A:ALA:H	1:576:A:LEU:HD21	5	1.16
(1,1612)	1:616:A:GLN:H	1:618:A:LEU:HD22	18	1.16
(1,1590)	1:583:A:LYS:H	1:618:A:LEU:HD23	16	1.16
(1,1489)	1:586:A:ALA:H	1:584:A:LEU:HD23	5	1.16
(1,1015)	1:609:A:ALA:HB3	1:605:A:GLN:HG3	14	1.16
(1,649)	1:591:A:VAL:HG12	1:596:A:PHE:HB2	15	1.16
(1,644)	1:591:A:VAL:HG12	1:607:A:VAL:HG12	13	1.16
(1,2155)	1:628:A:LEU:HD13	1:624:A:ARG:HB2	11	1.15
(1,2140)	1:628:A:LEU:HD11	1:625:A:TRP:HB3	9	1.15
(1,2125)	1:607:A:VAL:HG13	1:590:A:GLN:HA	17	1.15
(1,1945)	1:585:A:GLU:HG2	1:582:A:ALA:HB3	19	1.15
(1,1945)	1:585:A:GLU:HG2	1:582:A:ALA:HB2	20	1.15
(1,1898)	1:628:A:LEU:HG	1:631:A:LEU:HB2	17	1.15
(1,1713)	1:577:A:LEU:HD12	1:581:A:GLU:HB2	10	1.15
(1,1583)	1:611:A:MET:H	1:609:A:ALA:HB2	14	1.15
(1,1392)	1:621:A:ALA:HB1	1:625:A:TRP:HB3	3	1.15
(1,1174)	1:623:A:GLU:HG2	1:622:A:PHE:HB2	11	1.15
(1,1095)	1:565:A:LYS:HE2	1:566:A:LEU:HD12	19	1.15
(1,975)	1:615:A:GLU:HB2	1:584:A:LEU:HD11	10	1.15
(1,896)	1:617:A:GLU:HA	1:620:A:GLN:HG2	10	1.15
(1,649)	1:591:A:VAL:HG13	1:596:A:PHE:HB2	19	1.15
(1,644)	1:591:A:VAL:HG11	1:607:A:VAL:HG13	11	1.15
(1,637)	1:604:A:THR:HG22	1:607:A:VAL:HG21	18	1.15
(1,623)	1:577:A:LEU:HD11	1:618:A:LEU:HD22	6	1.15
(1,2125)	1:580:A:LEU:HD23	1:617:A:GLU:HA	20	1.14
(1,2119)	1:569:A:GLU:HB3	1:566:A:LEU:HD11	18	1.14
(1,1956)	1:627:A:TYR:HB3	1:630:A:ALA:HB1	7	1.14
(1,1945)	1:585:A:GLU:HG2	1:582:A:ALA:HB1	15	1.14
(1,1873)	1:613:A:ALA:HB2	1:587:A:LEU:HD12	12	1.14
(1,1612)	1:616:A:GLN:H	1:618:A:LEU:HD21	12	1.14
(1,1590)	1:583:A:LYS:H	1:618:A:LEU:HD23	2	1.14
(1,1590)	1:583:A:LYS:H	1:618:A:LEU:HD23	4	1.14
(1,1590)	1:583:A:LYS:H	1:618:A:LEU:HD22	12	1.14
(1,1583)	1:611:A:MET:H	1:609:A:ALA:HB3	4	1.14
(1,1583)	1:611:A:MET:H	1:612:A:ALA:HB2	18	1.14
(1,1392)	1:621:A:ALA:HB3	1:625:A:TRP:HB3	1	1.14
(1,1344)	1:577:A:LEU:HB3	1:618:A:LEU:HD23	19	1.14
(1,1192)	1:568:A:ARG:HD2	1:565:A:LYS:HA	6	1.14
(1,970)	1:632:A:LYS:HD3	1:570:A:LEU:HD11	1	1.14
(1,796)	1:577:A:LEU:HA	1:618:A:LEU:HD21	10	1.14
(1,637)	1:604:A:THR:HG21	1:607:A:VAL:HG22	8	1.14
(1,637)	1:604:A:THR:HG21	1:607:A:VAL:HG22	9	1.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2172)	1:625:A:TRP:HE3	1:573:A:LEU:HD23	10	1.13
(1,2161)	1:628:A:LEU:HA	1:630:A:ALA:HB3	20	1.13
(1,2149)	1:628:A:LEU:HD23	1:631:A:LEU:HD13	8	1.13
(1,2125)	1:607:A:VAL:HG12	1:590:A:GLN:HA	16	1.13
(1,2125)	1:607:A:VAL:HG13	1:590:A:GLN:HA	18	1.13
(1,2119)	1:569:A:GLU:HB3	1:566:A:LEU:HD13	20	1.13
(1,2104)	1:566:A:LEU:HD23	1:562:A:LEU:HB3	15	1.13
(1,1912)	1:585:A:GLU:HB2	1:582:A:ALA:HB3	7	1.13
(1,1898)	1:628:A:LEU:HG	1:631:A:LEU:HB2	15	1.13
(1,1713)	1:577:A:LEU:HD11	1:581:A:GLU:HB2	16	1.13
(1,1630)	1:621:A:ALA:H	1:576:A:LEU:HD23	6	1.13
(1,1590)	1:583:A:LYS:H	1:618:A:LEU:HD12	13	1.13
(1,1447)	1:568:A:ARG:HD2	1:564:A:TYR:HD1	8	1.13
(1,1392)	1:621:A:ALA:HB2	1:625:A:TRP:HB3	2	1.13
(1,1326)	1:566:A:LEU:HD22	1:563:A:SER:HB3	5	1.13
(1,1163)	1:599:A:GLN:HG3	1:600:A:PRO:HD3	7	1.13
(1,1015)	1:609:A:ALA:HB2	1:605:A:GLN:HG3	19	1.13
(1,970)	1:632:A:LYS:HD3	1:570:A:LEU:HD12	3	1.13
(1,796)	1:577:A:LEU:HA	1:618:A:LEU:HD23	1	1.13
(1,796)	1:577:A:LEU:HA	1:618:A:LEU:HD22	20	1.13
(1,644)	1:591:A:VAL:HG11	1:607:A:VAL:HG13	1	1.13
(1,623)	1:577:A:LEU:HD13	1:618:A:LEU:HD23	15	1.13
(1,2155)	1:628:A:LEU:HD13	1:624:A:ARG:HB2	14	1.12
(1,2140)	1:628:A:LEU:HD13	1:625:A:TRP:HB3	7	1.12
(1,2140)	1:628:A:LEU:HD13	1:625:A:TRP:HB3	12	1.12
(1,2119)	1:569:A:GLU:HB3	1:566:A:LEU:HD11	2	1.12
(1,2119)	1:569:A:GLU:HB3	1:566:A:LEU:HD13	11	1.12
(1,2104)	1:566:A:LEU:HD23	1:562:A:LEU:HB3	7	1.12
(1,1968)	1:579:A:ASP:HB3	1:576:A:LEU:HB3	17	1.12
(1,1873)	1:613:A:ALA:HB1	1:587:A:LEU:HD13	3	1.12
(1,1684)	1:625:A:TRP:HE3	1:573:A:LEU:HD21	9	1.12
(1,1684)	1:625:A:TRP:HE3	1:573:A:LEU:HD21	15	1.12
(1,1634)	1:622:A:PHE:H	1:576:A:LEU:HD21	6	1.12
(1,1583)	1:611:A:MET:H	1:609:A:ALA:HB2	7	1.12
(1,1583)	1:611:A:MET:H	1:612:A:ALA:HB1	12	1.12
(1,1583)	1:611:A:MET:H	1:609:A:ALA:HB1	17	1.12
(1,1294)	1:573:A:LEU:HD13	1:628:A:LEU:HD13	1	1.12
(1,1293)	1:577:A:LEU:HD12	1:573:A:LEU:HD12	16	1.12
(1,796)	1:577:A:LEU:HA	1:618:A:LEU:HD23	16	1.12
(1,649)	1:591:A:VAL:HG12	1:596:A:PHE:HB2	20	1.12
(1,2166)	1:561:A:LYS:HG3	1:562:A:LEU:HD22	5	1.11
(1,2163)	1:567:A:GLN:HA	1:570:A:LEU:HD13	10	1.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2161)	1:628:A:LEU:HA	1:630:A:ALA:HB1	8	1.11
(1,2138)	1:584:A:LEU:HD12	1:582:A:ALA:HA	14	1.11
(1,2135)	1:567:A:GLN:HA	1:570:A:LEU:HD13	10	1.11
(1,2125)	1:607:A:VAL:HG11	1:590:A:GLN:HA	7	1.11
(1,2119)	1:569:A:GLU:HB3	1:566:A:LEU:HD13	13	1.11
(1,2078)	1:562:A:LEU:HB3	1:566:A:LEU:HD12	8	1.11
(1,1991)	1:562:A:LEU:HB3	1:566:A:LEU:HD12	8	1.11
(1,1902)	1:567:A:GLN:HB2	1:562:A:LEU:HB2	11	1.11
(1,1743)	1:628:A:LEU:HD21	1:625:A:TRP:HA	16	1.11
(1,1713)	1:577:A:LEU:HD13	1:617:A:GLU:HG3	2	1.11
(1,1684)	1:625:A:TRP:HE3	1:573:A:LEU:HD22	2	1.11
(1,1684)	1:625:A:TRP:HE3	1:573:A:LEU:HD23	19	1.11
(1,1630)	1:621:A:ALA:H	1:576:A:LEU:HD22	1	1.11
(1,1366)	1:566:A:LEU:HD21	1:631:A:LEU:HD12	8	1.11
(1,672)	1:607:A:VAL:HG23	1:606:A:LYS:HE3	20	1.11
(1,649)	1:591:A:VAL:HG13	1:596:A:PHE:HB2	18	1.11
(1,644)	1:591:A:VAL:HG13	1:607:A:VAL:HG12	17	1.11
(1,623)	1:577:A:LEU:HD13	1:618:A:LEU:HD22	7	1.11
(1,1898)	1:628:A:LEU:HG	1:631:A:LEU:HB2	6	1.1
(1,1761)	1:621:A:ALA:HB3	1:580:A:LEU:HG	5	1.1
(1,1713)	1:577:A:LEU:HD11	1:581:A:GLU:HB2	8	1.1
(1,1684)	1:625:A:TRP:HE3	1:573:A:LEU:HD21	3	1.1
(1,1684)	1:625:A:TRP:HE3	1:573:A:LEU:HD22	7	1.1
(1,1681)	1:622:A:PHE:HD1	1:577:A:LEU:HD22	2	1.1
(1,1634)	1:622:A:PHE:H	1:576:A:LEU:HD22	19	1.1
(1,1630)	1:621:A:ALA:H	1:576:A:LEU:HD21	11	1.1
(1,1630)	1:621:A:ALA:H	1:576:A:LEU:HD22	20	1.1
(1,1612)	1:616:A:GLN:H	1:618:A:LEU:HD22	2	1.1
(1,1590)	1:583:A:LYS:H	1:618:A:LEU:HD11	17	1.1
(1,1583)	1:611:A:MET:H	1:609:A:ALA:HB2	11	1.1
(1,1518)	1:578:A:GLU:H	1:576:A:LEU:HD12	12	1.1
(1,1518)	1:578:A:GLU:H	1:576:A:LEU:HD11	16	1.1
(1,1447)	1:568:A:ARG:HD2	1:564:A:TYR:HD1	13	1.1
(1,1392)	1:621:A:ALA:HB2	1:625:A:TRP:HB3	19	1.1
(1,1344)	1:577:A:LEU:HB3	1:618:A:LEU:HD21	16	1.1
(1,1250)	1:626:A:GLU:HG2	1:623:A:GLU:HA	10	1.1
(1,1154)	1:603:A:GLN:HG2	1:600:A:PRO:HB3	14	1.1
(1,1015)	1:609:A:ALA:HB3	1:605:A:GLN:HG3	11	1.1
(1,1015)	1:609:A:ALA:HB3	1:605:A:GLN:HG3	12	1.1
(1,970)	1:632:A:LYS:HD3	1:570:A:LEU:HD13	9	1.1
(1,906)	1:596:A:PHE:HA	1:599:A:GLN:HG2	1	1.1
(1,637)	1:604:A:THR:HG23	1:607:A:VAL:HG22	1	1.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,637)	1:604:A:THR:HG22	1:607:A:VAL:HG23	11	1.1
(1,637)	1:604:A:THR:HG23	1:607:A:VAL:HG23	15	1.1
(1,623)	1:577:A:LEU:HD13	1:618:A:LEU:HD21	4	1.1
(1,623)	1:577:A:LEU:HD11	1:618:A:LEU:HD21	8	1.1
(1,623)	1:577:A:LEU:HD13	1:618:A:LEU:HD21	18	1.1
(1,623)	1:577:A:LEU:HD13	1:618:A:LEU:HD23	19	1.1
(1,2149)	1:628:A:LEU:HD23	1:631:A:LEU:HD11	12	1.09
(1,2140)	1:628:A:LEU:HD13	1:625:A:TRP:HB3	1	1.09
(1,2125)	1:580:A:LEU:HD22	1:617:A:GLU:HA	9	1.09
(1,2120)	1:573:A:LEU:HD21	1:624:A:ARG:HB2	11	1.09
(1,2078)	1:562:A:LEU:HB3	1:566:A:LEU:HD13	18	1.09
(1,1991)	1:562:A:LEU:HB3	1:566:A:LEU:HD13	18	1.09
(1,1956)	1:627:A:TYR:HB3	1:630:A:ALA:HB3	4	1.09
(1,1945)	1:585:A:GLU:HG2	1:582:A:ALA:HB2	13	1.09
(1,1912)	1:585:A:GLU:HB2	1:582:A:ALA:HB2	17	1.09
(1,1902)	1:567:A:GLN:HB2	1:562:A:LEU:HB2	16	1.09
(1,1888)	1:568:A:ARG:HG2	1:569:A:GLU:HB3	7	1.09
(1,1761)	1:621:A:ALA:HB1	1:580:A:LEU:HG	8	1.09
(1,1743)	1:628:A:LEU:HD21	1:570:A:LEU:HA	12	1.09
(1,1684)	1:625:A:TRP:HE3	1:573:A:LEU:HD21	14	1.09
(1,1684)	1:625:A:TRP:HE3	1:573:A:LEU:HD23	18	1.09
(1,1612)	1:616:A:GLN:H	1:618:A:LEU:HD23	6	1.09
(1,1583)	1:611:A:MET:H	1:609:A:ALA:HB2	15	1.09
(1,1392)	1:621:A:ALA:HB3	1:625:A:TRP:HB3	9	1.09
(1,1271)	1:576:A:LEU:HD12	1:621:A:ALA:HB3	3	1.09
(1,1095)	1:565:A:LYS:HE3	1:566:A:LEU:HD11	18	1.09
(1,1015)	1:609:A:ALA:HB3	1:605:A:GLN:HG3	7	1.09
(1,990)	1:591:A:VAL:HG22	1:611:A:MET:HG2	13	1.09
(1,796)	1:577:A:LEU:HA	1:618:A:LEU:HD22	12	1.09
(1,649)	1:591:A:VAL:HG13	1:596:A:PHE:HB2	17	1.09
(1,644)	1:591:A:VAL:HG11	1:607:A:VAL:HG12	9	1.09
(1,637)	1:604:A:THR:HG21	1:607:A:VAL:HG23	2	1.09
(1,637)	1:604:A:THR:HG21	1:607:A:VAL:HG21	17	1.09
(1,637)	1:604:A:THR:HG23	1:607:A:VAL:HG22	19	1.09
(1,623)	1:577:A:LEU:HD11	1:618:A:LEU:HD23	20	1.09
(1,223)	1:577:A:LEU:H	1:573:A:LEU:HD21	1	1.09
(1,2161)	1:628:A:LEU:HA	1:630:A:ALA:HB3	9	1.08
(1,2119)	1:569:A:GLU:HB3	1:566:A:LEU:HD13	8	1.08
(1,2078)	1:562:A:LEU:HB3	1:566:A:LEU:HD11	12	1.08
(1,1991)	1:562:A:LEU:HB3	1:566:A:LEU:HD11	12	1.08
(1,1986)	1:568:A:ARG:HD3	1:571:A:GLU:HB2	1	1.08
(1,1898)	1:628:A:LEU:HG	1:631:A:LEU:HB2	14	1.08

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1898)	1:628:A:LEU:HG	1:631:A:LEU:HB2	19	1.08
(1,1873)	1:613:A:ALA:HB3	1:587:A:LEU:HD12	15	1.08
(1,1722)	1:591:A:VAL:HG11	1:611:A:MET:HB2	8	1.08
(1,1713)	1:577:A:LEU:HD12	1:581:A:GLU:HB2	11	1.08
(1,1590)	1:583:A:LYS:H	1:618:A:LEU:HD11	11	1.08
(1,1583)	1:611:A:MET:H	1:609:A:ALA:HB3	8	1.08
(1,1583)	1:611:A:MET:H	1:609:A:ALA:HB1	13	1.08
(1,1393)	1:630:A:ALA:HB3	1:626:A:GLU:HB2	19	1.08
(1,1293)	1:577:A:LEU:HD11	1:573:A:LEU:HD12	15	1.08
(1,1271)	1:576:A:LEU:HD12	1:621:A:ALA:HB2	14	1.08
(1,1252)	1:580:A:LEU:HA	1:579:A:ASP:HB2	15	1.08
(1,1250)	1:626:A:GLU:HG2	1:623:A:GLU:HA	2	1.08
(1,1174)	1:623:A:GLU:HG2	1:622:A:PHE:HB2	9	1.08
(1,1067)	1:579:A:ASP:HB2	1:580:A:LEU:HD21	9	1.08
(1,1067)	1:579:A:ASP:HB2	1:580:A:LEU:HD22	10	1.08
(1,1067)	1:579:A:ASP:HB2	1:580:A:LEU:HD22	13	1.08
(1,1006)	1:567:A:GLN:HG3	1:562:A:LEU:HD11	19	1.08
(1,649)	1:591:A:VAL:HG11	1:596:A:PHE:HB2	1	1.08
(1,649)	1:591:A:VAL:HG12	1:596:A:PHE:HB2	11	1.08
(1,637)	1:604:A:THR:HG23	1:607:A:VAL:HG22	16	1.08
(1,623)	1:577:A:LEU:HD12	1:618:A:LEU:HD23	11	1.08
(1,2161)	1:628:A:LEU:HA	1:630:A:ALA:HB3	1	1.07
(1,2161)	1:628:A:LEU:HA	1:630:A:ALA:HB3	4	1.07
(1,2161)	1:628:A:LEU:HA	1:630:A:ALA:HB2	12	1.07
(1,2140)	1:628:A:LEU:HD11	1:625:A:TRP:HB3	13	1.07
(1,1956)	1:627:A:TYR:HB3	1:630:A:ALA:HB1	3	1.07
(1,1956)	1:627:A:TYR:HB3	1:630:A:ALA:HB3	14	1.07
(1,1945)	1:585:A:GLU:HG2	1:582:A:ALA:HB2	12	1.07
(1,1912)	1:585:A:GLU:HB2	1:582:A:ALA:HB2	1	1.07
(1,1856)	1:580:A:LEU:HA	1:583:A:LYS:HE2	7	1.07
(1,1713)	1:577:A:LEU:HD13	1:581:A:GLU:HB2	5	1.07
(1,1713)	1:577:A:LEU:HD13	1:581:A:GLU:HB2	19	1.07
(1,1681)	1:625:A:TRP:HE3	1:577:A:LEU:HD21	16	1.07
(1,1467)	1:593:A:ASP:H	1:591:A:VAL:HG12	4	1.07
(1,1366)	1:566:A:LEU:HD22	1:631:A:LEU:HD13	13	1.07
(1,1293)	1:577:A:LEU:HD13	1:573:A:LEU:HD12	13	1.07
(1,1252)	1:580:A:LEU:HA	1:579:A:ASP:HB2	6	1.07
(1,1252)	1:580:A:LEU:HA	1:579:A:ASP:HB2	7	1.07
(1,1252)	1:580:A:LEU:HA	1:579:A:ASP:HB2	16	1.07
(1,1250)	1:626:A:GLU:HG2	1:623:A:GLU:HA	14	1.07
(1,1174)	1:623:A:GLU:HG2	1:622:A:PHE:HB2	6	1.07
(1,1006)	1:567:A:GLN:HG3	1:562:A:LEU:HD13	14	1.07

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,672)	1:607:A:VAL:HG21	1:606:A:LYS:HE3	9	1.07
(1,644)	1:591:A:VAL:HG13	1:607:A:VAL:HG13	7	1.07
(1,644)	1:591:A:VAL:HG13	1:607:A:VAL:HG12	14	1.07
(1,637)	1:604:A:THR:HG22	1:607:A:VAL:HG22	4	1.07
(1,637)	1:604:A:THR:HG21	1:607:A:VAL:HG23	5	1.07
(1,623)	1:577:A:LEU:HD13	1:618:A:LEU:HD23	5	1.07
(1,611)	1:625:A:TRP:HH2	1:626:A:GLU:HG3	13	1.07
(1,579)	1:627:A:TYR:HD2	1:624:A:ARG:HD3	7	1.07
(1,33)	1:598:A:SER:H	1:599:A:GLN:HG2	1	1.07
(1,2149)	1:628:A:LEU:HD23	1:631:A:LEU:HD13	11	1.06
(1,2140)	1:628:A:LEU:HD11	1:625:A:TRP:HB3	4	1.06
(1,2125)	1:607:A:VAL:HG11	1:590:A:GLN:HA	1	1.06
(1,1888)	1:568:A:ARG:HG2	1:567:A:GLN:HB2	6	1.06
(1,1856)	1:580:A:LEU:HA	1:579:A:ASP:HB2	18	1.06
(1,1743)	1:628:A:LEU:HD23	1:625:A:TRP:HA	11	1.06
(1,1684)	1:625:A:TRP:HE3	1:573:A:LEU:HD21	12	1.06
(1,1684)	1:625:A:TRP:HE3	1:573:A:LEU:HD21	13	1.06
(1,1684)	1:625:A:TRP:HE3	1:573:A:LEU:HD21	17	1.06
(1,1583)	1:611:A:MET:H	1:609:A:ALA:HB1	5	1.06
(1,1583)	1:611:A:MET:H	1:613:A:ALA:HB3	19	1.06
(1,1449)	1:603:A:GLN:H	1:599:A:GLN:HB2	13	1.06
(1,1392)	1:621:A:ALA:HB3	1:625:A:TRP:HB3	13	1.06
(1,1366)	1:566:A:LEU:HD23	1:631:A:LEU:HD13	18	1.06
(1,1252)	1:580:A:LEU:HA	1:579:A:ASP:HB2	18	1.06
(1,838)	1:623:A:GLU:HA	1:626:A:GLU:HB3	6	1.06
(1,796)	1:577:A:LEU:HA	1:618:A:LEU:HD21	3	1.06
(1,649)	1:591:A:VAL:HG13	1:596:A:PHE:HB2	10	1.06
(1,33)	1:598:A:SER:H	1:599:A:GLN:HG2	3	1.06
(1,2161)	1:628:A:LEU:HA	1:630:A:ALA:HB1	13	1.05
(1,2125)	1:580:A:LEU:HD22	1:617:A:GLU:HA	4	1.05
(1,2078)	1:562:A:LEU:HB3	1:566:A:LEU:HD12	9	1.05
(1,1991)	1:562:A:LEU:HB3	1:566:A:LEU:HD12	9	1.05
(1,1968)	1:579:A:ASP:HB3	1:576:A:LEU:HB3	9	1.05
(1,1968)	1:579:A:ASP:HB3	1:576:A:LEU:HB3	12	1.05
(1,1968)	1:579:A:ASP:HB3	1:583:A:LYS:HD2	19	1.05
(1,1968)	1:579:A:ASP:HB3	1:576:A:LEU:HB3	20	1.05
(1,1873)	1:613:A:ALA:HB1	1:587:A:LEU:HD13	16	1.05
(1,1871)	1:594:A:ALA:HB2	1:595:A:SER:HB2	8	1.05
(1,1856)	1:580:A:LEU:HA	1:579:A:ASP:HB2	8	1.05
(1,1856)	1:580:A:LEU:HA	1:583:A:LYS:HE2	15	1.05
(1,1760)	1:594:A:ALA:HB2	1:595:A:SER:HB2	8	1.05
(1,1743)	1:628:A:LEU:HD22	1:625:A:TRP:HA	13	1.05

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1722)	1:591:A:VAL:HG11	1:611:A:MET:HB2	11	1.05
(1,1612)	1:616:A:GLN:H	1:618:A:LEU:HD22	16	1.05
(1,1612)	1:616:A:GLN:H	1:618:A:LEU:HD23	17	1.05
(1,1590)	1:583:A:LYS:H	1:618:A:LEU:HD23	18	1.05
(1,1583)	1:611:A:MET:H	1:609:A:ALA:HB1	20	1.05
(1,1392)	1:621:A:ALA:HB1	1:625:A:TRP:HB3	12	1.05
(1,1252)	1:580:A:LEU:HA	1:579:A:ASP:HB2	8	1.05
(1,1252)	1:580:A:LEU:HA	1:579:A:ASP:HB2	9	1.05
(1,1252)	1:580:A:LEU:HA	1:579:A:ASP:HB2	12	1.05
(1,1250)	1:626:A:GLU:HG2	1:623:A:GLU:HA	7	1.05
(1,776)	1:628:A:LEU:HA	1:562:A:LEU:HD23	19	1.05
(1,649)	1:591:A:VAL:HG11	1:596:A:PHE:HB2	14	1.05
(1,637)	1:604:A:THR:HG21	1:607:A:VAL:HG21	20	1.05
(1,623)	1:577:A:LEU:HD13	1:618:A:LEU:HD22	3	1.05
(1,623)	1:577:A:LEU:HD12	1:618:A:LEU:HD23	9	1.05
(1,2119)	1:569:A:GLU:HB3	1:566:A:LEU:HD12	19	1.04
(1,2078)	1:562:A:LEU:HB3	1:566:A:LEU:HD12	13	1.04
(1,1991)	1:562:A:LEU:HB3	1:566:A:LEU:HD12	13	1.04
(1,1991)	1:562:A:LEU:HB3	1:566:A:LEU:HD11	14	1.04
(1,1947)	1:615:A:GLU:HG2	1:584:A:LEU:HD12	13	1.04
(1,1894)	1:562:A:LEU:HG	1:567:A:GLN:HG3	15	1.04
(1,1871)	1:594:A:ALA:HB3	1:595:A:SER:HB2	4	1.04
(1,1856)	1:580:A:LEU:HA	1:579:A:ASP:HB2	11	1.04
(1,1761)	1:621:A:ALA:HB2	1:580:A:LEU:HG	4	1.04
(1,1761)	1:621:A:ALA:HB1	1:580:A:LEU:HG	17	1.04
(1,1741)	1:628:A:LEU:HD23	1:624:A:ARG:HA	16	1.04
(1,1722)	1:591:A:VAL:HG13	1:611:A:MET:HB2	4	1.04
(1,1713)	1:577:A:LEU:HD13	1:581:A:GLU:HB2	4	1.04
(1,1612)	1:616:A:GLN:H	1:618:A:LEU:HD21	15	1.04
(1,1489)	1:586:A:ALA:H	1:584:A:LEU:HD22	9	1.04
(1,1366)	1:566:A:LEU:HD23	1:631:A:LEU:HD11	12	1.04
(1,1252)	1:580:A:LEU:HA	1:579:A:ASP:HB2	4	1.04
(1,1252)	1:580:A:LEU:HA	1:579:A:ASP:HB2	11	1.04
(1,1192)	1:568:A:ARG:HD2	1:565:A:LYS:HA	1	1.04
(1,1192)	1:568:A:ARG:HD2	1:565:A:LYS:HA	8	1.04
(1,1174)	1:623:A:GLU:HG2	1:622:A:PHE:HB2	13	1.04
(1,964)	1:590:A:GLN:HB3	1:607:A:VAL:HG12	19	1.04
(1,644)	1:591:A:VAL:HG13	1:607:A:VAL:HG12	3	1.04
(1,644)	1:591:A:VAL:HG11	1:607:A:VAL:HG11	20	1.04
(1,623)	1:577:A:LEU:HD11	1:618:A:LEU:HD23	12	1.04
(1,33)	1:598:A:SER:H	1:599:A:GLN:HG2	9	1.04
(1,2161)	1:628:A:LEU:HA	1:630:A:ALA:HB3	14	1.03

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2155)	1:628:A:LEU:HD12	1:624:A:ARG:HB2	9	1.03
(1,2155)	1:628:A:LEU:HD11	1:624:A:ARG:HB2	19	1.03
(1,2037)	1:609:A:ALA:HA	1:605:A:GLN:HB3	18	1.03
(1,1968)	1:579:A:ASP:HB3	1:583:A:LYS:HD2	13	1.03
(1,1968)	1:579:A:ASP:HB3	1:576:A:LEU:HB3	18	1.03
(1,1947)	1:581:A:GLU:HG2	1:584:A:LEU:HD12	9	1.03
(1,1945)	1:585:A:GLU:HG2	1:582:A:ALA:HB1	11	1.03
(1,1894)	1:576:A:LEU:HG	1:617:A:GLU:HG3	7	1.03
(1,1888)	1:568:A:ARG:HG2	1:567:A:GLN:HB2	8	1.03
(1,1873)	1:613:A:ALA:HB2	1:587:A:LEU:HD12	9	1.03
(1,1856)	1:580:A:LEU:HA	1:579:A:ASP:HB2	14	1.03
(1,1790)	1:557:A:ARG:HA	1:555:A:VAL:HG21	12	1.03
(1,1743)	1:628:A:LEU:HD23	1:625:A:TRP:HA	10	1.03
(1,1634)	1:622:A:PHE:H	1:576:A:LEU:HD23	10	1.03
(1,1612)	1:616:A:GLN:H	1:618:A:LEU:HD22	1	1.03
(1,1612)	1:616:A:GLN:H	1:618:A:LEU:HD23	10	1.03
(1,1583)	1:611:A:MET:H	1:609:A:ALA:HB2	1	1.03
(1,1583)	1:611:A:MET:H	1:613:A:ALA:HB1	16	1.03
(1,1392)	1:621:A:ALA:HB2	1:625:A:TRP:HB3	20	1.03
(1,1331)	1:566:A:LEU:HD22	1:628:A:LEU:HA	2	1.03
(1,1252)	1:580:A:LEU:HA	1:579:A:ASP:HB2	2	1.03
(1,1252)	1:580:A:LEU:HA	1:579:A:ASP:HB2	14	1.03
(1,1192)	1:568:A:ARG:HD2	1:565:A:LYS:HA	13	1.03
(1,1015)	1:609:A:ALA:HB2	1:605:A:GLN:HG3	2	1.03
(1,637)	1:604:A:THR:HG23	1:607:A:VAL:HG21	3	1.03
(1,579)	1:627:A:TYR:HD2	1:624:A:ARG:HD3	20	1.03
(1,33)	1:598:A:SER:H	1:599:A:GLN:HG2	2	1.03
(1,2149)	1:628:A:LEU:HD21	1:631:A:LEU:HD11	16	1.02
(1,2125)	1:607:A:VAL:HG11	1:590:A:GLN:HA	11	1.02
(1,2120)	1:573:A:LEU:HD21	1:624:A:ARG:HB2	19	1.02
(1,1956)	1:627:A:TYR:HB3	1:630:A:ALA:HB2	17	1.02
(1,1945)	1:585:A:GLU:HG2	1:582:A:ALA:HB1	16	1.02
(1,1917)	1:585:A:GLU:HB2	1:584:A:LEU:HD12	18	1.02
(1,1902)	1:567:A:GLN:HB2	1:562:A:LEU:HG	14	1.02
(1,1856)	1:580:A:LEU:HA	1:579:A:ASP:HB2	20	1.02
(1,1761)	1:621:A:ALA:HB1	1:580:A:LEU:HG	13	1.02
(1,1741)	1:628:A:LEU:HD22	1:624:A:ARG:HA	15	1.02
(1,1722)	1:591:A:VAL:HG11	1:611:A:MET:HB2	6	1.02
(1,1684)	1:625:A:TRP:HE3	1:573:A:LEU:HD23	4	1.02
(1,1681)	1:625:A:TRP:HE3	1:577:A:LEU:HD22	15	1.02
(1,1590)	1:583:A:LYS:H	1:618:A:LEU:HD21	6	1.02
(1,1495)	1:584:A:LEU:H	1:584:A:LEU:HD13	6	1.02

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1279)	1:618:A:LEU:HD21	1:580:A:LEU:HD12	6	1.02
(1,1252)	1:580:A:LEU:HA	1:579:A:ASP:HB2	1	1.02
(1,1252)	1:580:A:LEU:HA	1:579:A:ASP:HB2	5	1.02
(1,1252)	1:580:A:LEU:HA	1:579:A:ASP:HB2	20	1.02
(1,1192)	1:568:A:ARG:HD2	1:565:A:LYS:HA	10	1.02
(1,1067)	1:579:A:ASP:HB2	1:580:A:LEU:HD22	20	1.02
(1,644)	1:591:A:VAL:HG12	1:607:A:VAL:HG11	15	1.02
(1,637)	1:604:A:THR:HG23	1:607:A:VAL:HG22	6	1.02
(1,623)	1:577:A:LEU:HD13	1:618:A:LEU:HD21	1	1.02
(1,623)	1:577:A:LEU:HD12	1:618:A:LEU:HD23	13	1.02
(1,623)	1:577:A:LEU:HD12	1:618:A:LEU:HD22	17	1.02
(1,2149)	1:631:A:LEU:HD13	1:566:A:LEU:HD11	10	1.01
(1,2078)	1:562:A:LEU:HB3	1:566:A:LEU:HD12	20	1.01
(1,1991)	1:562:A:LEU:HB3	1:566:A:LEU:HD12	20	1.01
(1,1918)	1:565:A:LYS:HD3	1:566:A:LEU:HD23	12	1.01
(1,1898)	1:628:A:LEU:HG	1:631:A:LEU:HB2	7	1.01
(1,1856)	1:580:A:LEU:HA	1:583:A:LYS:HE2	5	1.01
(1,1760)	1:613:A:ALA:HB3	1:611:A:MET:HA	19	1.01
(1,1743)	1:628:A:LEU:HD21	1:625:A:TRP:HA	20	1.01
(1,1684)	1:625:A:TRP:HE3	1:573:A:LEU:HD22	6	1.01
(1,1467)	1:593:A:ASP:H	1:591:A:VAL:HG11	17	1.01
(1,1445)	1:564:A:TYR:HE2	1:568:A:ARG:HD2	5	1.01
(1,1095)	1:565:A:LYS:HE2	1:566:A:LEU:HD13	13	1.01
(1,1067)	1:579:A:ASP:HB2	1:580:A:LEU:HD23	2	1.01
(1,1053)	1:577:A:LEU:HD12	1:617:A:GLU:HG3	17	1.01
(1,1015)	1:609:A:ALA:HB2	1:605:A:GLN:HG3	17	1.01
(1,1015)	1:609:A:ALA:HB2	1:605:A:GLN:HG3	20	1.01
(1,866)	1:582:A:ALA:HA	1:581:A:GLU:HG2	7	1.01
(1,33)	1:598:A:SER:H	1:599:A:GLN:HG2	11	1.01
(1,33)	1:598:A:SER:H	1:599:A:GLN:HG2	12	1.01
(1,2149)	1:628:A:LEU:HD23	1:631:A:LEU:HD13	1	1.0
(1,1992)	1:562:A:LEU:HB3	1:631:A:LEU:HG	7	1.0
(1,1968)	1:579:A:ASP:HB3	1:576:A:LEU:HB3	8	1.0
(1,1900)	1:567:A:GLN:HB2	1:562:A:LEU:HD11	6	1.0
(1,1888)	1:568:A:ARG:HG3	1:571:A:GLU:HB3	1	1.0
(1,1856)	1:580:A:LEU:HA	1:579:A:ASP:HB2	3	1.0
(1,1856)	1:580:A:LEU:HA	1:583:A:LYS:HE2	12	1.0
(1,1760)	1:613:A:ALA:HB3	1:611:A:MET:HA	4	1.0
(1,1684)	1:625:A:TRP:HE3	1:573:A:LEU:HD23	11	1.0
(1,1583)	1:611:A:MET:H	1:609:A:ALA:HB1	3	1.0
(1,1495)	1:584:A:LEU:H	1:584:A:LEU:HD12	8	1.0
(1,1489)	1:586:A:ALA:H	1:584:A:LEU:HD23	4	1.0

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1449)	1:603:A:GLN:H	1:605:A:GLN:HB2	16	1.0
(1,1392)	1:621:A:ALA:HB3	1:625:A:TRP:HB3	17	1.0
(1,1366)	1:566:A:LEU:HD21	1:631:A:LEU:HD13	17	1.0
(1,1366)	1:566:A:LEU:HD23	1:631:A:LEU:HD13	19	1.0
(1,1326)	1:566:A:LEU:HD23	1:563:A:SER:HB3	3	1.0
(1,1280)	1:573:A:LEU:HD23	1:580:A:LEU:HD12	12	1.0
(1,1271)	1:576:A:LEU:HD12	1:621:A:ALA:HB1	6	1.0
(1,1252)	1:580:A:LEU:HA	1:579:A:ASP:HB2	3	1.0
(1,1080)	1:576:A:LEU:HB3	1:573:A:LEU:HD23	1	1.0
(1,1067)	1:579:A:ASP:HB2	1:580:A:LEU:HD21	5	1.0
(1,1067)	1:579:A:ASP:HB2	1:580:A:LEU:HD21	19	1.0
(1,1015)	1:609:A:ALA:HB2	1:605:A:GLN:HG3	5	1.0
(1,975)	1:615:A:GLU:HB2	1:584:A:LEU:HD11	12	1.0
(1,695)	1:586:A:ALA:HB2	1:583:A:LYS:HB2	5	1.0
(1,649)	1:591:A:VAL:HG11	1:596:A:PHE:HB2	5	1.0
(1,33)	1:598:A:SER:H	1:599:A:GLN:HG2	15	1.0
(1,2161)	1:628:A:LEU:HA	1:630:A:ALA:HB2	5	0.99
(1,2119)	1:569:A:GLU:HB3	1:566:A:LEU:HD13	15	0.99
(1,1960)	1:622:A:PHE:HB3	1:619:A:GLU:HB2	20	0.99
(1,1958)	1:622:A:PHE:HB3	1:619:A:GLU:HB2	20	0.99
(1,1930)	1:556:A:LYS:HB3	1:555:A:VAL:HB	18	0.99
(1,1888)	1:568:A:ARG:HG2	1:569:A:GLU:HB3	11	0.99
(1,1856)	1:580:A:LEU:HA	1:583:A:LYS:HE2	2	0.99
(1,1856)	1:580:A:LEU:HA	1:579:A:ASP:HB2	10	0.99
(1,1856)	1:580:A:LEU:HA	1:579:A:ASP:HB2	17	0.99
(1,1761)	1:621:A:ALA:HB2	1:624:A:ARG:HG2	18	0.99
(1,1760)	1:613:A:ALA:HB2	1:611:A:MET:HA	1	0.99
(1,1743)	1:628:A:LEU:HD23	1:625:A:TRP:HA	6	0.99
(1,1722)	1:591:A:VAL:HG12	1:611:A:MET:HB2	17	0.99
(1,1592)	1:583:A:LYS:H	1:581:A:GLU:HB2	9	0.99
(1,1495)	1:584:A:LEU:H	1:584:A:LEU:HD11	9	0.99
(1,1495)	1:584:A:LEU:H	1:584:A:LEU:HD12	18	0.99
(1,1489)	1:586:A:ALA:H	1:584:A:LEU:HD23	1	0.99
(1,1271)	1:576:A:LEU:HD12	1:621:A:ALA:HB3	11	0.99
(1,1252)	1:580:A:LEU:HA	1:579:A:ASP:HB2	10	0.99
(1,1252)	1:580:A:LEU:HA	1:579:A:ASP:HB2	17	0.99
(1,1174)	1:623:A:GLU:HG2	1:622:A:PHE:HB2	5	0.99
(1,1095)	1:565:A:LYS:HE2	1:566:A:LEU:HD13	6	0.99
(1,975)	1:615:A:GLU:HB2	1:584:A:LEU:HD12	1	0.99
(1,672)	1:607:A:VAL:HG23	1:606:A:LYS:HE3	17	0.99
(1,2172)	1:625:A:TRP:HE3	1:573:A:LEU:HD22	20	0.98
(1,2155)	1:628:A:LEU:HD12	1:624:A:ARG:HB2	17	0.98

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2149)	1:628:A:LEU:HD22	1:631:A:LEU:HD13	2	0.98
(1,1968)	1:579:A:ASP:HB3	1:576:A:LEU:HB3	16	0.98
(1,1917)	1:585:A:GLU:HB2	1:584:A:LEU:HD13	2	0.98
(1,1917)	1:585:A:GLU:HB2	1:584:A:LEU:HD13	6	0.98
(1,1902)	1:567:A:GLN:HB2	1:562:A:LEU:HB2	7	0.98
(1,1900)	1:567:A:GLN:HB3	1:562:A:LEU:HD13	15	0.98
(1,1856)	1:580:A:LEU:HA	1:583:A:LYS:HE2	6	0.98
(1,1761)	1:621:A:ALA:HB2	1:624:A:ARG:HG2	19	0.98
(1,1743)	1:628:A:LEU:HD21	1:570:A:LEU:HA	8	0.98
(1,1722)	1:591:A:VAL:HG13	1:611:A:MET:HB2	16	0.98
(1,1720)	1:604:A:THR:HG23	1:600:A:PRO:HD3	8	0.98
(1,1612)	1:616:A:GLN:H	1:618:A:LEU:HD21	19	0.98
(1,1583)	1:611:A:MET:H	1:609:A:ALA:HB2	6	0.98
(1,1495)	1:584:A:LEU:H	1:584:A:LEU:HD11	11	0.98
(1,1489)	1:586:A:ALA:H	1:584:A:LEU:HD22	13	0.98
(1,1467)	1:593:A:ASP:H	1:591:A:VAL:HG12	1	0.98
(1,1366)	1:566:A:LEU:HD22	1:631:A:LEU:HD12	1	0.98
(1,1366)	1:566:A:LEU:HD23	1:631:A:LEU:HD13	14	0.98
(1,1362)	1:631:A:LEU:HB3	1:562:A:LEU:HD22	19	0.98
(1,1280)	1:573:A:LEU:HD22	1:580:A:LEU:HD11	18	0.98
(1,1280)	1:573:A:LEU:HD21	1:580:A:LEU:HD13	20	0.98
(1,1250)	1:626:A:GLU:HG2	1:623:A:GLU:HA	12	0.98
(1,1015)	1:609:A:ALA:HB3	1:605:A:GLN:HG3	1	0.98
(1,1015)	1:609:A:ALA:HB3	1:605:A:GLN:HG3	6	0.98
(1,1015)	1:609:A:ALA:HB3	1:605:A:GLN:HG3	15	0.98
(1,989)	1:611:A:MET:HG2	1:587:A:LEU:HD12	12	0.98
(1,695)	1:586:A:ALA:HB3	1:583:A:LYS:HB2	7	0.98
(1,649)	1:591:A:VAL:HG11	1:596:A:PHE:HB2	3	0.98
(1,649)	1:591:A:VAL:HG12	1:596:A:PHE:HB2	6	0.98
(1,43)	1:597:A:PHE:H	1:596:A:PHE:HB2	7	0.98
(1,2172)	1:625:A:TRP:HE3	1:573:A:LEU:HD21	16	0.97
(1,2161)	1:628:A:LEU:HA	1:630:A:ALA:HB1	3	0.97
(1,2155)	1:628:A:LEU:HD11	1:624:A:ARG:HB2	1	0.97
(1,2155)	1:624:A:ARG:HB2	1:628:A:LEU:HD23	4	0.97
(1,2120)	1:573:A:LEU:HD22	1:624:A:ARG:HB2	5	0.97
(1,2119)	1:569:A:GLU:HB3	1:566:A:LEU:HD11	7	0.97
(1,2119)	1:569:A:GLU:HB3	1:566:A:LEU:HD12	14	0.97
(1,2078)	1:562:A:LEU:HB3	1:566:A:LEU:HD12	17	0.97
(1,2037)	1:609:A:ALA:HA	1:605:A:GLN:HB3	4	0.97
(1,2037)	1:609:A:ALA:HA	1:605:A:GLN:HB2	9	0.97
(1,1991)	1:562:A:LEU:HB3	1:566:A:LEU:HD12	17	0.97
(1,1968)	1:579:A:ASP:HB3	1:576:A:LEU:HB3	3	0.97

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1968)	1:579:A:ASP:HB3	1:576:A:LEU:HB3	14	0.97
(1,1885)	1:624:A:ARG:HG2	1:628:A:LEU:HD11	8	0.97
(1,1871)	1:594:A:ALA:HB3	1:595:A:SER:HB2	2	0.97
(1,1761)	1:621:A:ALA:HB2	1:624:A:ARG:HG2	6	0.97
(1,1760)	1:594:A:ALA:HB3	1:595:A:SER:HB2	2	0.97
(1,1743)	1:628:A:LEU:HD22	1:625:A:TRP:HA	1	0.97
(1,1684)	1:625:A:TRP:HE3	1:573:A:LEU:HD23	8	0.97
(1,1681)	1:622:A:PHE:HE1	1:577:A:LEU:HD23	10	0.97
(1,1681)	1:622:A:PHE:HD1	1:577:A:LEU:HD21	18	0.97
(1,1583)	1:611:A:MET:H	1:609:A:ALA:HB1	2	0.97
(1,1583)	1:611:A:MET:H	1:609:A:ALA:HB2	9	0.97
(1,1495)	1:584:A:LEU:H	1:584:A:LEU:HD12	12	0.97
(1,1467)	1:593:A:ASP:H	1:591:A:VAL:HG13	6	0.97
(1,1288)	1:566:A:LEU:HD22	1:562:A:LEU:HD21	11	0.97
(1,1271)	1:576:A:LEU:HD11	1:621:A:ALA:HB2	8	0.97
(1,1271)	1:576:A:LEU:HD11	1:621:A:ALA:HB2	13	0.97
(1,1271)	1:576:A:LEU:HD13	1:621:A:ALA:HB2	17	0.97
(1,1250)	1:626:A:GLU:HG2	1:623:A:GLU:HA	3	0.97
(1,1067)	1:579:A:ASP:HB2	1:580:A:LEU:HD23	11	0.97
(1,964)	1:590:A:GLN:HB3	1:607:A:VAL:HG13	3	0.97
(1,964)	1:590:A:GLN:HB3	1:607:A:VAL:HG13	9	0.97
(1,695)	1:586:A:ALA:HB1	1:583:A:LYS:HB2	8	0.97
(1,672)	1:607:A:VAL:HG22	1:606:A:LYS:HE3	11	0.97
(1,649)	1:591:A:VAL:HG11	1:596:A:PHE:HB2	2	0.97
(1,637)	1:604:A:THR:HG22	1:607:A:VAL:HG21	14	0.97
(1,2161)	1:628:A:LEU:HA	1:630:A:ALA:HB1	16	0.96
(1,2123)	1:573:A:LEU:HD12	1:624:A:ARG:HB2	10	0.96
(1,2104)	1:566:A:LEU:HD21	1:562:A:LEU:HB3	10	0.96
(1,2104)	1:566:A:LEU:HD21	1:562:A:LEU:HB2	11	0.96
(1,1991)	1:562:A:LEU:HB3	1:566:A:LEU:HD11	19	0.96
(1,1968)	1:579:A:ASP:HB3	1:576:A:LEU:HB3	5	0.96
(1,1902)	1:567:A:GLN:HB2	1:562:A:LEU:HG	19	0.96
(1,1888)	1:568:A:ARG:HG2	1:569:A:GLU:HB3	15	0.96
(1,1871)	1:594:A:ALA:HB3	1:595:A:SER:HB2	14	0.96
(1,1856)	1:580:A:LEU:HA	1:583:A:LYS:HE2	9	0.96
(1,1856)	1:580:A:LEU:HA	1:579:A:ASP:HB2	19	0.96
(1,1760)	1:594:A:ALA:HB3	1:595:A:SER:HB2	14	0.96
(1,1743)	1:628:A:LEU:HD21	1:625:A:TRP:HA	17	0.96
(1,1665)	1:632:A:LYS:H	1:570:A:LEU:HD13	14	0.96
(1,1495)	1:584:A:LEU:H	1:584:A:LEU:HD13	2	0.96
(1,1495)	1:584:A:LEU:H	1:584:A:LEU:HD11	4	0.96
(1,1495)	1:584:A:LEU:H	1:584:A:LEU:HD12	5	0.96

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1392)	1:621:A:ALA:HB1	1:625:A:TRP:HB3	4	0.96
(1,1392)	1:621:A:ALA:HB2	1:625:A:TRP:HB3	5	0.96
(1,1381)	1:573:A:LEU:HD12	1:624:A:ARG:HB2	10	0.96
(1,1252)	1:580:A:LEU:HA	1:579:A:ASP:HB2	19	0.96
(1,1067)	1:579:A:ASP:HB2	1:580:A:LEU:HD22	15	0.96
(1,1024)	1:590:A:GLN:HG3	1:589:A:THR:HG23	3	0.96
(1,1015)	1:609:A:ALA:HB1	1:605:A:GLN:HG3	4	0.96
(1,1015)	1:609:A:ALA:HB3	1:605:A:GLN:HG3	10	0.96
(1,695)	1:586:A:ALA:HB1	1:583:A:LYS:HB2	15	0.96
(1,670)	1:591:A:VAL:HG21	1:607:A:VAL:HG21	17	0.96
(1,2161)	1:628:A:LEU:HA	1:630:A:ALA:HB2	2	0.95
(1,2161)	1:628:A:LEU:HA	1:630:A:ALA:HB3	11	0.95
(1,2161)	1:628:A:LEU:HA	1:630:A:ALA:HB2	15	0.95
(1,2161)	1:628:A:LEU:HA	1:630:A:ALA:HB2	17	0.95
(1,2037)	1:609:A:ALA:HA	1:605:A:GLN:HB2	13	0.95
(1,2037)	1:603:A:GLN:HA	1:605:A:GLN:HB2	17	0.95
(1,1947)	1:581:A:GLU:HG2	1:584:A:LEU:HD12	4	0.95
(1,1930)	1:556:A:LYS:HB3	1:555:A:VAL:HB	9	0.95
(1,1912)	1:585:A:GLU:HB2	1:582:A:ALA:HB1	4	0.95
(1,1743)	1:628:A:LEU:HD23	1:625:A:TRP:HA	18	0.95
(1,1722)	1:591:A:VAL:HG13	1:611:A:MET:HB2	1	0.95
(1,1619)	1:618:A:LEU:H	1:618:A:LEU:HD21	14	0.95
(1,1489)	1:586:A:ALA:H	1:584:A:LEU:HD22	6	0.95
(1,1489)	1:586:A:ALA:H	1:584:A:LEU:HD23	8	0.95
(1,1392)	1:621:A:ALA:HB3	1:625:A:TRP:HB3	7	0.95
(1,1294)	1:573:A:LEU:HD13	1:628:A:LEU:HD13	10	0.95
(1,1293)	1:577:A:LEU:HD11	1:573:A:LEU:HD13	7	0.95
(1,1293)	1:577:A:LEU:HD13	1:573:A:LEU:HD11	11	0.95
(1,1252)	1:580:A:LEU:HA	1:579:A:ASP:HB2	13	0.95
(1,1067)	1:579:A:ASP:HB2	1:580:A:LEU:HD22	12	0.95
(1,1053)	1:577:A:LEU:HD12	1:617:A:GLU:HG3	9	0.95
(1,1015)	1:609:A:ALA:HB2	1:605:A:GLN:HG3	13	0.95
(1,1015)	1:609:A:ALA:HB1	1:605:A:GLN:HG3	16	0.95
(1,1011)	1:567:A:GLN:HG2	1:562:A:LEU:HD13	14	0.95
(1,975)	1:615:A:GLU:HB2	1:584:A:LEU:HD12	6	0.95
(1,975)	1:615:A:GLU:HB2	1:584:A:LEU:HD11	17	0.95
(1,796)	1:577:A:LEU:HA	1:618:A:LEU:HD23	18	0.95
(1,695)	1:586:A:ALA:HB2	1:583:A:LYS:HB2	19	0.95
(1,670)	1:591:A:VAL:HG23	1:607:A:VAL:HG22	1	0.95
(1,649)	1:591:A:VAL:HG11	1:596:A:PHE:HB2	12	0.95
(1,644)	1:591:A:VAL:HG13	1:607:A:VAL:HG11	2	0.95
(1,644)	1:591:A:VAL:HG11	1:607:A:VAL:HG11	4	0.95

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,637)	1:604:A:THR:HG21	1:607:A:VAL:HG22	12	0.95
(1,2172)	1:625:A:TRP:HE3	1:573:A:LEU:HD21	9	0.94
(1,2161)	1:628:A:LEU:HA	1:630:A:ALA:HB1	6	0.94
(1,2119)	1:569:A:GLU:HB3	1:566:A:LEU:HD12	10	0.94
(1,2078)	1:562:A:LEU:HB3	1:566:A:LEU:HD13	4	0.94
(1,1991)	1:562:A:LEU:HB3	1:566:A:LEU:HD13	4	0.94
(1,1968)	1:579:A:ASP:HB3	1:583:A:LYS:HD2	2	0.94
(1,1947)	1:581:A:GLU:HG2	1:584:A:LEU:HD13	8	0.94
(1,1902)	1:567:A:GLN:HB2	1:562:A:LEU:HB3	1	0.94
(1,1898)	1:628:A:LEU:HG	1:631:A:LEU:HB2	20	0.94
(1,1761)	1:621:A:ALA:HB1	1:624:A:ARG:HG2	11	0.94
(1,1743)	1:628:A:LEU:HD23	1:625:A:TRP:HA	15	0.94
(1,1733)	1:607:A:VAL:HG23	1:610:A:ASP:HB3	3	0.94
(1,1630)	1:621:A:ALA:H	1:576:A:LEU:HD23	12	0.94
(1,1619)	1:618:A:LEU:H	1:618:A:LEU:HD12	2	0.94
(1,1545)	1:569:A:GLU:H	1:628:A:LEU:HD12	10	0.94
(1,1495)	1:584:A:LEU:H	1:584:A:LEU:HD13	1	0.94
(1,1495)	1:584:A:LEU:H	1:584:A:LEU:HD13	13	0.94
(1,1489)	1:586:A:ALA:H	1:584:A:LEU:HD23	11	0.94
(1,1484)	1:587:A:LEU:H	1:588:A:GLN:HG2	7	0.94
(1,1392)	1:621:A:ALA:HB1	1:625:A:TRP:HB3	11	0.94
(1,1392)	1:621:A:ALA:HB2	1:625:A:TRP:HB3	16	0.94
(1,1293)	1:577:A:LEU:HD12	1:573:A:LEU:HD13	20	0.94
(1,1067)	1:579:A:ASP:HB2	1:580:A:LEU:HD22	3	0.94
(1,1067)	1:579:A:ASP:HB2	1:580:A:LEU:HD22	16	0.94
(1,1053)	1:577:A:LEU:HD13	1:617:A:GLU:HG3	4	0.94
(1,964)	1:590:A:GLN:HB3	1:607:A:VAL:HG12	10	0.94
(1,43)	1:597:A:PHE:H	1:596:A:PHE:HB2	4	0.94
(1,43)	1:597:A:PHE:H	1:596:A:PHE:HB2	6	0.94
(1,43)	1:597:A:PHE:H	1:596:A:PHE:HB2	19	0.94
(1,35)	1:598:A:SER:H	1:599:A:GLN:HB3	15	0.94
(1,33)	1:598:A:SER:H	1:599:A:GLN:HG2	20	0.94
(1,2172)	1:625:A:TRP:HE3	1:573:A:LEU:HD22	2	0.93
(1,2172)	1:625:A:TRP:HE3	1:573:A:LEU:HD21	15	0.93
(1,2166)	1:561:A:LYS:HG3	1:562:A:LEU:HD23	18	0.93
(1,2124)	1:612:A:ALA:HA	1:611:A:MET:HE1	13	0.93
(1,2118)	1:583:A:LYS:HE2	1:580:A:LEU:HD22	20	0.93
(1,1968)	1:579:A:ASP:HB3	1:583:A:LYS:HD2	11	0.93
(1,1962)	1:610:A:ASP:HB3	1:609:A:ALA:HB2	7	0.93
(1,1947)	1:581:A:GLU:HG2	1:584:A:LEU:HD12	11	0.93
(1,1898)	1:628:A:LEU:HG	1:631:A:LEU:HB2	11	0.93
(1,1888)	1:568:A:ARG:HG2	1:569:A:GLU:HB3	17	0.93

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1888)	1:568:A:ARG:HG3	1:571:A:GLU:HB3	18	0.93
(1,1722)	1:591:A:VAL:HG11	1:611:A:MET:HB2	20	0.93
(1,1720)	1:604:A:THR:HG22	1:597:A:PHE:HB2	20	0.93
(1,1713)	1:577:A:LEU:HD12	1:581:A:GLU:HB2	17	0.93
(1,1681)	1:625:A:TRP:HE3	1:577:A:LEU:HD21	4	0.93
(1,1681)	1:625:A:TRP:HE3	1:577:A:LEU:HD23	13	0.93
(1,1681)	1:622:A:PHE:HD1	1:577:A:LEU:HD21	17	0.93
(1,1630)	1:621:A:ALA:H	1:576:A:LEU:HD22	15	0.93
(1,1590)	1:583:A:LYS:H	1:618:A:LEU:HD23	14	0.93
(1,1495)	1:584:A:LEU:H	1:584:A:LEU:HD11	3	0.93
(1,1495)	1:584:A:LEU:H	1:584:A:LEU:HD12	10	0.93
(1,1495)	1:584:A:LEU:H	1:584:A:LEU:HD12	17	0.93
(1,1495)	1:584:A:LEU:H	1:584:A:LEU:HD13	19	0.93
(1,1495)	1:584:A:LEU:H	1:584:A:LEU:HD13	20	0.93
(1,1489)	1:586:A:ALA:H	1:584:A:LEU:HD23	2	0.93
(1,1489)	1:586:A:ALA:H	1:584:A:LEU:HD22	17	0.93
(1,1467)	1:593:A:ASP:H	1:591:A:VAL:HG13	11	0.93
(1,1280)	1:573:A:LEU:HD23	1:580:A:LEU:HD13	16	0.93
(1,1067)	1:579:A:ASP:HB2	1:580:A:LEU:HD22	14	0.93
(1,1053)	1:577:A:LEU:HD11	1:617:A:GLU:HG3	12	0.93
(1,1015)	1:609:A:ALA:HB1	1:605:A:GLN:HG3	8	0.93
(1,695)	1:586:A:ALA:HB3	1:583:A:LYS:HB2	1	0.93
(1,695)	1:586:A:ALA:HB2	1:583:A:LYS:HB2	9	0.93
(1,649)	1:591:A:VAL:HG11	1:596:A:PHE:HB2	16	0.93
(1,43)	1:597:A:PHE:H	1:596:A:PHE:HB2	20	0.93
(1,2172)	1:625:A:TRP:HE3	1:573:A:LEU:HD23	19	0.92
(1,2161)	1:628:A:LEU:HA	1:630:A:ALA:HB2	19	0.92
(1,2149)	1:628:A:LEU:HD21	1:631:A:LEU:HD11	5	0.92
(1,2104)	1:562:A:LEU:HG	1:566:A:LEU:HD23	5	0.92
(1,1968)	1:579:A:ASP:HB3	1:576:A:LEU:HB3	7	0.92
(1,1962)	1:610:A:ASP:HB3	1:613:A:ALA:HB2	10	0.92
(1,1930)	1:556:A:LYS:HB3	1:555:A:VAL:HB	7	0.92
(1,1900)	1:567:A:GLN:HB2	1:562:A:LEU:HD12	1	0.92
(1,1898)	1:628:A:LEU:HG	1:631:A:LEU:HB2	18	0.92
(1,1761)	1:621:A:ALA:HB1	1:580:A:LEU:HG	9	0.92
(1,1741)	1:628:A:LEU:HD22	1:624:A:ARG:HA	11	0.92
(1,1722)	1:591:A:VAL:HG12	1:611:A:MET:HB2	18	0.92
(1,1720)	1:604:A:THR:HG21	1:600:A:PRO:HD3	18	0.92
(1,1681)	1:622:A:PHE:HD1	1:577:A:LEU:HD22	9	0.92
(1,1619)	1:618:A:LEU:H	1:618:A:LEU:HD11	5	0.92
(1,1545)	1:569:A:GLU:H	1:628:A:LEU:HD13	2	0.92
(1,1545)	1:569:A:GLU:H	1:628:A:LEU:HD13	15	0.92

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1489)	1:586:A:ALA:H	1:584:A:LEU:HD23	15	0.92
(1,1489)	1:586:A:ALA:H	1:584:A:LEU:HD23	19	0.92
(1,1293)	1:577:A:LEU:HD11	1:573:A:LEU:HD12	2	0.92
(1,1291)	1:608:A:LEU:HD11	1:604:A:THR:HG21	10	0.92
(1,1067)	1:579:A:ASP:HB2	1:580:A:LEU:HD21	4	0.92
(1,1053)	1:577:A:LEU:HD13	1:617:A:GLU:HG3	5	0.92
(1,975)	1:615:A:GLU:HB2	1:584:A:LEU:HD11	8	0.92
(1,964)	1:590:A:GLN:HB3	1:607:A:VAL:HG12	20	0.92
(1,695)	1:586:A:ALA:HB1	1:583:A:LYS:HB2	3	0.92
(1,695)	1:586:A:ALA:HB3	1:583:A:LYS:HB2	4	0.92
(1,695)	1:586:A:ALA:HB3	1:583:A:LYS:HB2	18	0.92
(1,644)	1:591:A:VAL:HG12	1:607:A:VAL:HG11	19	0.92
(1,125)	1:589:A:THR:H	1:586:A:ALA:HB2	1	0.92
(1,33)	1:598:A:SER:H	1:599:A:GLN:HG2	10	0.92
(1,2172)	1:625:A:TRP:HE3	1:573:A:LEU:HD21	3	0.91
(1,2172)	1:625:A:TRP:HE3	1:573:A:LEU:HD22	7	0.91
(1,2172)	1:625:A:TRP:HE3	1:573:A:LEU:HD21	14	0.91
(1,2161)	1:628:A:LEU:HA	1:630:A:ALA:HB1	7	0.91
(1,2155)	1:628:A:LEU:HD13	1:624:A:ARG:HB2	20	0.91
(1,2118)	1:583:A:LYS:HE2	1:580:A:LEU:HD23	17	0.91
(1,2118)	1:579:A:ASP:HB2	1:580:A:LEU:HD22	18	0.91
(1,2105)	1:566:A:LEU:HD21	1:628:A:LEU:HG	16	0.91
(1,1962)	1:610:A:ASP:HB3	1:613:A:ALA:HB3	4	0.91
(1,1871)	1:594:A:ALA:HB1	1:595:A:SER:HB2	3	0.91
(1,1760)	1:594:A:ALA:HB1	1:595:A:SER:HB2	3	0.91
(1,1733)	1:607:A:VAL:HG22	1:610:A:ASP:HB3	11	0.91
(1,1713)	1:577:A:LEU:HD12	1:581:A:GLU:HB2	13	0.91
(1,1681)	1:622:A:PHE:HE1	1:577:A:LEU:HD22	6	0.91
(1,1630)	1:621:A:ALA:H	1:576:A:LEU:HD23	7	0.91
(1,1619)	1:618:A:LEU:H	1:618:A:LEU:HD12	19	0.91
(1,1592)	1:613:A:ALA:H	1:615:A:GLU:HG3	17	0.91
(1,1592)	1:583:A:LYS:H	1:581:A:GLU:HB2	19	0.91
(1,1495)	1:584:A:LEU:H	1:584:A:LEU:HD13	16	0.91
(1,1293)	1:577:A:LEU:HD12	1:573:A:LEU:HD12	12	0.91
(1,1271)	1:576:A:LEU:HD13	1:621:A:ALA:HB3	4	0.91
(1,1067)	1:579:A:ASP:HB2	1:580:A:LEU:HD23	7	0.91
(1,1067)	1:579:A:ASP:HB2	1:580:A:LEU:HD22	8	0.91
(1,1067)	1:579:A:ASP:HB2	1:580:A:LEU:HD22	17	0.91
(1,1067)	1:579:A:ASP:HB2	1:580:A:LEU:HD22	18	0.91
(1,1053)	1:577:A:LEU:HD13	1:617:A:GLU:HG3	3	0.91
(1,975)	1:615:A:GLU:HB2	1:584:A:LEU:HD13	11	0.91
(1,695)	1:586:A:ALA:HB1	1:583:A:LYS:HB2	12	0.91

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,644)	1:591:A:VAL:HG11	1:607:A:VAL:HG13	6	0.91
(1,125)	1:589:A:THR:H	1:586:A:ALA:HB1	9	0.91
(1,125)	1:589:A:THR:H	1:586:A:ALA:HB1	14	0.91
(1,43)	1:597:A:PHE:H	1:596:A:PHE:HB2	3	0.91
(1,43)	1:597:A:PHE:H	1:596:A:PHE:HB2	18	0.91
(1,2172)	1:625:A:TRP:HE3	1:573:A:LEU:HD23	18	0.9
(1,2118)	1:583:A:LYS:HE3	1:580:A:LEU:HD23	11	0.9
(1,2105)	1:566:A:LEU:HD23	1:628:A:LEU:HG	1	0.9
(1,2056)	1:572:A:GLN:HG3	1:569:A:GLU:HA	1	0.9
(1,2037)	1:609:A:ALA:HA	1:605:A:GLN:HB3	1	0.9
(1,1995)	1:557:A:ARG:HD2	1:555:A:VAL:HG12	15	0.9
(1,1956)	1:627:A:TYR:HB3	1:630:A:ALA:HB2	19	0.9
(1,1947)	1:581:A:GLU:HG2	1:584:A:LEU:HD13	10	0.9
(1,1917)	1:585:A:GLU:HB2	1:584:A:LEU:HD12	5	0.9
(1,1917)	1:585:A:GLU:HB2	1:584:A:LEU:HD11	9	0.9
(1,1888)	1:568:A:ARG:HG2	1:569:A:GLU:HB3	2	0.9
(1,1871)	1:594:A:ALA:HB3	1:595:A:SER:HB2	18	0.9
(1,1871)	1:594:A:ALA:HB3	1:595:A:SER:HB2	20	0.9
(1,1812)	1:632:A:LYS:HA	1:631:A:LEU:HD23	18	0.9
(1,1807)	1:587:A:LEU:HA	1:590:A:GLN:HB2	2	0.9
(1,1760)	1:594:A:ALA:HB3	1:595:A:SER:HB2	18	0.9
(1,1760)	1:594:A:ALA:HB3	1:595:A:SER:HB2	20	0.9
(1,1733)	1:607:A:VAL:HG23	1:610:A:ASP:HB3	20	0.9
(1,1681)	1:622:A:PHE:HD1	1:577:A:LEU:HD22	19	0.9
(1,1612)	1:616:A:GLN:H	1:618:A:LEU:HD21	20	0.9
(1,1538)	1:571:A:GLU:H	1:628:A:LEU:HD11	14	0.9
(1,1280)	1:573:A:LEU:HD21	1:580:A:LEU:HD12	6	0.9
(1,1053)	1:577:A:LEU:HD11	1:617:A:GLU:HG3	8	0.9
(1,1015)	1:609:A:ALA:HB3	1:605:A:GLN:HG3	18	0.9
(1,695)	1:586:A:ALA:HB2	1:583:A:LYS:HB2	2	0.9
(1,695)	1:586:A:ALA:HB3	1:583:A:LYS:HB2	20	0.9
(1,125)	1:589:A:THR:H	1:586:A:ALA:HB3	16	0.9
(1,43)	1:597:A:PHE:H	1:596:A:PHE:HB2	2	0.9
(1,43)	1:597:A:PHE:H	1:596:A:PHE:HB2	12	0.9
(1,43)	1:597:A:PHE:H	1:596:A:PHE:HB2	17	0.9
(1,35)	1:598:A:SER:H	1:599:A:GLN:HB3	7	0.9
(1,2163)	1:567:A:GLN:HA	1:570:A:LEU:HD11	7	0.89
(1,2155)	1:628:A:LEU:HD13	1:624:A:ARG:HB2	18	0.89
(1,2135)	1:567:A:GLN:HA	1:570:A:LEU:HD11	7	0.89
(1,2120)	1:573:A:LEU:HD23	1:624:A:ARG:HB2	6	0.89
(1,2118)	1:583:A:LYS:HE2	1:580:A:LEU:HD23	8	0.89
(1,2029)	1:568:A:ARG:HD3	1:565:A:LYS:HA	5	0.89

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2029)	1:568:A:ARG:HD3	1:565:A:LYS:HA	10	0.89
(1,1962)	1:610:A:ASP:HB3	1:613:A:ALA:HB3	18	0.89
(1,1913)	1:585:A:GLU:HB3	1:586:A:ALA:HB2	12	0.89
(1,1898)	1:628:A:LEU:HG	1:631:A:LEU:HB2	13	0.89
(1,1856)	1:580:A:LEU:HA	1:583:A:LYS:HE2	13	0.89
(1,1850)	1:589:A:THR:HA	1:590:A:GLN:HB2	11	0.89
(1,1761)	1:621:A:ALA:HB2	1:624:A:ARG:HG2	2	0.89
(1,1733)	1:607:A:VAL:HG22	1:610:A:ASP:HB3	2	0.89
(1,1733)	1:607:A:VAL:HG21	1:610:A:ASP:HB3	6	0.89
(1,1729)	1:631:A:LEU:HD23	1:561:A:LYS:HA	12	0.89
(1,1619)	1:618:A:LEU:H	1:618:A:LEU:HD11	4	0.89
(1,1619)	1:618:A:LEU:H	1:618:A:LEU:HD13	16	0.89
(1,1619)	1:618:A:LEU:H	1:618:A:LEU:HD12	17	0.89
(1,1619)	1:618:A:LEU:H	1:618:A:LEU:HD12	18	0.89
(1,1545)	1:569:A:GLU:H	1:628:A:LEU:HD11	11	0.89
(1,1495)	1:584:A:LEU:H	1:584:A:LEU:HD12	7	0.89
(1,1489)	1:586:A:ALA:H	1:584:A:LEU:HD21	3	0.89
(1,1489)	1:586:A:ALA:H	1:584:A:LEU:HD22	14	0.89
(1,1293)	1:577:A:LEU:HD11	1:573:A:LEU:HD13	5	0.89
(1,1291)	1:608:A:LEU:HD12	1:604:A:THR:HG21	1	0.89
(1,1288)	1:566:A:LEU:HD22	1:562:A:LEU:HD23	14	0.89
(1,1280)	1:573:A:LEU:HD23	1:580:A:LEU:HD12	5	0.89
(1,1111)	1:631:A:LEU:HD23	1:562:A:LEU:HB3	1	0.89
(1,1095)	1:565:A:LYS:HE2	1:566:A:LEU:HD13	8	0.89
(1,1053)	1:577:A:LEU:HD11	1:617:A:GLU:HG3	14	0.89
(1,644)	1:591:A:VAL:HG13	1:607:A:VAL:HG11	16	0.89
(1,317)	1:563:A:SER:H	1:566:A:LEU:HD21	15	0.89
(1,149)	1:586:A:ALA:H	1:589:A:THR:HG23	5	0.89
(1,125)	1:589:A:THR:H	1:586:A:ALA:HB1	2	0.89
(1,125)	1:589:A:THR:H	1:586:A:ALA:HB2	20	0.89
(1,43)	1:597:A:PHE:H	1:596:A:PHE:HB2	1	0.89
(1,43)	1:597:A:PHE:H	1:596:A:PHE:HB2	5	0.89
(1,43)	1:597:A:PHE:H	1:596:A:PHE:HB2	11	0.89
(1,33)	1:598:A:SER:H	1:599:A:GLN:HG2	7	0.89
(1,2172)	1:625:A:TRP:HE3	1:573:A:LEU:HD21	13	0.88
(1,2172)	1:625:A:TRP:HE3	1:573:A:LEU:HD21	17	0.88
(1,2163)	1:567:A:GLN:HA	1:570:A:LEU:HD12	15	0.88
(1,2158)	1:591:A:VAL:HG21	1:596:A:PHE:HB2	4	0.88
(1,2158)	1:591:A:VAL:HG23	1:596:A:PHE:HB2	7	0.88
(1,2135)	1:567:A:GLN:HA	1:570:A:LEU:HD12	15	0.88
(1,2119)	1:569:A:GLU:HB3	1:566:A:LEU:HD11	3	0.88
(1,2119)	1:569:A:GLU:HB3	1:566:A:LEU:HD12	5	0.88

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2037)	1:609:A:ALA:HA	1:605:A:GLN:HB3	8	0.88
(1,1966)	1:579:A:ASP:HB2	1:576:A:LEU:HB3	1	0.88
(1,1962)	1:610:A:ASP:HB3	1:609:A:ALA:HB1	13	0.88
(1,1958)	1:622:A:PHE:HB3	1:619:A:GLU:HB2	13	0.88
(1,1917)	1:585:A:GLU:HB2	1:584:A:LEU:HD12	12	0.88
(1,1888)	1:568:A:ARG:HG3	1:571:A:GLU:HB3	10	0.88
(1,1871)	1:594:A:ALA:HB1	1:595:A:SER:HB2	11	0.88
(1,1760)	1:594:A:ALA:HB1	1:595:A:SER:HB2	11	0.88
(1,1722)	1:591:A:VAL:HG13	1:611:A:MET:HB2	3	0.88
(1,1705)	1:622:A:PHE:HD1	1:577:A:LEU:HD21	16	0.88
(1,1681)	1:622:A:PHE:HD1	1:577:A:LEU:HD21	20	0.88
(1,1619)	1:618:A:LEU:H	1:618:A:LEU:HD11	9	0.88
(1,1619)	1:618:A:LEU:H	1:618:A:LEU:HD12	11	0.88
(1,1619)	1:618:A:LEU:H	1:618:A:LEU:HD13	13	0.88
(1,1619)	1:618:A:LEU:H	1:618:A:LEU:HD13	15	0.88
(1,1592)	1:613:A:ALA:H	1:616:A:GLN:HB2	1	0.88
(1,1538)	1:571:A:GLU:H	1:628:A:LEU:HD11	20	0.88
(1,1489)	1:586:A:ALA:H	1:584:A:LEU:HD21	12	0.88
(1,1489)	1:586:A:ALA:H	1:584:A:LEU:HD21	18	0.88
(1,1489)	1:586:A:ALA:H	1:584:A:LEU:HD21	20	0.88
(1,1466)	1:606:A:LYS:H	1:609:A:ALA:HB1	20	0.88
(1,1449)	1:603:A:GLN:H	1:605:A:GLN:HB2	4	0.88
(1,1366)	1:566:A:LEU:HD23	1:631:A:LEU:HD11	16	0.88
(1,1293)	1:577:A:LEU:HD13	1:573:A:LEU:HD13	17	0.88
(1,1291)	1:608:A:LEU:HD13	1:604:A:THR:HG22	4	0.88
(1,1280)	1:573:A:LEU:HD22	1:580:A:LEU:HD12	19	0.88
(1,1271)	1:576:A:LEU:HD13	1:621:A:ALA:HB1	2	0.88
(1,1163)	1:599:A:GLN:HG3	1:600:A:PRO:HD3	15	0.88
(1,1053)	1:577:A:LEU:HD12	1:617:A:GLU:HG3	1	0.88
(1,929)	1:565:A:LYS:HG2	1:566:A:LEU:HD12	11	0.88
(1,838)	1:623:A:GLU:HA	1:626:A:GLU:HB3	10	0.88
(1,695)	1:586:A:ALA:HB1	1:583:A:LYS:HB2	17	0.88
(1,670)	1:591:A:VAL:HG21	1:607:A:VAL:HG22	4	0.88
(1,670)	1:591:A:VAL:HG23	1:607:A:VAL:HG23	7	0.88
(1,649)	1:591:A:VAL:HG11	1:596:A:PHE:HB2	9	0.88
(1,644)	1:591:A:VAL:HG13	1:607:A:VAL:HG11	5	0.88
(1,579)	1:627:A:TYR:HD2	1:624:A:ARG:HD3	3	0.88
(1,2172)	1:625:A:TRP:HE3	1:573:A:LEU:HD21	12	0.87
(1,2161)	1:628:A:LEU:HA	1:630:A:ALA:HB2	10	0.87
(1,2121)	1:581:A:GLU:HG2	1:618:A:LEU:HD22	14	0.87
(1,1792)	1:610:A:ASP:HA	1:587:A:LEU:HD23	17	0.87
(1,1761)	1:621:A:ALA:HB3	1:624:A:ARG:HG2	7	0.87

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1761)	1:621:A:ALA:HB1	1:580:A:LEU:HG	14	0.87
(1,1761)	1:621:A:ALA:HB2	1:624:A:ARG:HG2	16	0.87
(1,1722)	1:591:A:VAL:HG13	1:611:A:MET:HB2	12	0.87
(1,1722)	1:591:A:VAL:HG11	1:611:A:MET:HB2	15	0.87
(1,1720)	1:604:A:THR:HG22	1:597:A:PHE:HB2	2	0.87
(1,1720)	1:604:A:THR:HG22	1:597:A:PHE:HB2	12	0.87
(1,1619)	1:618:A:LEU:H	1:618:A:LEU:HD12	8	0.87
(1,1592)	1:583:A:LYS:H	1:581:A:GLU:HB2	4	0.87
(1,1592)	1:583:A:LYS:H	1:581:A:GLU:HB2	10	0.87
(1,1545)	1:569:A:GLU:H	1:628:A:LEU:HD12	1	0.87
(1,1366)	1:566:A:LEU:HD22	1:631:A:LEU:HD12	9	0.87
(1,1293)	1:577:A:LEU:HD11	1:573:A:LEU:HD13	19	0.87
(1,1291)	1:608:A:LEU:HD13	1:604:A:THR:HG21	13	0.87
(1,975)	1:615:A:GLU:HB2	1:584:A:LEU:HD11	18	0.87
(1,929)	1:565:A:LYS:HG2	1:566:A:LEU:HD11	5	0.87
(1,695)	1:586:A:ALA:HB1	1:583:A:LYS:HB2	13	0.87
(1,125)	1:589:A:THR:H	1:586:A:ALA:HB2	6	0.87
(1,43)	1:597:A:PHE:H	1:596:A:PHE:HB2	15	0.87
(1,35)	1:598:A:SER:H	1:599:A:GLN:HB3	5	0.87
(1,1966)	1:579:A:ASP:HB2	1:576:A:LEU:HB3	6	0.86
(1,1966)	1:579:A:ASP:HB2	1:576:A:LEU:HB3	15	0.86
(1,1958)	1:622:A:PHE:HB3	1:623:A:GLU:HB2	6	0.86
(1,1913)	1:585:A:GLU:HB3	1:586:A:ALA:HB3	10	0.86
(1,1902)	1:567:A:GLN:HB2	1:562:A:LEU:HG	5	0.86
(1,1871)	1:594:A:ALA:HB3	1:595:A:SER:HB2	9	0.86
(1,1871)	1:594:A:ALA:HB3	1:595:A:SER:HB2	15	0.86
(1,1761)	1:621:A:ALA:HB2	1:624:A:ARG:HG2	10	0.86
(1,1760)	1:594:A:ALA:HB3	1:595:A:SER:HB2	9	0.86
(1,1760)	1:594:A:ALA:HB3	1:595:A:SER:HB2	15	0.86
(1,1733)	1:607:A:VAL:HG21	1:610:A:ASP:HB3	13	0.86
(1,1733)	1:607:A:VAL:HG22	1:610:A:ASP:HB3	15	0.86
(1,1733)	1:607:A:VAL:HG23	1:610:A:ASP:HB3	17	0.86
(1,1729)	1:631:A:LEU:HD23	1:563:A:SER:HB2	2	0.86
(1,1722)	1:591:A:VAL:HG13	1:611:A:MET:HB2	7	0.86
(1,1720)	1:604:A:THR:HG21	1:597:A:PHE:HB2	6	0.86
(1,1720)	1:604:A:THR:HG21	1:597:A:PHE:HB2	15	0.86
(1,1715)	1:577:A:LEU:HD13	1:617:A:GLU:HG2	19	0.86
(1,1681)	1:625:A:TRP:HE3	1:577:A:LEU:HD21	7	0.86
(1,1619)	1:618:A:LEU:H	1:618:A:LEU:HD11	6	0.86
(1,1619)	1:618:A:LEU:H	1:618:A:LEU:HD13	10	0.86
(1,1592)	1:583:A:LYS:H	1:581:A:GLU:HB2	11	0.86
(1,1506)	1:582:A:ALA:H	1:618:A:LEU:HD11	2	0.86

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1306)	1:589:A:THR:HG22	1:590:A:GLN:HB2	5	0.86
(1,1271)	1:576:A:LEU:HD13	1:621:A:ALA:HB2	9	0.86
(1,1067)	1:579:A:ASP:HB2	1:580:A:LEU:HD23	1	0.86
(1,1053)	1:577:A:LEU:HD13	1:617:A:GLU:HG3	18	0.86
(1,989)	1:611:A:MET:HG2	1:587:A:LEU:HD11	7	0.86
(1,964)	1:590:A:GLN:HB3	1:607:A:VAL:HG12	2	0.86
(1,149)	1:586:A:ALA:H	1:589:A:THR:HG23	15	0.86
(1,43)	1:597:A:PHE:H	1:596:A:PHE:HB2	10	0.86
(1,43)	1:597:A:PHE:H	1:596:A:PHE:HB2	16	0.86
(1,2166)	1:562:A:LEU:HD13	1:561:A:LYS:HG3	10	0.85
(1,2155)	1:628:A:LEU:HD12	1:624:A:ARG:HB2	13	0.85
(1,2125)	1:607:A:VAL:HG13	1:590:A:GLN:HA	14	0.85
(1,2118)	1:583:A:LYS:HE2	1:580:A:LEU:HD22	3	0.85
(1,1968)	1:579:A:ASP:HB3	1:576:A:LEU:HB3	4	0.85
(1,1966)	1:579:A:ASP:HB2	1:576:A:LEU:HB3	18	0.85
(1,1947)	1:581:A:GLU:HG2	1:584:A:LEU:HD12	3	0.85
(1,1792)	1:610:A:ASP:HA	1:587:A:LEU:HD22	16	0.85
(1,1761)	1:621:A:ALA:HB1	1:580:A:LEU:HG	15	0.85
(1,1743)	1:628:A:LEU:HD22	1:625:A:TRP:HA	7	0.85
(1,1729)	1:631:A:LEU:HD23	1:561:A:LYS:HA	11	0.85
(1,1729)	1:631:A:LEU:HD22	1:561:A:LYS:HA	19	0.85
(1,1720)	1:604:A:THR:HG21	1:597:A:PHE:HB2	1	0.85
(1,1720)	1:604:A:THR:HG21	1:597:A:PHE:HB2	3	0.85
(1,1720)	1:604:A:THR:HG22	1:597:A:PHE:HB2	9	0.85
(1,1720)	1:604:A:THR:HG23	1:597:A:PHE:HB2	11	0.85
(1,1715)	1:577:A:LEU:HD13	1:617:A:GLU:HG2	15	0.85
(1,1681)	1:622:A:PHE:HD1	1:577:A:LEU:HD21	12	0.85
(1,1619)	1:618:A:LEU:H	1:618:A:LEU:HD11	3	0.85
(1,1619)	1:618:A:LEU:H	1:618:A:LEU:HD11	7	0.85
(1,1619)	1:618:A:LEU:H	1:618:A:LEU:HD12	12	0.85
(1,1495)	1:584:A:LEU:H	1:584:A:LEU:HD13	15	0.85
(1,1319)	1:567:A:GLN:HA	1:562:A:LEU:HD11	19	0.85
(1,1306)	1:589:A:THR:HG22	1:590:A:GLN:HB2	3	0.85
(1,1280)	1:573:A:LEU:HD23	1:580:A:LEU:HD13	3	0.85
(1,1280)	1:573:A:LEU:HD22	1:580:A:LEU:HD11	8	0.85
(1,1271)	1:576:A:LEU:HD11	1:621:A:ALA:HB1	5	0.85
(1,1271)	1:576:A:LEU:HD13	1:621:A:ALA:HB1	18	0.85
(1,1192)	1:568:A:ARG:HD2	1:565:A:LYS:HA	20	0.85
(1,1174)	1:623:A:GLU:HG2	1:622:A:PHE:HB2	15	0.85
(1,1067)	1:579:A:ASP:HB2	1:580:A:LEU:HD22	6	0.85
(1,975)	1:615:A:GLU:HB2	1:584:A:LEU:HD11	5	0.85
(1,975)	1:615:A:GLU:HB2	1:584:A:LEU:HD12	19	0.85

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,670)	1:591:A:VAL:HG23	1:607:A:VAL:HG23	11	0.85
(1,125)	1:589:A:THR:H	1:586:A:ALA:HB3	8	0.85
(1,43)	1:597:A:PHE:H	1:596:A:PHE:HB2	14	0.85
(1,35)	1:598:A:SER:H	1:599:A:GLN:HB3	3	0.85
(1,35)	1:598:A:SER:H	1:599:A:GLN:HB3	17	0.85
(1,2158)	1:591:A:VAL:HG21	1:596:A:PHE:HB2	17	0.84
(1,2155)	1:628:A:LEU:HD11	1:624:A:ARG:HB2	3	0.84
(1,2118)	1:583:A:LYS:HE2	1:580:A:LEU:HD23	7	0.84
(1,1966)	1:579:A:ASP:HB2	1:576:A:LEU:HB3	4	0.84
(1,1966)	1:579:A:ASP:HB2	1:576:A:LEU:HB3	7	0.84
(1,1962)	1:610:A:ASP:HB3	1:613:A:ALA:HB2	12	0.84
(1,1792)	1:610:A:ASP:HA	1:587:A:LEU:HD21	2	0.84
(1,1792)	1:610:A:ASP:HA	1:587:A:LEU:HD23	18	0.84
(1,1792)	1:610:A:ASP:HA	1:587:A:LEU:HD21	19	0.84
(1,1792)	1:610:A:ASP:HA	1:587:A:LEU:HD23	20	0.84
(1,1729)	1:631:A:LEU:HD22	1:563:A:SER:HB2	7	0.84
(1,1722)	1:591:A:VAL:HG13	1:611:A:MET:HB2	2	0.84
(1,1720)	1:604:A:THR:HG22	1:600:A:PRO:HD3	19	0.84
(1,1684)	1:625:A:TRP:HE3	1:573:A:LEU:HD21	5	0.84
(1,1592)	1:613:A:ALA:H	1:615:A:GLU:HG3	8	0.84
(1,1535)	1:572:A:GLN:H	1:573:A:LEU:HD21	10	0.84
(1,1489)	1:586:A:ALA:H	1:584:A:LEU:HD21	7	0.84
(1,1466)	1:606:A:LYS:H	1:609:A:ALA:HB3	8	0.84
(1,1392)	1:621:A:ALA:HB3	1:625:A:TRP:HB3	15	0.84
(1,1365)	1:631:A:LEU:HD21	1:566:A:LEU:HD11	16	0.84
(1,1291)	1:608:A:LEU:HD12	1:604:A:THR:HG22	18	0.84
(1,1264)	1:568:A:ARG:HD2	1:564:A:TYR:HA	18	0.84
(1,989)	1:611:A:MET:HG2	1:587:A:LEU:HD12	9	0.84
(1,956)	1:605:A:GLN:HB3	1:608:A:LEU:HD11	3	0.84
(1,929)	1:565:A:LYS:HG2	1:566:A:LEU:HD12	15	0.84
(1,695)	1:586:A:ALA:HB3	1:583:A:LYS:HB2	6	0.84
(1,695)	1:586:A:ALA:HB2	1:583:A:LYS:HB2	14	0.84
(1,670)	1:591:A:VAL:HG21	1:607:A:VAL:HG21	14	0.84
(1,43)	1:597:A:PHE:H	1:596:A:PHE:HB2	8	0.84
(1,2172)	1:625:A:TRP:HE3	1:573:A:LEU:HD23	4	0.83
(1,2158)	1:591:A:VAL:HG23	1:596:A:PHE:HB2	11	0.83
(1,2155)	1:628:A:LEU:HD12	1:624:A:ARG:HB2	2	0.83
(1,2125)	1:607:A:VAL:HG13	1:590:A:GLN:HA	8	0.83
(1,2118)	1:583:A:LYS:HE2	1:580:A:LEU:HD21	19	0.83
(1,2114)	1:615:A:GLU:HB2	1:584:A:LEU:HD12	2	0.83
(1,2104)	1:566:A:LEU:HD22	1:562:A:LEU:HB2	2	0.83
(1,2014)	1:601:A:HIS:HB3	1:602:A:GLU:HB2	1	0.83

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1947)	1:615:A:GLU:HG2	1:584:A:LEU:HD11	5	0.83
(1,1871)	1:594:A:ALA:HB3	1:595:A:SER:HB2	17	0.83
(1,1853)	1:554:A:THR:HB	1:555:A:VAL:HG13	5	0.83
(1,1850)	1:589:A:THR:HA	1:590:A:GLN:HB2	6	0.83
(1,1792)	1:610:A:ASP:HA	1:587:A:LEU:HD21	6	0.83
(1,1760)	1:594:A:ALA:HB3	1:595:A:SER:HB2	17	0.83
(1,1690)	1:564:A:TYR:HE1	1:567:A:GLN:HB2	5	0.83
(1,1681)	1:622:A:PHE:HD1	1:577:A:LEU:HD23	1	0.83
(1,1671)	1:633:A:ASN:H	1:570:A:LEU:HD11	14	0.83
(1,1619)	1:618:A:LEU:H	1:618:A:LEU:HD11	1	0.83
(1,1619)	1:618:A:LEU:H	1:618:A:LEU:HD12	20	0.83
(1,1552)	1:567:A:GLN:H	1:568:A:ARG:HB3	16	0.83
(1,1489)	1:586:A:ALA:H	1:584:A:LEU:HD22	10	0.83
(1,1489)	1:586:A:ALA:H	1:584:A:LEU:HD23	16	0.83
(1,1331)	1:566:A:LEU:HD23	1:628:A:LEU:HA	15	0.83
(1,1291)	1:608:A:LEU:HD13	1:604:A:THR:HG21	19	0.83
(1,1280)	1:573:A:LEU:HD21	1:580:A:LEU:HD12	7	0.83
(1,1280)	1:573:A:LEU:HD23	1:580:A:LEU:HD13	9	0.83
(1,1271)	1:576:A:LEU:HD11	1:621:A:ALA:HB1	20	0.83
(1,1015)	1:609:A:ALA:HB2	1:605:A:GLN:HG3	3	0.83
(1,990)	1:591:A:VAL:HG22	1:611:A:MET:HG2	14	0.83
(1,975)	1:615:A:GLU:HB2	1:584:A:LEU:HD12	2	0.83
(1,964)	1:590:A:GLN:HB3	1:607:A:VAL:HG12	5	0.83
(1,964)	1:590:A:GLN:HB3	1:607:A:VAL:HG13	12	0.83
(1,964)	1:590:A:GLN:HB3	1:607:A:VAL:HG12	15	0.83
(1,695)	1:586:A:ALA:HB2	1:583:A:LYS:HB2	10	0.83
(1,670)	1:591:A:VAL:HG21	1:607:A:VAL:HG22	16	0.83
(1,644)	1:591:A:VAL:HG12	1:607:A:VAL:HG12	18	0.83
(1,637)	1:604:A:THR:HG22	1:607:A:VAL:HG23	7	0.83
(1,125)	1:589:A:THR:H	1:586:A:ALA:HB3	17	0.83
(1,125)	1:589:A:THR:H	1:586:A:ALA:HB1	19	0.83
(1,2172)	1:625:A:TRP:HE3	1:573:A:LEU:HD22	6	0.82
(1,2155)	1:628:A:LEU:HD11	1:624:A:ARG:HB2	12	0.82
(1,2120)	1:573:A:LEU:HD22	1:624:A:ARG:HB2	17	0.82
(1,2037)	1:609:A:ALA:HA	1:605:A:GLN:HB3	2	0.82
(1,1966)	1:579:A:ASP:HB2	1:576:A:LEU:HB3	16	0.82
(1,1962)	1:610:A:ASP:HB3	1:609:A:ALA:HB1	17	0.82
(1,1960)	1:622:A:PHE:HB3	1:623:A:GLU:HB2	18	0.82
(1,1958)	1:622:A:PHE:HB3	1:623:A:GLU:HB2	18	0.82
(1,1945)	1:585:A:GLU:HG2	1:582:A:ALA:HB2	17	0.82
(1,1856)	1:580:A:LEU:HA	1:583:A:LYS:HE3	1	0.82
(1,1850)	1:589:A:THR:HA	1:590:A:GLN:HB2	17	0.82

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1807)	1:587:A:LEU:HA	1:590:A:GLN:HB2	12	0.82
(1,1807)	1:587:A:LEU:HA	1:590:A:GLN:HB2	13	0.82
(1,1807)	1:587:A:LEU:HA	1:590:A:GLN:HB2	20	0.82
(1,1792)	1:610:A:ASP:HA	1:587:A:LEU:HD21	10	0.82
(1,1722)	1:591:A:VAL:HG13	1:611:A:MET:HB2	5	0.82
(1,1711)	1:577:A:LEU:HD23	1:624:A:ARG:HB3	11	0.82
(1,1704)	1:622:A:PHE:HD2	1:618:A:LEU:HB3	6	0.82
(1,1690)	1:564:A:TYR:HE1	1:567:A:GLN:HB2	10	0.82
(1,1681)	1:622:A:PHE:HD1	1:577:A:LEU:HD22	3	0.82
(1,1506)	1:582:A:ALA:H	1:618:A:LEU:HD11	12	0.82
(1,1326)	1:566:A:LEU:HD21	1:563:A:SER:HB3	11	0.82
(1,1293)	1:577:A:LEU:HD11	1:573:A:LEU:HD13	4	0.82
(1,1287)	1:566:A:LEU:HD22	1:631:A:LEU:HD23	2	0.82
(1,1154)	1:603:A:GLN:HG2	1:600:A:PRO:HB3	5	0.82
(1,989)	1:611:A:MET:HG2	1:587:A:LEU:HD13	17	0.82
(1,906)	1:596:A:PHE:HA	1:599:A:GLN:HG2	3	0.82
(1,695)	1:586:A:ALA:HB3	1:583:A:LYS:HB2	11	0.82
(1,644)	1:591:A:VAL:HG11	1:607:A:VAL:HG12	12	0.82
(1,2172)	1:625:A:TRP:HE3	1:573:A:LEU:HD23	11	0.81
(1,2158)	1:591:A:VAL:HG21	1:596:A:PHE:HB2	18	0.81
(1,2149)	1:631:A:LEU:HD13	1:566:A:LEU:HD12	15	0.81
(1,2118)	1:583:A:LYS:HE2	1:580:A:LEU:HD21	5	0.81
(1,2037)	1:603:A:GLN:HA	1:605:A:GLN:HB2	11	0.81
(1,2029)	1:568:A:ARG:HD3	1:565:A:LYS:HA	13	0.81
(1,1992)	1:562:A:LEU:HB2	1:632:A:LYS:HG2	15	0.81
(1,1968)	1:579:A:ASP:HB3	1:583:A:LYS:HD2	10	0.81
(1,1917)	1:585:A:GLU:HB2	1:584:A:LEU:HD12	10	0.81
(1,1898)	1:628:A:LEU:HG	1:631:A:LEU:HB2	16	0.81
(1,1792)	1:610:A:ASP:HA	1:587:A:LEU:HD21	4	0.81
(1,1792)	1:610:A:ASP:HA	1:587:A:LEU:HD23	8	0.81
(1,1761)	1:621:A:ALA:HB1	1:624:A:ARG:HG2	12	0.81
(1,1720)	1:604:A:THR:HG23	1:597:A:PHE:HB2	14	0.81
(1,1681)	1:625:A:TRP:HE3	1:577:A:LEU:HD23	8	0.81
(1,1681)	1:622:A:PHE:HD1	1:577:A:LEU:HD23	11	0.81
(1,1681)	1:625:A:TRP:HE3	1:577:A:LEU:HD23	14	0.81
(1,1592)	1:583:A:LYS:H	1:581:A:GLU:HB2	16	0.81
(1,1545)	1:569:A:GLU:H	1:628:A:LEU:HD12	5	0.81
(1,1545)	1:569:A:GLU:H	1:628:A:LEU:HD12	7	0.81
(1,1545)	1:569:A:GLU:H	1:628:A:LEU:HD11	14	0.81
(1,1545)	1:569:A:GLU:H	1:628:A:LEU:HD13	16	0.81
(1,1467)	1:593:A:ASP:H	1:591:A:VAL:HG12	14	0.81
(1,1287)	1:566:A:LEU:HD23	1:631:A:LEU:HD22	5	0.81

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1250)	1:626:A:GLU:HG2	1:623:A:GLU:HA	5	0.81
(1,989)	1:611:A:MET:HG2	1:587:A:LEU:HD12	1	0.81
(1,989)	1:611:A:MET:HG2	1:587:A:LEU:HD11	2	0.81
(1,989)	1:611:A:MET:HG2	1:587:A:LEU:HD11	4	0.81
(1,989)	1:611:A:MET:HG2	1:587:A:LEU:HD12	10	0.81
(1,989)	1:611:A:MET:HG2	1:587:A:LEU:HD13	16	0.81
(1,975)	1:615:A:GLU:HB2	1:584:A:LEU:HD13	9	0.81
(1,906)	1:596:A:PHE:HA	1:599:A:GLN:HG2	13	0.81
(1,670)	1:591:A:VAL:HG21	1:607:A:VAL:HG21	18	0.81
(1,649)	1:591:A:VAL:HG12	1:596:A:PHE:HB2	8	0.81
(1,644)	1:591:A:VAL:HG12	1:607:A:VAL:HG11	10	0.81
(1,317)	1:563:A:SER:H	1:566:A:LEU:HD23	2	0.81
(1,2163)	1:567:A:GLN:HA	1:570:A:LEU:HD12	14	0.8
(1,2158)	1:591:A:VAL:HG21	1:596:A:PHE:HB2	15	0.8
(1,2155)	1:628:A:LEU:HD11	1:624:A:ARG:HB2	6	0.8
(1,2135)	1:567:A:GLN:HA	1:570:A:LEU:HD12	14	0.8
(1,2037)	1:603:A:GLN:HA	1:605:A:GLN:HB2	20	0.8
(1,1966)	1:579:A:ASP:HB2	1:576:A:LEU:HB3	12	0.8
(1,1959)	1:622:A:PHE:HB2	1:619:A:GLU:HB2	9	0.8
(1,1871)	1:594:A:ALA:HB3	1:595:A:SER:HB2	10	0.8
(1,1792)	1:610:A:ASP:HA	1:587:A:LEU:HD22	5	0.8
(1,1792)	1:610:A:ASP:HA	1:587:A:LEU:HD21	11	0.8
(1,1792)	1:610:A:ASP:HA	1:587:A:LEU:HD22	13	0.8
(1,1760)	1:594:A:ALA:HB3	1:595:A:SER:HB2	10	0.8
(1,1720)	1:604:A:THR:HG23	1:597:A:PHE:HB2	7	0.8
(1,1711)	1:577:A:LEU:HD21	1:626:A:GLU:HG3	6	0.8
(1,1630)	1:621:A:ALA:H	1:576:A:LEU:HD22	10	0.8
(1,1552)	1:567:A:GLN:H	1:566:A:LEU:HG	3	0.8
(1,1552)	1:567:A:GLN:H	1:566:A:LEU:HG	14	0.8
(1,1467)	1:593:A:ASP:H	1:591:A:VAL:HG12	7	0.8
(1,1467)	1:593:A:ASP:H	1:591:A:VAL:HG11	10	0.8
(1,1467)	1:593:A:ASP:H	1:591:A:VAL:HG12	16	0.8
(1,1466)	1:606:A:LYS:H	1:609:A:ALA:HB1	3	0.8
(1,1449)	1:603:A:GLN:H	1:599:A:GLN:HB2	9	0.8
(1,1280)	1:573:A:LEU:HD23	1:580:A:LEU:HD13	17	0.8
(1,989)	1:611:A:MET:HG2	1:587:A:LEU:HD13	8	0.8
(1,989)	1:611:A:MET:HG2	1:587:A:LEU:HD13	18	0.8
(1,896)	1:617:A:GLU:HA	1:620:A:GLN:HG2	16	0.8
(1,695)	1:586:A:ALA:HB1	1:583:A:LYS:HB2	16	0.8
(1,670)	1:591:A:VAL:HG22	1:607:A:VAL:HG22	9	0.8
(1,125)	1:589:A:THR:H	1:586:A:ALA:HB2	11	0.8
(1,35)	1:598:A:SER:H	1:599:A:GLN:HB3	12	0.8

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,35)	1:598:A:SER:H	1:599:A:GLN:HB3	14	0.8
(1,2172)	1:625:A:TRP:HE3	1:573:A:LEU:HD23	8	0.79
(1,2158)	1:591:A:VAL:HG21	1:596:A:PHE:HB2	14	0.79
(1,2155)	1:628:A:LEU:HD11	1:624:A:ARG:HB2	7	0.79
(1,2118)	1:583:A:LYS:HE2	1:580:A:LEU:HD23	2	0.79
(1,2029)	1:568:A:ARG:HD3	1:565:A:LYS:HA	8	0.79
(1,2029)	1:568:A:ARG:HD3	1:565:A:LYS:HA	12	0.79
(1,2029)	1:568:A:ARG:HD3	1:565:A:LYS:HA	20	0.79
(1,1966)	1:579:A:ASP:HB2	1:576:A:LEU:HB3	3	0.79
(1,1966)	1:579:A:ASP:HB2	1:576:A:LEU:HB3	8	0.79
(1,1962)	1:610:A:ASP:HB3	1:609:A:ALA:HB2	15	0.79
(1,1947)	1:581:A:GLU:HG2	1:584:A:LEU:HD11	16	0.79
(1,1945)	1:585:A:GLU:HG2	1:582:A:ALA:HB3	1	0.79
(1,1945)	1:585:A:GLU:HG2	1:582:A:ALA:HB2	4	0.79
(1,1944)	1:582:A:ALA:HB1	1:585:A:GLU:HG3	10	0.79
(1,1898)	1:628:A:LEU:HG	1:631:A:LEU:HB2	12	0.79
(1,1850)	1:589:A:THR:HA	1:590:A:GLN:HB2	1	0.79
(1,1743)	1:628:A:LEU:HD23	1:625:A:TRP:HA	19	0.79
(1,1733)	1:607:A:VAL:HG23	1:610:A:ASP:HB3	14	0.79
(1,1722)	1:591:A:VAL:HG13	1:611:A:MET:HB2	9	0.79
(1,1722)	1:591:A:VAL:HG12	1:611:A:MET:HB2	10	0.79
(1,1690)	1:564:A:TYR:HE1	1:567:A:GLN:HB3	6	0.79
(1,1592)	1:613:A:ALA:H	1:615:A:GLU:HG3	12	0.79
(1,1506)	1:582:A:ALA:H	1:618:A:LEU:HD21	6	0.79
(1,1495)	1:584:A:LEU:H	1:584:A:LEU:HD11	14	0.79
(1,1366)	1:566:A:LEU:HD22	1:631:A:LEU:HD13	6	0.79
(1,1293)	1:577:A:LEU:HD13	1:573:A:LEU:HD11	9	0.79
(1,1271)	1:576:A:LEU:HD11	1:621:A:ALA:HB2	1	0.79
(1,1014)	1:605:A:GLN:HG3	1:608:A:LEU:HD12	13	0.79
(1,989)	1:611:A:MET:HG2	1:587:A:LEU:HD13	11	0.79
(1,906)	1:596:A:PHE:HA	1:599:A:GLN:HG2	2	0.79
(1,637)	1:604:A:THR:HG23	1:607:A:VAL:HG22	13	0.79
(1,2155)	1:628:A:LEU:HD11	1:624:A:ARG:HB2	10	0.78
(1,2037)	1:609:A:ALA:HA	1:605:A:GLN:HB3	3	0.78
(1,2037)	1:603:A:GLN:HA	1:605:A:GLN:HB2	6	0.78
(1,2029)	1:568:A:ARG:HD3	1:565:A:LYS:HA	6	0.78
(1,1962)	1:610:A:ASP:HB3	1:606:A:LYS:HG2	14	0.78
(1,1947)	1:581:A:GLU:HG2	1:618:A:LEU:HD13	2	0.78
(1,1944)	1:582:A:ALA:HB3	1:585:A:GLU:HG3	19	0.78
(1,1913)	1:585:A:GLU:HB3	1:586:A:ALA:HB3	2	0.78
(1,1913)	1:585:A:GLU:HB3	1:586:A:ALA:HB1	18	0.78
(1,1856)	1:580:A:LEU:HA	1:583:A:LYS:HE2	16	0.78

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1853)	1:554:A:THR:HB	1:555:A:VAL:HG23	15	0.78
(1,1850)	1:589:A:THR:HA	1:590:A:GLN:HB2	7	0.78
(1,1850)	1:589:A:THR:HA	1:590:A:GLN:HB2	8	0.78
(1,1850)	1:589:A:THR:HA	1:590:A:GLN:HB2	16	0.78
(1,1807)	1:587:A:LEU:HA	1:590:A:GLN:HB2	10	0.78
(1,1743)	1:628:A:LEU:HD23	1:625:A:TRP:HA	14	0.78
(1,1704)	1:622:A:PHE:HD2	1:618:A:LEU:HB3	14	0.78
(1,1690)	1:564:A:TYR:HE1	1:567:A:GLN:HB3	11	0.78
(1,1630)	1:621:A:ALA:H	1:576:A:LEU:HD21	19	0.78
(1,1513)	1:579:A:ASP:H	1:576:A:LEU:HG	1	0.78
(1,1469)	1:592:A:ALA:H	1:591:A:VAL:HG22	7	0.78
(1,1449)	1:603:A:GLN:H	1:605:A:GLN:HB2	18	0.78
(1,1280)	1:573:A:LEU:HD23	1:580:A:LEU:HD11	13	0.78
(1,1264)	1:568:A:ARG:HD2	1:564:A:TYR:HA	1	0.78
(1,1264)	1:568:A:ARG:HD2	1:564:A:TYR:HA	6	0.78
(1,989)	1:611:A:MET:HG2	1:587:A:LEU:HD13	3	0.78
(1,975)	1:615:A:GLU:HB2	1:584:A:LEU:HD12	13	0.78
(1,672)	1:607:A:VAL:HG22	1:606:A:LYS:HE3	15	0.78
(1,670)	1:591:A:VAL:HG23	1:607:A:VAL:HG22	19	0.78
(1,670)	1:591:A:VAL:HG23	1:607:A:VAL:HG21	20	0.78
(1,43)	1:597:A:PHE:H	1:596:A:PHE:HB2	9	0.78
(1,33)	1:598:A:SER:H	1:599:A:GLN:HG2	13	0.78
(1,2163)	1:567:A:GLN:HA	1:570:A:LEU:HD13	4	0.77
(1,2158)	1:591:A:VAL:HG23	1:596:A:PHE:HB2	20	0.77
(1,2135)	1:567:A:GLN:HA	1:570:A:LEU:HD13	4	0.77
(1,2105)	1:566:A:LEU:HD21	1:569:A:GLU:HG3	10	0.77
(1,1962)	1:610:A:ASP:HB3	1:609:A:ALA:HB1	19	0.77
(1,1917)	1:585:A:GLU:HB2	1:584:A:LEU:HD13	16	0.77
(1,1913)	1:585:A:GLU:HB3	1:586:A:ALA:HB3	14	0.77
(1,1807)	1:587:A:LEU:HA	1:590:A:GLN:HB2	3	0.77
(1,1792)	1:610:A:ASP:HA	1:587:A:LEU:HD21	14	0.77
(1,1729)	1:631:A:LEU:HD23	1:561:A:LYS:HA	17	0.77
(1,1715)	1:577:A:LEU:HD13	1:617:A:GLU:HG2	7	0.77
(1,1690)	1:564:A:TYR:HE2	1:567:A:GLN:HB2	4	0.77
(1,1690)	1:564:A:TYR:HE1	1:567:A:GLN:HB3	13	0.77
(1,1306)	1:589:A:THR:HG22	1:590:A:GLN:HB2	15	0.77
(1,1291)	1:608:A:LEU:HD13	1:604:A:THR:HG22	12	0.77
(1,1154)	1:603:A:GLN:HG2	1:600:A:PRO:HB3	6	0.77
(1,1053)	1:577:A:LEU:HD11	1:617:A:GLU:HG3	13	0.77
(1,644)	1:591:A:VAL:HG11	1:607:A:VAL:HG12	8	0.77
(1,35)	1:598:A:SER:H	1:599:A:GLN:HB3	11	0.77
(1,2158)	1:591:A:VAL:HG23	1:596:A:PHE:HB2	6	0.76

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2120)	1:573:A:LEU:HD22	1:624:A:ARG:HB2	3	0.76
(1,2118)	1:583:A:LYS:HE2	1:580:A:LEU:HD23	12	0.76
(1,1968)	1:579:A:ASP:HB3	1:576:A:LEU:HB3	6	0.76
(1,1966)	1:579:A:ASP:HB2	1:576:A:LEU:HB3	2	0.76
(1,1966)	1:579:A:ASP:HB2	1:576:A:LEU:HB3	17	0.76
(1,1962)	1:610:A:ASP:HB3	1:609:A:ALA:HB3	8	0.76
(1,1960)	1:622:A:PHE:HB3	1:623:A:GLU:HB2	12	0.76
(1,1958)	1:622:A:PHE:HB3	1:623:A:GLU:HB2	12	0.76
(1,1944)	1:582:A:ALA:HB3	1:585:A:GLU:HG3	3	0.76
(1,1944)	1:582:A:ALA:HB1	1:585:A:GLU:HG3	15	0.76
(1,1930)	1:556:A:LYS:HB3	1:555:A:VAL:HB	11	0.76
(1,1917)	1:585:A:GLU:HB2	1:584:A:LEU:HD11	3	0.76
(1,1917)	1:585:A:GLU:HB2	1:584:A:LEU:HD13	15	0.76
(1,1850)	1:589:A:THR:HA	1:590:A:GLN:HB2	4	0.76
(1,1836)	1:619:A:GLU:HA	1:618:A:LEU:HD12	20	0.76
(1,1792)	1:610:A:ASP:HA	1:587:A:LEU:HD23	1	0.76
(1,1729)	1:631:A:LEU:HD23	1:563:A:SER:HB2	15	0.76
(1,1722)	1:591:A:VAL:HG12	1:611:A:MET:HB2	19	0.76
(1,1720)	1:604:A:THR:HG21	1:600:A:PRO:HD3	4	0.76
(1,1704)	1:622:A:PHE:HD2	1:618:A:LEU:HB3	15	0.76
(1,1552)	1:567:A:GLN:H	1:566:A:LEU:HG	19	0.76
(1,1469)	1:592:A:ALA:H	1:591:A:VAL:HG22	11	0.76
(1,1466)	1:606:A:LYS:H	1:609:A:ALA:HB2	1	0.76
(1,1466)	1:606:A:LYS:H	1:609:A:ALA:HB2	11	0.76
(1,1466)	1:606:A:LYS:H	1:609:A:ALA:HB2	15	0.76
(1,1293)	1:577:A:LEU:HD11	1:573:A:LEU:HD11	3	0.76
(1,1280)	1:573:A:LEU:HD21	1:580:A:LEU:HD13	2	0.76
(1,1280)	1:573:A:LEU:HD22	1:580:A:LEU:HD13	4	0.76
(1,1280)	1:573:A:LEU:HD23	1:580:A:LEU:HD11	14	0.76
(1,1192)	1:568:A:ARG:HD2	1:565:A:LYS:HA	12	0.76
(1,989)	1:611:A:MET:HG2	1:587:A:LEU:HD12	5	0.76
(1,989)	1:611:A:MET:HG2	1:587:A:LEU:HD12	15	0.76
(1,989)	1:611:A:MET:HG2	1:587:A:LEU:HD13	19	0.76
(1,968)	1:604:A:THR:HG22	1:603:A:GLN:HB3	16	0.76
(1,43)	1:597:A:PHE:H	1:596:A:PHE:HB2	13	0.76
(1,35)	1:598:A:SER:H	1:599:A:GLN:HB3	2	0.76
(1,2158)	1:591:A:VAL:HG23	1:596:A:PHE:HB2	10	0.75
(1,2158)	1:591:A:VAL:HG22	1:596:A:PHE:HB2	12	0.75
(1,2118)	1:583:A:LYS:HE2	1:580:A:LEU:HD22	10	0.75
(1,2037)	1:603:A:GLN:HA	1:605:A:GLN:HB2	5	0.75
(1,2037)	1:603:A:GLN:HA	1:605:A:GLN:HB2	12	0.75
(1,2037)	1:603:A:GLN:HA	1:605:A:GLN:HB2	16	0.75

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2037)	1:603:A:GLN:HA	1:605:A:GLN:HB2	19	0.75
(1,1960)	1:622:A:PHE:HB3	1:623:A:GLU:HB2	3	0.75
(1,1958)	1:622:A:PHE:HB3	1:623:A:GLU:HB2	3	0.75
(1,1939)	1:572:A:GLN:HG3	1:573:A:LEU:HB3	5	0.75
(1,1913)	1:585:A:GLU:HB3	1:586:A:ALA:HB2	3	0.75
(1,1898)	1:628:A:LEU:HG	1:631:A:LEU:HB2	1	0.75
(1,1898)	1:628:A:LEU:HG	1:631:A:LEU:HB2	8	0.75
(1,1792)	1:610:A:ASP:HA	1:587:A:LEU:HD23	3	0.75
(1,1792)	1:610:A:ASP:HA	1:587:A:LEU:HD22	7	0.75
(1,1792)	1:610:A:ASP:HA	1:587:A:LEU:HD23	9	0.75
(1,1733)	1:607:A:VAL:HG21	1:610:A:ASP:HB3	9	0.75
(1,1729)	1:631:A:LEU:HD23	1:561:A:LYS:HA	20	0.75
(1,1720)	1:604:A:THR:HG23	1:600:A:PRO:HD3	5	0.75
(1,1720)	1:604:A:THR:HG23	1:600:A:PRO:HD3	17	0.75
(1,1704)	1:622:A:PHE:HD2	1:618:A:LEU:HB3	2	0.75
(1,1690)	1:564:A:TYR:HE1	1:567:A:GLN:HB3	8	0.75
(1,1690)	1:564:A:TYR:HE1	1:567:A:GLN:HB2	12	0.75
(1,1690)	1:564:A:TYR:HE2	1:567:A:GLN:HB2	14	0.75
(1,1621)	1:619:A:GLU:H	1:618:A:LEU:HD12	12	0.75
(1,1611)	1:616:A:GLN:H	1:612:A:ALA:HB2	5	0.75
(1,1611)	1:616:A:GLN:H	1:612:A:ALA:HB1	14	0.75
(1,1566)	1:607:A:VAL:H	1:606:A:LYS:HB3	19	0.75
(1,1506)	1:582:A:ALA:H	1:618:A:LEU:HD13	16	0.75
(1,1363)	1:562:A:LEU:HD23	1:631:A:LEU:HB2	4	0.75
(1,1271)	1:576:A:LEU:HD12	1:621:A:ALA:HB1	16	0.75
(1,1095)	1:565:A:LYS:HE3	1:566:A:LEU:HD12	14	0.75
(1,1053)	1:577:A:LEU:HD11	1:617:A:GLU:HG3	6	0.75
(1,975)	1:615:A:GLU:HB2	1:584:A:LEU:HD13	3	0.75
(1,975)	1:615:A:GLU:HB2	1:584:A:LEU:HD13	14	0.75
(1,968)	1:604:A:THR:HG22	1:603:A:GLN:HB3	10	0.75
(1,956)	1:605:A:GLN:HB3	1:608:A:LEU:HD12	12	0.75
(1,896)	1:617:A:GLU:HA	1:620:A:GLN:HG2	11	0.75
(1,2158)	1:591:A:VAL:HG21	1:596:A:PHE:HB2	5	0.74
(1,2109)	1:608:A:LEU:HD13	1:591:A:VAL:HG11	9	0.74
(1,2037)	1:603:A:GLN:HA	1:605:A:GLN:HB2	10	0.74
(1,1995)	1:557:A:ARG:HD2	1:555:A:VAL:HG12	6	0.74
(1,1966)	1:579:A:ASP:HB2	1:576:A:LEU:HB3	13	0.74
(1,1966)	1:579:A:ASP:HB2	1:576:A:LEU:HB3	14	0.74
(1,1962)	1:610:A:ASP:HB3	1:609:A:ALA:HB1	20	0.74
(1,1959)	1:622:A:PHE:HB2	1:619:A:GLU:HB2	3	0.74
(1,1939)	1:572:A:GLN:HG3	1:573:A:LEU:HB3	18	0.74
(1,1917)	1:585:A:GLU:HB2	1:584:A:LEU:HD13	19	0.74

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1913)	1:585:A:GLU:HB3	1:586:A:ALA:HB2	16	0.74
(1,1853)	1:554:A:THR:HB	1:555:A:VAL:HG23	11	0.74
(1,1836)	1:619:A:GLU:HA	1:618:A:LEU:HD11	7	0.74
(1,1743)	1:628:A:LEU:HD22	1:625:A:TRP:HA	9	0.74
(1,1729)	1:631:A:LEU:HD23	1:563:A:SER:HB2	6	0.74
(1,1705)	1:622:A:PHE:HD1	1:577:A:LEU:HD22	15	0.74
(1,1671)	1:633:A:ASN:H	1:570:A:LEU:HD11	5	0.74
(1,1611)	1:616:A:GLN:H	1:612:A:ALA:HB2	15	0.74
(1,1592)	1:613:A:ALA:H	1:616:A:GLN:HB2	14	0.74
(1,1538)	1:571:A:GLU:H	1:628:A:LEU:HD12	10	0.74
(1,1532)	1:573:A:LEU:H	1:573:A:LEU:HD21	10	0.74
(1,1506)	1:582:A:ALA:H	1:618:A:LEU:HD23	18	0.74
(1,1466)	1:606:A:LYS:H	1:609:A:ALA:HB2	6	0.74
(1,1449)	1:603:A:GLN:H	1:599:A:GLN:HB2	17	0.74
(1,1365)	1:631:A:LEU:HD23	1:566:A:LEU:HD13	1	0.74
(1,1325)	1:628:A:LEU:HD11	1:569:A:GLU:HA	11	0.74
(1,1291)	1:608:A:LEU:HD12	1:604:A:THR:HG23	7	0.74
(1,1291)	1:608:A:LEU:HD12	1:604:A:THR:HG23	16	0.74
(1,1232)	1:606:A:LYS:HB2	1:603:A:GLN:HA	19	0.74
(1,989)	1:611:A:MET:HG2	1:587:A:LEU:HD13	6	0.74
(1,975)	1:615:A:GLU:HB2	1:584:A:LEU:HD13	4	0.74
(1,970)	1:632:A:LYS:HD3	1:570:A:LEU:HD11	7	0.74
(1,796)	1:577:A:LEU:HA	1:618:A:LEU:HD21	6	0.74
(1,670)	1:591:A:VAL:HG23	1:607:A:VAL:HG22	6	0.74
(1,586)	1:625:A:TRP:HD1	1:577:A:LEU:HD23	12	0.74
(1,586)	1:625:A:TRP:HD1	1:577:A:LEU:HD22	13	0.74
(1,35)	1:598:A:SER:H	1:599:A:GLN:HB3	4	0.74
(1,35)	1:598:A:SER:H	1:599:A:GLN:HB3	19	0.74
(1,2158)	1:591:A:VAL:HG23	1:596:A:PHE:HB2	1	0.73
(1,2120)	1:573:A:LEU:HD22	1:624:A:ARG:HB2	9	0.73
(1,1995)	1:557:A:ARG:HD3	1:555:A:VAL:HG21	4	0.73
(1,1966)	1:579:A:ASP:HB2	1:576:A:LEU:HB3	10	0.73
(1,1947)	1:581:A:GLU:HG2	1:618:A:LEU:HD12	7	0.73
(1,1923)	1:614:A:ALA:HB1	1:611:A:MET:HG3	13	0.73
(1,1898)	1:628:A:LEU:HG	1:631:A:LEU:HB2	2	0.73
(1,1850)	1:589:A:THR:HA	1:590:A:GLN:HB2	18	0.73
(1,1834)	1:583:A:LYS:HA	1:587:A:LEU:HD21	8	0.73
(1,1834)	1:583:A:LYS:HA	1:587:A:LEU:HD22	14	0.73
(1,1762)	1:621:A:ALA:HB1	1:580:A:LEU:HB2	8	0.73
(1,1761)	1:621:A:ALA:HB1	1:624:A:ARG:HG2	3	0.73
(1,1723)	1:591:A:VAL:HG13	1:611:A:MET:HG3	16	0.73
(1,1711)	1:577:A:LEU:HD22	1:624:A:ARG:HB3	15	0.73

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1704)	1:622:A:PHE:HD2	1:618:A:LEU:HB3	18	0.73
(1,1506)	1:582:A:ALA:H	1:618:A:LEU:HD11	20	0.73
(1,1469)	1:592:A:ALA:H	1:591:A:VAL:HG22	1	0.73
(1,1469)	1:592:A:ALA:H	1:591:A:VAL:HG23	18	0.73
(1,1466)	1:606:A:LYS:H	1:609:A:ALA:HB1	2	0.73
(1,1387)	1:577:A:LEU:HD22	1:574:A:PRO:HB2	1	0.73
(1,1367)	1:570:A:LEU:HD22	1:628:A:LEU:HB3	18	0.73
(1,1271)	1:576:A:LEU:HD11	1:621:A:ALA:HB1	10	0.73
(1,1264)	1:568:A:ARG:HD2	1:564:A:TYR:HA	20	0.73
(1,1136)	1:600:A:PRO:HD3	1:603:A:GLN:HB2	12	0.73
(1,1095)	1:565:A:LYS:HE3	1:566:A:LEU:HD13	3	0.73
(1,1053)	1:577:A:LEU:HD11	1:617:A:GLU:HG3	11	0.73
(1,1014)	1:605:A:GLN:HG3	1:608:A:LEU:HD12	9	0.73
(1,956)	1:605:A:GLN:HB3	1:608:A:LEU:HD11	17	0.73
(1,670)	1:591:A:VAL:HG22	1:607:A:VAL:HG22	12	0.73
(1,670)	1:591:A:VAL:HG21	1:607:A:VAL:HG22	13	0.73
(1,670)	1:591:A:VAL:HG21	1:607:A:VAL:HG23	15	0.73
(1,586)	1:625:A:TRP:HD1	1:577:A:LEU:HD22	11	0.73
(1,586)	1:625:A:TRP:HD1	1:577:A:LEU:HD23	17	0.73
(1,125)	1:589:A:THR:H	1:586:A:ALA:HB2	18	0.73
(1,35)	1:598:A:SER:H	1:599:A:GLN:HB3	10	0.73
(1,24)	1:599:A:GLN:H	1:599:A:GLN:HG2	1	0.73
(1,2029)	1:568:A:ARG:HD3	1:565:A:LYS:HA	1	0.72
(1,2025)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	19	0.72
(1,2014)	1:601:A:HIS:HB3	1:602:A:GLU:HB2	5	0.72
(1,2014)	1:601:A:HIS:HB3	1:602:A:GLU:HB2	14	0.72
(1,1968)	1:579:A:ASP:HB3	1:583:A:LYS:HD2	15	0.72
(1,1966)	1:579:A:ASP:HB2	1:576:A:LEU:HB3	5	0.72
(1,1945)	1:585:A:GLU:HG2	1:582:A:ALA:HB3	7	0.72
(1,1944)	1:582:A:ALA:HB1	1:585:A:GLU:HG3	18	0.72
(1,1901)	1:612:A:ALA:HB2	1:616:A:GLN:HB3	13	0.72
(1,1856)	1:580:A:LEU:HA	1:583:A:LYS:HE2	4	0.72
(1,1836)	1:619:A:GLU:HA	1:618:A:LEU:HD12	8	0.72
(1,1834)	1:583:A:LYS:HA	1:587:A:LEU:HD21	18	0.72
(1,1812)	1:632:A:LYS:HA	1:631:A:LEU:HD21	14	0.72
(1,1807)	1:587:A:LEU:HA	1:590:A:GLN:HB2	9	0.72
(1,1792)	1:610:A:ASP:HA	1:587:A:LEU:HD21	12	0.72
(1,1733)	1:607:A:VAL:HG22	1:610:A:ASP:HB3	7	0.72
(1,1729)	1:631:A:LEU:HD22	1:563:A:SER:HB2	10	0.72
(1,1705)	1:622:A:PHE:HD1	1:577:A:LEU:HD22	2	0.72
(1,1705)	1:622:A:PHE:HD1	1:577:A:LEU:HD21	7	0.72
(1,1690)	1:564:A:TYR:HE1	1:567:A:GLN:HB2	20	0.72

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1552)	1:567:A:GLN:H	1:568:A:ARG:HB2	8	0.72
(1,1552)	1:567:A:GLN:H	1:566:A:LEU:HG	13	0.72
(1,1544)	1:569:A:GLU:H	1:566:A:LEU:HB3	12	0.72
(1,1467)	1:593:A:ASP:H	1:591:A:VAL:HG13	8	0.72
(1,1467)	1:593:A:ASP:H	1:591:A:VAL:HG11	18	0.72
(1,1466)	1:606:A:LYS:H	1:609:A:ALA:HB1	19	0.72
(1,1376)	1:566:A:LEU:HD23	1:563:A:SER:HB2	17	0.72
(1,1367)	1:570:A:LEU:HD23	1:628:A:LEU:HB3	8	0.72
(1,1278)	1:632:A:LYS:HG2	1:562:A:LEU:HD13	9	0.72
(1,1136)	1:600:A:PRO:HD3	1:603:A:GLN:HB2	15	0.72
(1,1019)	1:604:A:THR:HG22	1:599:A:GLN:HG2	13	0.72
(1,866)	1:582:A:ALA:HA	1:581:A:GLU:HG2	2	0.72
(1,35)	1:598:A:SER:H	1:599:A:GLN:HB3	13	0.72
(1,2163)	1:567:A:GLN:HA	1:570:A:LEU:HD12	16	0.71
(1,2158)	1:591:A:VAL:HG21	1:596:A:PHE:HB2	8	0.71
(1,2135)	1:567:A:GLN:HA	1:570:A:LEU:HD12	16	0.71
(1,2118)	1:583:A:LYS:HE2	1:580:A:LEU:HD22	15	0.71
(1,2056)	1:572:A:GLN:HG3	1:569:A:GLU:HA	10	0.71
(1,2037)	1:603:A:GLN:HA	1:605:A:GLN:HB2	7	0.71
(1,2014)	1:601:A:HIS:HB3	1:602:A:GLU:HB2	10	0.71
(1,1966)	1:579:A:ASP:HB2	1:576:A:LEU:HB3	9	0.71
(1,1962)	1:610:A:ASP:HB3	1:609:A:ALA:HB2	9	0.71
(1,1947)	1:581:A:GLU:HG2	1:584:A:LEU:HD11	1	0.71
(1,1944)	1:582:A:ALA:HB2	1:585:A:GLU:HG3	6	0.71
(1,1900)	1:567:A:GLN:HB3	1:562:A:LEU:HD12	10	0.71
(1,1888)	1:568:A:ARG:HG2	1:567:A:GLN:HB2	5	0.71
(1,1850)	1:589:A:THR:HA	1:590:A:GLN:HB2	14	0.71
(1,1834)	1:583:A:LYS:HA	1:587:A:LEU:HD22	19	0.71
(1,1733)	1:607:A:VAL:HG22	1:610:A:ASP:HB3	5	0.71
(1,1733)	1:607:A:VAL:HG21	1:610:A:ASP:HB3	12	0.71
(1,1712)	1:577:A:LEU:HD21	1:625:A:TRP:HA	6	0.71
(1,1612)	1:616:A:GLN:H	1:618:A:LEU:HD21	5	0.71
(1,1552)	1:567:A:GLN:H	1:568:A:ARG:HB2	18	0.71
(1,1545)	1:569:A:GLU:H	1:628:A:LEU:HD11	20	0.71
(1,1538)	1:571:A:GLU:H	1:628:A:LEU:HD13	17	0.71
(1,1532)	1:573:A:LEU:H	1:573:A:LEU:HD11	13	0.71
(1,1513)	1:579:A:ASP:H	1:576:A:LEU:HG	16	0.71
(1,1506)	1:582:A:ALA:H	1:618:A:LEU:HD13	3	0.71
(1,1506)	1:582:A:ALA:H	1:618:A:LEU:HD11	8	0.71
(1,1506)	1:582:A:ALA:H	1:618:A:LEU:HD13	9	0.71
(1,1469)	1:592:A:ALA:H	1:591:A:VAL:HG23	4	0.71
(1,1469)	1:592:A:ALA:H	1:591:A:VAL:HG23	17	0.71

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1467)	1:593:A:ASP:H	1:591:A:VAL:HG11	19	0.71
(1,1376)	1:566:A:LEU:HD21	1:563:A:SER:HB2	9	0.71
(1,1293)	1:577:A:LEU:HD12	1:573:A:LEU:HD11	6	0.71
(1,1287)	1:566:A:LEU:HD22	1:631:A:LEU:HD22	10	0.71
(1,1280)	1:573:A:LEU:HD22	1:580:A:LEU:HD11	11	0.71
(1,1053)	1:577:A:LEU:HD11	1:617:A:GLU:HG3	20	0.71
(1,838)	1:623:A:GLU:HA	1:626:A:GLU:HB3	8	0.71
(1,670)	1:591:A:VAL:HG23	1:607:A:VAL:HG21	3	0.71
(1,586)	1:625:A:TRP:HD1	1:577:A:LEU:HD23	5	0.71
(1,586)	1:625:A:TRP:HD1	1:577:A:LEU:HD23	16	0.71
(1,438)	1:619:A:GLU:H	1:619:A:GLU:HB3	3	0.71
(1,438)	1:619:A:GLU:H	1:619:A:GLU:HB3	6	0.71
(1,438)	1:619:A:GLU:H	1:619:A:GLU:HB3	9	0.71
(1,438)	1:619:A:GLU:H	1:619:A:GLU:HB3	18	0.71
(1,125)	1:589:A:THR:H	1:586:A:ALA:HB2	4	0.71
(1,125)	1:589:A:THR:H	1:586:A:ALA:HB1	10	0.71
(1,2120)	1:573:A:LEU:HD23	1:624:A:ARG:HB2	20	0.7
(1,2118)	1:583:A:LYS:HE2	1:580:A:LEU:HD23	14	0.7
(1,1968)	1:579:A:ASP:HB3	1:583:A:LYS:HD2	1	0.7
(1,1966)	1:579:A:ASP:HB2	1:576:A:LEU:HB3	11	0.7
(1,1966)	1:579:A:ASP:HB2	1:576:A:LEU:HB3	19	0.7
(1,1966)	1:579:A:ASP:HB2	1:576:A:LEU:HB3	20	0.7
(1,1944)	1:582:A:ALA:HB2	1:585:A:GLU:HG3	12	0.7
(1,1944)	1:582:A:ALA:HB3	1:585:A:GLU:HG3	14	0.7
(1,1923)	1:614:A:ALA:HB3	1:611:A:MET:HG3	14	0.7
(1,1834)	1:583:A:LYS:HA	1:587:A:LEU:HD23	7	0.7
(1,1834)	1:583:A:LYS:HA	1:587:A:LEU:HD21	20	0.7
(1,1790)	1:557:A:ARG:HA	1:555:A:VAL:HG22	4	0.7
(1,1752)	1:614:A:ALA:HB3	1:611:A:MET:HG3	14	0.7
(1,1741)	1:628:A:LEU:HD22	1:624:A:ARG:HA	12	0.7
(1,1733)	1:607:A:VAL:HG21	1:610:A:ASP:HB3	4	0.7
(1,1723)	1:591:A:VAL:HG12	1:611:A:MET:HG3	17	0.7
(1,1712)	1:577:A:LEU:HD21	1:625:A:TRP:HA	12	0.7
(1,1712)	1:577:A:LEU:HD21	1:625:A:TRP:HA	18	0.7
(1,1712)	1:577:A:LEU:HD22	1:625:A:TRP:HA	19	0.7
(1,1690)	1:564:A:TYR:HE2	1:567:A:GLN:HB2	3	0.7
(1,1612)	1:616:A:GLN:H	1:618:A:LEU:HD23	7	0.7
(1,1552)	1:567:A:GLN:H	1:566:A:LEU:HG	9	0.7
(1,1545)	1:569:A:GLU:H	1:628:A:LEU:HD12	8	0.7
(1,1545)	1:569:A:GLU:H	1:628:A:LEU:HD13	17	0.7
(1,1544)	1:569:A:GLU:H	1:566:A:LEU:HB3	6	0.7
(1,1513)	1:579:A:ASP:H	1:576:A:LEU:HG	17	0.7

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1484)	1:587:A:LEU:H	1:588:A:GLN:HG2	5	0.7
(1,1467)	1:593:A:ASP:H	1:591:A:VAL:HG13	20	0.7
(1,1466)	1:606:A:LYS:H	1:609:A:ALA:HB1	5	0.7
(1,1449)	1:603:A:GLN:H	1:605:A:GLN:HB2	10	0.7
(1,1291)	1:608:A:LEU:HD11	1:604:A:THR:HG22	2	0.7
(1,989)	1:611:A:MET:HG2	1:587:A:LEU:HD11	20	0.7
(1,438)	1:619:A:GLU:H	1:619:A:GLU:HB3	12	0.7
(1,2165)	1:606:A:LYS:HA	1:610:A:ASP:HB2	3	0.69
(1,2165)	1:606:A:LYS:HA	1:606:A:LYS:HE2	9	0.69
(1,2158)	1:591:A:VAL:HG21	1:596:A:PHE:HB2	16	0.69
(1,2109)	1:608:A:LEU:HD12	1:591:A:VAL:HG12	8	0.69
(1,2025)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	18	0.69
(1,2014)	1:601:A:HIS:HB3	1:602:A:GLU:HB2	6	0.69
(1,1962)	1:610:A:ASP:HB3	1:609:A:ALA:HB1	2	0.69
(1,1962)	1:610:A:ASP:HB3	1:609:A:ALA:HB1	3	0.69
(1,1944)	1:582:A:ALA:HB3	1:585:A:GLU:HG3	5	0.69
(1,1836)	1:619:A:GLU:HA	1:618:A:LEU:HD23	17	0.69
(1,1834)	1:583:A:LYS:HA	1:587:A:LEU:HD22	15	0.69
(1,1807)	1:587:A:LEU:HA	1:590:A:GLN:HB2	19	0.69
(1,1792)	1:610:A:ASP:HA	1:587:A:LEU:HD21	15	0.69
(1,1741)	1:628:A:LEU:HD22	1:624:A:ARG:HA	1	0.69
(1,1741)	1:628:A:LEU:HD21	1:624:A:ARG:HA	2	0.69
(1,1729)	1:631:A:LEU:HD23	1:561:A:LYS:HA	16	0.69
(1,1723)	1:591:A:VAL:HG13	1:611:A:MET:HG3	4	0.69
(1,1611)	1:616:A:GLN:H	1:612:A:ALA:HB1	4	0.69
(1,1544)	1:569:A:GLU:H	1:566:A:LEU:HB3	18	0.69
(1,1544)	1:569:A:GLU:H	1:566:A:LEU:HB3	20	0.69
(1,1467)	1:593:A:ASP:H	1:591:A:VAL:HG12	2	0.69
(1,1466)	1:606:A:LYS:H	1:609:A:ALA:HB2	7	0.69
(1,1466)	1:606:A:LYS:H	1:609:A:ALA:HB2	14	0.69
(1,1466)	1:606:A:LYS:H	1:609:A:ALA:HB3	16	0.69
(1,1449)	1:603:A:GLN:H	1:605:A:GLN:HB2	2	0.69
(1,1449)	1:603:A:GLN:H	1:605:A:GLN:HB2	5	0.69
(1,1449)	1:603:A:GLN:H	1:605:A:GLN:HB2	6	0.69
(1,1449)	1:603:A:GLN:H	1:605:A:GLN:HB2	8	0.69
(1,1396)	1:632:A:LYS:HG3	1:562:A:LEU:HB3	16	0.69
(1,1367)	1:570:A:LEU:HD22	1:628:A:LEU:HB3	9	0.69
(1,1095)	1:565:A:LYS:HE2	1:566:A:LEU:HD12	12	0.69
(1,1054)	1:604:A:THR:HG22	1:597:A:PHE:HB2	8	0.69
(1,809)	1:605:A:GLN:HA	1:608:A:LEU:HD22	17	0.69
(1,631)	1:577:A:LEU:HD12	1:622:A:PHE:HB3	6	0.69
(1,631)	1:577:A:LEU:HD11	1:622:A:PHE:HB3	18	0.69

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,586)	1:625:A:TRP:HD1	1:577:A:LEU:HD21	9	0.69
(1,438)	1:619:A:GLU:H	1:619:A:GLU:HB3	1	0.69
(1,149)	1:586:A:ALA:H	1:589:A:THR:HG23	7	0.69
(1,35)	1:598:A:SER:H	1:599:A:GLN:HB3	9	0.69
(1,2160)	1:630:A:ALA:HB2	1:627:A:TYR:HB2	5	0.68
(1,2160)	1:630:A:ALA:HB2	1:627:A:TYR:HB2	12	0.68
(1,2160)	1:630:A:ALA:HB2	1:627:A:TYR:HB2	15	0.68
(1,2158)	1:591:A:VAL:HG22	1:596:A:PHE:HB2	9	0.68
(1,2092)	1:562:A:LEU:HD11	1:570:A:LEU:HB2	19	0.68
(1,2014)	1:601:A:HIS:HB3	1:602:A:GLU:HB2	3	0.68
(1,2014)	1:601:A:HIS:HB3	1:602:A:GLU:HB2	18	0.68
(1,1962)	1:610:A:ASP:HB3	1:609:A:ALA:HB2	1	0.68
(1,1944)	1:582:A:ALA:HB1	1:585:A:GLU:HG3	9	0.68
(1,1939)	1:572:A:GLN:HG3	1:573:A:LEU:HB3	17	0.68
(1,1902)	1:567:A:GLN:HB2	1:562:A:LEU:HB3	6	0.68
(1,1852)	1:604:A:THR:HB	1:599:A:GLN:HB2	19	0.68
(1,1836)	1:619:A:GLU:HA	1:618:A:LEU:HD11	9	0.68
(1,1836)	1:619:A:GLU:HA	1:618:A:LEU:HD13	10	0.68
(1,1834)	1:583:A:LYS:HA	1:587:A:LEU:HD21	17	0.68
(1,1720)	1:604:A:THR:HG22	1:600:A:PRO:HD3	16	0.68
(1,1704)	1:622:A:PHE:HD2	1:618:A:LEU:HB3	13	0.68
(1,1690)	1:564:A:TYR:HE1	1:567:A:GLN:HB3	1	0.68
(1,1621)	1:619:A:GLU:H	1:618:A:LEU:HD23	3	0.68
(1,1592)	1:613:A:ALA:H	1:616:A:GLN:HB2	3	0.68
(1,1545)	1:569:A:GLU:H	1:628:A:LEU:HD11	18	0.68
(1,1538)	1:571:A:GLU:H	1:570:A:LEU:HD11	1	0.68
(1,1532)	1:573:A:LEU:H	1:573:A:LEU:HD13	6	0.68
(1,1513)	1:579:A:ASP:H	1:576:A:LEU:HG	2	0.68
(1,1513)	1:579:A:ASP:H	1:576:A:LEU:HG	7	0.68
(1,1469)	1:592:A:ALA:H	1:591:A:VAL:HG22	6	0.68
(1,1449)	1:603:A:GLN:H	1:605:A:GLN:HB2	7	0.68
(1,1387)	1:577:A:LEU:HD23	1:574:A:PRO:HB2	12	0.68
(1,1306)	1:589:A:THR:HG22	1:590:A:GLN:HB2	19	0.68
(1,1293)	1:577:A:LEU:HD11	1:573:A:LEU:HD13	18	0.68
(1,1291)	1:608:A:LEU:HD13	1:604:A:THR:HG22	9	0.68
(1,1278)	1:632:A:LYS:HG2	1:562:A:LEU:HD12	19	0.68
(1,1136)	1:600:A:PRO:HD3	1:603:A:GLN:HB2	2	0.68
(1,1111)	1:631:A:LEU:HD21	1:562:A:LEU:HB3	3	0.68
(1,970)	1:632:A:LYS:HD3	1:570:A:LEU:HD12	12	0.68
(1,838)	1:623:A:GLU:HA	1:626:A:GLU:HB3	2	0.68
(1,838)	1:623:A:GLU:HA	1:626:A:GLU:HB3	7	0.68
(1,838)	1:623:A:GLU:HA	1:626:A:GLU:HB3	14	0.68

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,672)	1:607:A:VAL:HG21	1:606:A:LYS:HE2	13	0.68
(1,670)	1:591:A:VAL:HG23	1:607:A:VAL:HG22	10	0.68
(1,631)	1:577:A:LEU:HD12	1:622:A:PHE:HB3	16	0.68
(1,2160)	1:630:A:ALA:HB2	1:627:A:TYR:HB2	10	0.67
(1,2093)	1:587:A:LEU:HD22	1:587:A:LEU:HD12	19	0.67
(1,2013)	1:565:A:LYS:HA	1:568:A:ARG:HB3	2	0.67
(1,1959)	1:622:A:PHE:HB2	1:619:A:GLU:HB2	1	0.67
(1,1959)	1:622:A:PHE:HB2	1:619:A:GLU:HB2	6	0.67
(1,1944)	1:582:A:ALA:HB2	1:585:A:GLU:HG3	2	0.67
(1,1913)	1:613:A:ALA:HB2	1:617:A:GLU:HB3	15	0.67
(1,1898)	1:628:A:LEU:HG	1:631:A:LEU:HB2	10	0.67
(1,1845)	1:554:A:THR:HA	1:555:A:VAL:HG11	12	0.67
(1,1836)	1:619:A:GLU:HA	1:618:A:LEU:HD13	13	0.67
(1,1812)	1:632:A:LYS:HA	1:631:A:LEU:HD21	20	0.67
(1,1733)	1:607:A:VAL:HG21	1:610:A:ASP:HB3	19	0.67
(1,1729)	1:631:A:LEU:HD22	1:561:A:LYS:HA	18	0.67
(1,1712)	1:577:A:LEU:HD22	1:625:A:TRP:HA	2	0.67
(1,1712)	1:577:A:LEU:HD22	1:625:A:TRP:HA	3	0.67
(1,1712)	1:577:A:LEU:HD22	1:625:A:TRP:HA	15	0.67
(1,1621)	1:619:A:GLU:H	1:618:A:LEU:HD22	18	0.67
(1,1552)	1:567:A:GLN:H	1:566:A:LEU:HG	4	0.67
(1,1552)	1:567:A:GLN:H	1:568:A:ARG:HB2	6	0.67
(1,1552)	1:567:A:GLN:H	1:568:A:ARG:HB2	20	0.67
(1,1545)	1:569:A:GLU:H	1:628:A:LEU:HD12	6	0.67
(1,1544)	1:569:A:GLU:H	1:566:A:LEU:HB3	10	0.67
(1,1544)	1:569:A:GLU:H	1:566:A:LEU:HB3	13	0.67
(1,1538)	1:571:A:GLU:H	1:628:A:LEU:HD11	11	0.67
(1,1538)	1:571:A:GLU:H	1:628:A:LEU:HD13	13	0.67
(1,1535)	1:572:A:GLN:H	1:573:A:LEU:HD11	16	0.67
(1,1534)	1:572:A:GLN:H	1:572:A:GLN:HB3	14	0.67
(1,1532)	1:573:A:LEU:H	1:573:A:LEU:HD11	1	0.67
(1,1513)	1:579:A:ASP:H	1:576:A:LEU:HG	5	0.67
(1,1506)	1:582:A:ALA:H	1:618:A:LEU:HD12	15	0.67
(1,1466)	1:606:A:LYS:H	1:609:A:ALA:HB3	4	0.67
(1,1376)	1:566:A:LEU:HD22	1:563:A:SER:HB2	18	0.67
(1,1333)	1:573:A:LEU:HD13	1:624:A:ARG:HD2	5	0.67
(1,1288)	1:566:A:LEU:HD21	1:562:A:LEU:HD22	10	0.67
(1,1019)	1:604:A:THR:HG21	1:599:A:GLN:HG2	7	0.67
(1,956)	1:605:A:GLN:HB3	1:608:A:LEU:HD13	14	0.67
(1,670)	1:591:A:VAL:HG22	1:607:A:VAL:HG23	2	0.67
(1,670)	1:591:A:VAL:HG21	1:607:A:VAL:HG23	5	0.67
(1,630)	1:577:A:LEU:HD13	1:580:A:LEU:HG	20	0.67

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,586)	1:625:A:TRP:HD1	1:577:A:LEU:HD21	2	0.67
(1,586)	1:625:A:TRP:HD1	1:577:A:LEU:HD21	15	0.67
(1,2172)	1:625:A:TRP:HE3	1:573:A:LEU:HD21	5	0.66
(1,2160)	1:630:A:ALA:HB3	1:627:A:TYR:HB2	11	0.66
(1,2160)	1:630:A:ALA:HB1	1:627:A:TYR:HB2	16	0.66
(1,2109)	1:608:A:LEU:HD13	1:591:A:VAL:HG12	20	0.66
(1,2014)	1:601:A:HIS:HB3	1:602:A:GLU:HB2	4	0.66
(1,2013)	1:565:A:LYS:HA	1:568:A:ARG:HB3	16	0.66
(1,1947)	1:581:A:GLU:HG2	1:584:A:LEU:HD12	14	0.66
(1,1946)	1:581:A:GLU:HG2	1:584:A:LEU:HD12	14	0.66
(1,1912)	1:585:A:GLU:HB2	1:582:A:ALA:HB3	8	0.66
(1,1853)	1:554:A:THR:HB	1:555:A:VAL:HG12	4	0.66
(1,1729)	1:631:A:LEU:HD23	1:561:A:LYS:HA	13	0.66
(1,1723)	1:591:A:VAL:HG12	1:611:A:MET:HG3	18	0.66
(1,1712)	1:577:A:LEU:HD21	1:625:A:TRP:HA	20	0.66
(1,1704)	1:622:A:PHE:HD2	1:618:A:LEU:HB3	3	0.66
(1,1538)	1:571:A:GLU:H	1:628:A:LEU:HD13	15	0.66
(1,1532)	1:573:A:LEU:H	1:573:A:LEU:HD11	16	0.66
(1,1480)	1:588:A:GLN:H	1:586:A:ALA:HB3	1	0.66
(1,1469)	1:592:A:ALA:H	1:591:A:VAL:HG23	8	0.66
(1,1469)	1:592:A:ALA:H	1:591:A:VAL:HG23	16	0.66
(1,1466)	1:606:A:LYS:H	1:609:A:ALA:HB3	9	0.66
(1,1466)	1:606:A:LYS:H	1:609:A:ALA:HB1	17	0.66
(1,1396)	1:632:A:LYS:HG3	1:562:A:LEU:HB2	1	0.66
(1,1376)	1:566:A:LEU:HD22	1:563:A:SER:HB2	4	0.66
(1,1367)	1:570:A:LEU:HD21	1:628:A:LEU:HB3	4	0.66
(1,1367)	1:570:A:LEU:HD22	1:628:A:LEU:HB3	20	0.66
(1,1287)	1:566:A:LEU:HD21	1:631:A:LEU:HD22	15	0.66
(1,1136)	1:600:A:PRO:HD3	1:603:A:GLN:HB2	9	0.66
(1,1136)	1:600:A:PRO:HD3	1:603:A:GLN:HB2	20	0.66
(1,1120)	1:588:A:GLN:HA	1:611:A:MET:HE2	3	0.66
(1,1120)	1:588:A:GLN:HA	1:611:A:MET:HE2	9	0.66
(1,1019)	1:604:A:THR:HG23	1:599:A:GLN:HG2	8	0.66
(1,956)	1:605:A:GLN:HB3	1:608:A:LEU:HD13	11	0.66
(1,906)	1:596:A:PHE:HA	1:599:A:GLN:HG2	11	0.66
(1,809)	1:605:A:GLN:HA	1:608:A:LEU:HD21	16	0.66
(1,631)	1:577:A:LEU:HD13	1:622:A:PHE:HB3	10	0.66
(1,631)	1:577:A:LEU:HD12	1:622:A:PHE:HB3	14	0.66
(1,586)	1:625:A:TRP:HD1	1:577:A:LEU:HD22	8	0.66
(1,125)	1:589:A:THR:H	1:586:A:ALA:HB3	13	0.66
(1,35)	1:598:A:SER:H	1:599:A:GLN:HB3	20	0.66
(1,2160)	1:630:A:ALA:HB2	1:627:A:TYR:HB2	2	0.65

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2160)	1:630:A:ALA:HB1	1:627:A:TYR:HB2	8	0.65
(1,2078)	1:562:A:LEU:HB3	1:566:A:LEU:HD13	1	0.65
(1,2029)	1:568:A:ARG:HD3	1:567:A:GLN:HA	18	0.65
(1,2014)	1:601:A:HIS:HB3	1:602:A:GLU:HB2	7	0.65
(1,2014)	1:601:A:HIS:HB3	1:602:A:GLU:HB2	19	0.65
(1,2013)	1:565:A:LYS:HA	1:568:A:ARG:HB3	7	0.65
(1,2013)	1:565:A:LYS:HA	1:568:A:ARG:HB3	9	0.65
(1,1991)	1:562:A:LEU:HB3	1:566:A:LEU:HD13	1	0.65
(1,1962)	1:610:A:ASP:HB3	1:609:A:ALA:HB2	6	0.65
(1,1944)	1:585:A:GLU:HG3	1:586:A:ALA:HB1	4	0.65
(1,1944)	1:582:A:ALA:HB3	1:578:A:GLU:HG3	16	0.65
(1,1939)	1:572:A:GLN:HG3	1:573:A:LEU:HB3	4	0.65
(1,1913)	1:585:A:GLU:HB3	1:586:A:ALA:HB3	9	0.65
(1,1913)	1:585:A:GLU:HB3	1:586:A:ALA:HB3	19	0.65
(1,1901)	1:612:A:ALA:HB1	1:616:A:GLN:HB3	11	0.65
(1,1900)	1:567:A:GLN:HB3	1:562:A:LEU:HD13	3	0.65
(1,1834)	1:583:A:LYS:HA	1:587:A:LEU:HD22	6	0.65
(1,1834)	1:583:A:LYS:HA	1:587:A:LEU:HD22	10	0.65
(1,1812)	1:632:A:LYS:HA	1:631:A:LEU:HD22	8	0.65
(1,1807)	1:587:A:LEU:HA	1:590:A:GLN:HB2	5	0.65
(1,1733)	1:607:A:VAL:HG21	1:610:A:ASP:HB3	10	0.65
(1,1712)	1:577:A:LEU:HD21	1:625:A:TRP:HA	4	0.65
(1,1671)	1:633:A:ASN:H	1:562:A:LEU:HD22	19	0.65
(1,1611)	1:616:A:GLN:H	1:612:A:ALA:HB3	1	0.65
(1,1592)	1:613:A:ALA:H	1:616:A:GLN:HB2	15	0.65
(1,1588)	1:583:A:LYS:H	1:581:A:GLU:HG2	17	0.65
(1,1567)	1:607:A:VAL:H	1:606:A:LYS:HB2	19	0.65
(1,1552)	1:567:A:GLN:H	1:568:A:ARG:HB2	1	0.65
(1,1545)	1:569:A:GLU:H	1:628:A:LEU:HD13	13	0.65
(1,1544)	1:569:A:GLU:H	1:566:A:LEU:HB3	5	0.65
(1,1513)	1:579:A:ASP:H	1:576:A:LEU:HG	14	0.65
(1,1387)	1:577:A:LEU:HD22	1:574:A:PRO:HB2	13	0.65
(1,1326)	1:566:A:LEU:HD23	1:563:A:SER:HB3	17	0.65
(1,1271)	1:576:A:LEU:HD12	1:621:A:ALA:HB2	7	0.65
(1,1136)	1:600:A:PRO:HD3	1:603:A:GLN:HB2	11	0.65
(1,1120)	1:588:A:GLN:HA	1:611:A:MET:HE3	8	0.65
(1,1054)	1:604:A:THR:HG22	1:597:A:PHE:HB2	17	0.65
(1,968)	1:604:A:THR:HG22	1:603:A:GLN:HB3	6	0.65
(1,870)	1:556:A:LYS:HA	1:556:A:LYS:HE2	10	0.65
(1,851)	1:604:A:THR:HA	1:608:A:LEU:HD13	10	0.65
(1,630)	1:577:A:LEU:HD12	1:580:A:LEU:HG	3	0.65
(1,300)	1:567:A:GLN:H	1:566:A:LEU:HD21	9	0.65

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,146)	1:586:A:ALA:H	1:585:A:GLU:HB2	11	0.65
(1,125)	1:589:A:THR:H	1:586:A:ALA:HB3	12	0.65
(1,2109)	1:608:A:LEU:HD13	1:591:A:VAL:HG11	12	0.64
(1,2093)	1:570:A:LEU:HD22	1:570:A:LEU:HD11	12	0.64
(1,2078)	1:562:A:LEU:HB3	1:566:A:LEU:HD12	6	0.64
(1,2025)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	12	0.64
(1,2022)	1:599:A:GLN:HG3	1:600:A:PRO:HD2	13	0.64
(1,1998)	1:562:A:LEU:HB3	1:566:A:LEU:HB2	18	0.64
(1,1992)	1:562:A:LEU:HB2	1:632:A:LYS:HG2	14	0.64
(1,1991)	1:562:A:LEU:HB3	1:566:A:LEU:HD12	6	0.64
(1,1879)	1:551:A:LYS:HG3	1:551:A:LYS:HD2	3	0.64
(1,1874)	1:632:A:LYS:HG2	1:562:A:LEU:HD22	17	0.64
(1,1874)	1:632:A:LYS:HG2	1:562:A:LEU:HD23	20	0.64
(1,1834)	1:583:A:LYS:HA	1:587:A:LEU:HD22	2	0.64
(1,1812)	1:632:A:LYS:HA	1:631:A:LEU:HD23	19	0.64
(1,1743)	1:628:A:LEU:HD23	1:625:A:TRP:HA	3	0.64
(1,1723)	1:591:A:VAL:HG11	1:611:A:MET:HG3	11	0.64
(1,1712)	1:577:A:LEU:HD22	1:625:A:TRP:HA	9	0.64
(1,1704)	1:622:A:PHE:HD2	1:618:A:LEU:HB3	1	0.64
(1,1704)	1:622:A:PHE:HD2	1:618:A:LEU:HB3	16	0.64
(1,1690)	1:564:A:TYR:HE1	1:567:A:GLN:HB2	7	0.64
(1,1690)	1:564:A:TYR:HE1	1:567:A:GLN:HB2	15	0.64
(1,1633)	1:622:A:PHE:H	1:619:A:GLU:HB3	8	0.64
(1,1621)	1:619:A:GLU:H	1:618:A:LEU:HD21	9	0.64
(1,1545)	1:569:A:GLU:H	1:628:A:LEU:HD13	4	0.64
(1,1545)	1:569:A:GLU:H	1:628:A:LEU:HD12	19	0.64
(1,1544)	1:569:A:GLU:H	1:566:A:LEU:HB3	8	0.64
(1,1534)	1:572:A:GLN:H	1:572:A:GLN:HB3	15	0.64
(1,1513)	1:579:A:ASP:H	1:576:A:LEU:HG	19	0.64
(1,1469)	1:592:A:ALA:H	1:591:A:VAL:HG23	14	0.64
(1,1469)	1:592:A:ALA:H	1:591:A:VAL:HG13	20	0.64
(1,1468)	1:592:A:ALA:H	1:593:A:ASP:HB2	7	0.64
(1,1467)	1:593:A:ASP:H	1:591:A:VAL:HG12	9	0.64
(1,1466)	1:606:A:LYS:H	1:609:A:ALA:HB1	13	0.64
(1,1449)	1:603:A:GLN:H	1:605:A:GLN:HB2	1	0.64
(1,1390)	1:599:A:GLN:HG3	1:600:A:PRO:HD2	13	0.64
(1,1387)	1:577:A:LEU:HD23	1:574:A:PRO:HB2	7	0.64
(1,1306)	1:589:A:THR:HG23	1:590:A:GLN:HB2	13	0.64
(1,1265)	1:593:A:ASP:HB3	1:595:A:SER:HB3	13	0.64
(1,1165)	1:601:A:HIS:HB2	1:605:A:GLN:HG2	9	0.64
(1,1136)	1:600:A:PRO:HD3	1:603:A:GLN:HB2	3	0.64
(1,1054)	1:604:A:THR:HG23	1:597:A:PHE:HB2	18	0.64

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1019)	1:604:A:THR:HG23	1:599:A:GLN:HG2	9	0.64
(1,970)	1:632:A:LYS:HD3	1:570:A:LEU:HD13	4	0.64
(1,968)	1:604:A:THR:HG21	1:603:A:GLN:HB3	14	0.64
(1,956)	1:605:A:GLN:HB3	1:608:A:LEU:HD12	4	0.64
(1,956)	1:605:A:GLN:HB3	1:608:A:LEU:HD11	8	0.64
(1,838)	1:623:A:GLU:HA	1:626:A:GLU:HB3	3	0.64
(1,809)	1:605:A:GLN:HA	1:608:A:LEU:HD21	12	0.64
(1,630)	1:577:A:LEU:HD13	1:580:A:LEU:HG	8	0.64
(1,586)	1:625:A:TRP:HD1	1:577:A:LEU:HD23	20	0.64
(1,300)	1:567:A:GLN:H	1:566:A:LEU:HD22	12	0.64
(1,300)	1:567:A:GLN:H	1:566:A:LEU:HD22	14	0.64
(1,146)	1:586:A:ALA:H	1:585:A:GLU:HB2	20	0.64
(1,125)	1:589:A:THR:H	1:586:A:ALA:HB2	7	0.64
(1,2171)	1:591:A:VAL:HG22	1:597:A:PHE:HZ	12	0.63
(1,2160)	1:630:A:ALA:HB1	1:627:A:TYR:HB2	13	0.63
(1,2106)	1:569:A:GLU:HG3	1:573:A:LEU:HD13	1	0.63
(1,2093)	1:570:A:LEU:HD21	1:570:A:LEU:HD11	3	0.63
(1,2093)	1:570:A:LEU:HD21	1:570:A:LEU:HD13	17	0.63
(1,2042)	1:625:A:TRP:HA	1:573:A:LEU:HG	9	0.63
(1,2014)	1:601:A:HIS:HB3	1:602:A:GLU:HB2	16	0.63
(1,2014)	1:601:A:HIS:HB3	1:602:A:GLU:HB2	17	0.63
(1,1962)	1:610:A:ASP:HB3	1:613:A:ALA:HB1	16	0.63
(1,1959)	1:622:A:PHE:HB2	1:619:A:GLU:HB2	18	0.63
(1,1812)	1:632:A:LYS:HA	1:631:A:LEU:HD23	2	0.63
(1,1812)	1:632:A:LYS:HA	1:631:A:LEU:HD22	10	0.63
(1,1723)	1:591:A:VAL:HG11	1:611:A:MET:HG3	6	0.63
(1,1711)	1:577:A:LEU:HD22	1:626:A:GLU:HG3	2	0.63
(1,1705)	1:622:A:PHE:HD1	1:577:A:LEU:HD21	4	0.63
(1,1704)	1:622:A:PHE:HD2	1:618:A:LEU:HB3	10	0.63
(1,1683)	1:622:A:PHE:HE2	1:618:A:LEU:HD21	2	0.63
(1,1621)	1:619:A:GLU:H	1:618:A:LEU:HD22	4	0.63
(1,1545)	1:569:A:GLU:H	1:628:A:LEU:HD12	12	0.63
(1,1534)	1:572:A:GLN:H	1:572:A:GLN:HB3	11	0.63
(1,1513)	1:579:A:ASP:H	1:576:A:LEU:HG	6	0.63
(1,1513)	1:579:A:ASP:H	1:576:A:LEU:HG	9	0.63
(1,1506)	1:582:A:ALA:H	1:618:A:LEU:HD13	7	0.63
(1,1467)	1:593:A:ASP:H	1:591:A:VAL:HG12	5	0.63
(1,1466)	1:606:A:LYS:H	1:609:A:ALA:HB2	18	0.63
(1,1387)	1:577:A:LEU:HD21	1:574:A:PRO:HB2	15	0.63
(1,1367)	1:570:A:LEU:HD23	1:628:A:LEU:HB3	13	0.63
(1,1306)	1:589:A:THR:HG23	1:590:A:GLN:HB2	2	0.63
(1,1306)	1:589:A:THR:HG21	1:590:A:GLN:HB2	16	0.63

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1291)	1:608:A:LEU:HD11	1:604:A:THR:HG23	11	0.63
(1,1278)	1:632:A:LYS:HG2	1:562:A:LEU:HD13	5	0.63
(1,1271)	1:576:A:LEU:HD12	1:621:A:ALA:HB2	15	0.63
(1,1264)	1:568:A:ARG:HD2	1:564:A:TYR:HA	8	0.63
(1,1136)	1:600:A:PRO:HD3	1:603:A:GLN:HB2	1	0.63
(1,1036)	1:569:A:GLU:HG3	1:573:A:LEU:HD13	1	0.63
(1,1024)	1:590:A:GLN:HG3	1:589:A:THR:HG22	14	0.63
(1,1019)	1:604:A:THR:HG21	1:599:A:GLN:HG2	11	0.63
(1,1019)	1:604:A:THR:HG22	1:599:A:GLN:HG2	16	0.63
(1,956)	1:605:A:GLN:HB3	1:608:A:LEU:HD13	10	0.63
(1,838)	1:623:A:GLU:HA	1:626:A:GLU:HB3	18	0.63
(1,649)	1:591:A:VAL:HG13	1:596:A:PHE:HB2	13	0.63
(1,559)	1:596:A:PHE:HE2	1:604:A:THR:HG21	9	0.63
(1,308)	1:566:A:LEU:H	1:566:A:LEU:HD23	17	0.63
(1,146)	1:586:A:ALA:H	1:585:A:GLU:HB2	7	0.63
(1,24)	1:599:A:GLN:H	1:599:A:GLN:HG2	20	0.63
(1,2158)	1:591:A:VAL:HG23	1:596:A:PHE:HB2	19	0.62
(1,2093)	1:570:A:LEU:HD21	1:570:A:LEU:HD12	4	0.62
(1,2093)	1:570:A:LEU:HD21	1:570:A:LEU:HD11	10	0.62
(1,2093)	1:570:A:LEU:HD23	1:570:A:LEU:HD12	13	0.62
(1,2093)	1:570:A:LEU:HD21	1:570:A:LEU:HD11	14	0.62
(1,2093)	1:570:A:LEU:HD21	1:570:A:LEU:HD13	15	0.62
(1,2014)	1:601:A:HIS:HB3	1:602:A:GLU:HB2	11	0.62
(1,1901)	1:612:A:ALA:HB1	1:616:A:GLN:HB3	4	0.62
(1,1885)	1:628:A:LEU:HD22	1:624:A:ARG:HG2	15	0.62
(1,1879)	1:565:A:LYS:HG2	1:565:A:LYS:HD2	12	0.62
(1,1852)	1:604:A:THR:HB	1:608:A:LEU:HB2	18	0.62
(1,1733)	1:607:A:VAL:HG21	1:610:A:ASP:HB3	16	0.62
(1,1733)	1:607:A:VAL:HG23	1:610:A:ASP:HB3	18	0.62
(1,1729)	1:631:A:LEU:HD23	1:561:A:LYS:HA	3	0.62
(1,1723)	1:591:A:VAL:HG13	1:611:A:MET:HG3	12	0.62
(1,1720)	1:604:A:THR:HG22	1:600:A:PRO:HD3	13	0.62
(1,1704)	1:622:A:PHE:HD2	1:618:A:LEU:HB3	4	0.62
(1,1668)	1:633:A:ASN:H	1:629:A:GLU:HA	18	0.62
(1,1633)	1:622:A:PHE:H	1:619:A:GLU:HB3	17	0.62
(1,1621)	1:619:A:GLU:H	1:618:A:LEU:HD22	16	0.62
(1,1611)	1:616:A:GLN:H	1:612:A:ALA:HB1	11	0.62
(1,1611)	1:616:A:GLN:H	1:612:A:ALA:HB2	13	0.62
(1,1538)	1:571:A:GLU:H	1:628:A:LEU:HD12	7	0.62
(1,1532)	1:573:A:LEU:H	1:573:A:LEU:HD13	14	0.62
(1,1513)	1:579:A:ASP:H	1:576:A:LEU:HG	20	0.62
(1,1452)	1:599:A:GLN:H	1:600:A:PRO:HG2	7	0.62

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1449)	1:603:A:GLN:H	1:605:A:GLN:HB2	3	0.62
(1,1431)	1:622:A:PHE:HE2	1:618:A:LEU:HD21	2	0.62
(1,1397)	1:587:A:LEU:HD11	1:583:A:LYS:HA	10	0.62
(1,1387)	1:577:A:LEU:HD21	1:574:A:PRO:HB2	2	0.62
(1,1387)	1:577:A:LEU:HD21	1:574:A:PRO:HB2	3	0.62
(1,1387)	1:577:A:LEU:HD23	1:574:A:PRO:HB2	4	0.62
(1,1387)	1:577:A:LEU:HD23	1:574:A:PRO:HB2	5	0.62
(1,1387)	1:577:A:LEU:HD23	1:574:A:PRO:HB2	16	0.62
(1,1376)	1:566:A:LEU:HD23	1:563:A:SER:HB2	20	0.62
(1,1367)	1:570:A:LEU:HD22	1:628:A:LEU:HB3	1	0.62
(1,1367)	1:570:A:LEU:HD21	1:628:A:LEU:HB3	2	0.62
(1,1367)	1:570:A:LEU:HD21	1:628:A:LEU:HB3	14	0.62
(1,1331)	1:566:A:LEU:HD23	1:628:A:LEU:HA	7	0.62
(1,1326)	1:566:A:LEU:HD21	1:563:A:SER:HB3	9	0.62
(1,1306)	1:589:A:THR:HG22	1:590:A:GLN:HB2	8	0.62
(1,1264)	1:568:A:ARG:HD2	1:564:A:TYR:HA	13	0.62
(1,1230)	1:612:A:ALA:HA	1:611:A:MET:HG3	13	0.62
(1,1177)	1:623:A:GLU:HG2	1:622:A:PHE:HB3	9	0.62
(1,1120)	1:588:A:GLN:HA	1:611:A:MET:HE1	11	0.62
(1,1095)	1:565:A:LYS:HE2	1:566:A:LEU:HD13	17	0.62
(1,968)	1:604:A:THR:HG23	1:603:A:GLN:HB3	5	0.62
(1,956)	1:605:A:GLN:HB3	1:608:A:LEU:HD11	16	0.62
(1,956)	1:605:A:GLN:HB3	1:608:A:LEU:HD11	18	0.62
(1,929)	1:565:A:LYS:HG2	1:566:A:LEU:HD13	16	0.62
(1,906)	1:596:A:PHE:HA	1:599:A:GLN:HG2	9	0.62
(1,586)	1:625:A:TRP:HD1	1:577:A:LEU:HD21	3	0.62
(1,586)	1:625:A:TRP:HD1	1:577:A:LEU:HD23	18	0.62
(1,586)	1:625:A:TRP:HD1	1:577:A:LEU:HD21	19	0.62
(1,300)	1:567:A:GLN:H	1:566:A:LEU:HD22	4	0.62
(1,146)	1:586:A:ALA:H	1:585:A:GLU:HB2	17	0.62
(1,35)	1:598:A:SER:H	1:599:A:GLN:HB3	1	0.62
(1,24)	1:599:A:GLN:H	1:599:A:GLN:HG2	9	0.62
(1,2166)	1:561:A:LYS:HG3	1:562:A:LEU:HD22	9	0.61
(1,2158)	1:591:A:VAL:HG23	1:596:A:PHE:HB2	3	0.61
(1,2118)	1:583:A:LYS:HE2	1:580:A:LEU:HD22	6	0.61
(1,2117)	1:561:A:LYS:HG3	1:561:A:LYS:HD2	4	0.61
(1,2117)	1:551:A:LYS:HG3	1:551:A:LYS:HD3	15	0.61
(1,2093)	1:570:A:LEU:HD22	1:570:A:LEU:HD13	7	0.61
(1,2093)	1:570:A:LEU:HD22	1:570:A:LEU:HD12	9	0.61
(1,2093)	1:587:A:LEU:HD23	1:587:A:LEU:HD12	16	0.61
(1,2042)	1:573:A:LEU:HG	1:570:A:LEU:HA	4	0.61
(1,2042)	1:625:A:TRP:HA	1:573:A:LEU:HG	19	0.61

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1962)	1:610:A:ASP:HB3	1:606:A:LYS:HG2	11	0.61
(1,1934)	1:567:A:GLN:HG3	1:562:A:LEU:HB3	18	0.61
(1,1891)	1:562:A:LEU:HG	1:562:A:LEU:HD11	5	0.61
(1,1891)	1:562:A:LEU:HG	1:562:A:LEU:HD11	19	0.61
(1,1879)	1:565:A:LYS:HG2	1:565:A:LYS:HD2	4	0.61
(1,1865)	1:622:A:PHE:HA	1:623:A:GLU:HA	7	0.61
(1,1853)	1:554:A:THR:HB	1:555:A:VAL:HG12	3	0.61
(1,1836)	1:619:A:GLU:HA	1:618:A:LEU:HD11	3	0.61
(1,1812)	1:632:A:LYS:HA	1:631:A:LEU:HD23	11	0.61
(1,1812)	1:632:A:LYS:HA	1:631:A:LEU:HD21	17	0.61
(1,1758)	1:612:A:ALA:HB1	1:612:A:ALA:HA	5	0.61
(1,1758)	1:609:A:ALA:HB1	1:609:A:ALA:HA	10	0.61
(1,1758)	1:609:A:ALA:HB3	1:609:A:ALA:HA	15	0.61
(1,1723)	1:591:A:VAL:HG13	1:611:A:MET:HG3	1	0.61
(1,1532)	1:573:A:LEU:H	1:573:A:LEU:HD12	5	0.61
(1,1532)	1:573:A:LEU:H	1:573:A:LEU:HD12	19	0.61
(1,1513)	1:579:A:ASP:H	1:576:A:LEU:HG	10	0.61
(1,1467)	1:593:A:ASP:H	1:591:A:VAL:HG12	3	0.61
(1,1466)	1:606:A:LYS:H	1:609:A:ALA:HB2	10	0.61
(1,1457)	1:597:A:PHE:H	1:598:A:SER:HB2	1	0.61
(1,1457)	1:597:A:PHE:H	1:598:A:SER:HB2	6	0.61
(1,1457)	1:597:A:PHE:H	1:598:A:SER:HB2	7	0.61
(1,1397)	1:587:A:LEU:HD12	1:583:A:LYS:HA	14	0.61
(1,1397)	1:587:A:LEU:HD12	1:583:A:LYS:HA	17	0.61
(1,1387)	1:577:A:LEU:HD21	1:574:A:PRO:HB2	10	0.61
(1,1333)	1:573:A:LEU:HD11	1:624:A:ARG:HD2	6	0.61
(1,1333)	1:573:A:LEU:HD13	1:624:A:ARG:HD2	19	0.61
(1,1306)	1:589:A:THR:HG21	1:590:A:GLN:HB2	6	0.61
(1,1291)	1:608:A:LEU:HD12	1:604:A:THR:HG21	15	0.61
(1,1280)	1:573:A:LEU:HD23	1:580:A:LEU:HD12	15	0.61
(1,1271)	1:576:A:LEU:HD13	1:621:A:ALA:HB3	12	0.61
(1,1164)	1:601:A:HIS:HB3	1:605:A:GLN:HG3	20	0.61
(1,1163)	1:599:A:GLN:HG3	1:600:A:PRO:HD3	6	0.61
(1,1120)	1:588:A:GLN:HA	1:611:A:MET:HE3	1	0.61
(1,1120)	1:588:A:GLN:HA	1:611:A:MET:HE2	6	0.61
(1,1111)	1:631:A:LEU:HD21	1:562:A:LEU:HB2	4	0.61
(1,637)	1:604:A:THR:HG23	1:607:A:VAL:HG22	10	0.61
(1,586)	1:625:A:TRP:HD1	1:577:A:LEU:HD23	4	0.61
(1,543)	1:625:A:TRP:HE1	1:570:A:LEU:HD22	19	0.61
(1,317)	1:563:A:SER:H	1:566:A:LEU:HD23	11	0.61
(1,300)	1:567:A:GLN:H	1:566:A:LEU:HD21	6	0.61
(1,35)	1:598:A:SER:H	1:599:A:GLN:HB3	16	0.61

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,35)	1:598:A:SER:H	1:599:A:GLN:HB3	18	0.61
(1,24)	1:599:A:GLN:H	1:599:A:GLN:HG2	10	0.61
(1,2171)	1:591:A:VAL:HG23	1:597:A:PHE:HZ	10	0.6
(1,2166)	1:561:A:LYS:HG3	1:562:A:LEU:HD23	13	0.6
(1,2158)	1:591:A:VAL:HG22	1:596:A:PHE:HB2	2	0.6
(1,2120)	1:573:A:LEU:HD21	1:624:A:ARG:HB2	18	0.6
(1,2117)	1:551:A:LYS:HG2	1:551:A:LYS:HD3	3	0.6
(1,2117)	1:556:A:LYS:HG2	1:556:A:LYS:HD2	17	0.6
(1,2114)	1:581:A:GLU:HG3	1:618:A:LEU:HD12	6	0.6
(1,2103)	1:562:A:LEU:HG	1:562:A:LEU:HD21	1	0.6
(1,2103)	1:562:A:LEU:HG	1:562:A:LEU:HD23	8	0.6
(1,2103)	1:562:A:LEU:HG	1:562:A:LEU:HD21	9	0.6
(1,2103)	1:562:A:LEU:HG	1:562:A:LEU:HD22	18	0.6
(1,2093)	1:570:A:LEU:HD22	1:570:A:LEU:HD13	1	0.6
(1,2093)	1:570:A:LEU:HD22	1:570:A:LEU:HD11	5	0.6
(1,2093)	1:570:A:LEU:HD21	1:570:A:LEU:HD11	6	0.6
(1,2093)	1:570:A:LEU:HD22	1:570:A:LEU:HD12	18	0.6
(1,2025)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	10	0.6
(1,2014)	1:601:A:HIS:HB3	1:602:A:GLU:HB2	20	0.6
(1,2013)	1:565:A:LYS:HA	1:568:A:ARG:HB3	4	0.6
(1,2013)	1:565:A:LYS:HA	1:568:A:ARG:HB3	14	0.6
(1,2013)	1:565:A:LYS:HA	1:568:A:ARG:HB3	15	0.6
(1,2010)	1:551:A:LYS:HE3	1:551:A:LYS:HD2	7	0.6
(1,2010)	1:561:A:LYS:HE2	1:561:A:LYS:HD2	20	0.6
(1,1992)	1:562:A:LEU:HB2	1:631:A:LEU:HG	19	0.6
(1,1982)	1:632:A:LYS:HE2	1:632:A:LYS:HD3	12	0.6
(1,1980)	1:565:A:LYS:HE3	1:565:A:LYS:HD2	20	0.6
(1,1960)	1:622:A:PHE:HB3	1:623:A:GLU:HB2	10	0.6
(1,1958)	1:622:A:PHE:HB3	1:623:A:GLU:HB2	10	0.6
(1,1958)	1:622:A:PHE:HB3	1:623:A:GLU:HB2	14	0.6
(1,1946)	1:581:A:GLU:HG2	1:618:A:LEU:HD22	6	0.6
(1,1937)	1:616:A:GLN:HG3	1:613:A:ALA:HB2	20	0.6
(1,1924)	1:614:A:ALA:HB3	1:611:A:MET:HG2	10	0.6
(1,1898)	1:628:A:LEU:HG	1:631:A:LEU:HB2	5	0.6
(1,1891)	1:562:A:LEU:HG	1:562:A:LEU:HD13	1	0.6
(1,1891)	1:562:A:LEU:HG	1:562:A:LEU:HD13	9	0.6
(1,1880)	1:632:A:LYS:HG2	1:632:A:LYS:HD2	1	0.6
(1,1880)	1:632:A:LYS:HG2	1:632:A:LYS:HD2	9	0.6
(1,1845)	1:554:A:THR:HA	1:555:A:VAL:HG23	16	0.6
(1,1834)	1:583:A:LYS:HA	1:587:A:LEU:HD23	16	0.6
(1,1758)	1:582:A:ALA:HB3	1:582:A:ALA:HA	3	0.6
(1,1758)	1:609:A:ALA:HB2	1:609:A:ALA:HA	4	0.6

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1758)	1:609:A:ALA:HB1	1:609:A:ALA:HA	7	0.6
(1,1758)	1:609:A:ALA:HB1	1:609:A:ALA:HA	11	0.6
(1,1758)	1:582:A:ALA:HB2	1:582:A:ALA:HA	12	0.6
(1,1758)	1:609:A:ALA:HB3	1:609:A:ALA:HA	13	0.6
(1,1758)	1:612:A:ALA:HB1	1:612:A:ALA:HA	17	0.6
(1,1732)	1:607:A:VAL:HG23	1:606:A:LYS:HB2	19	0.6
(1,1712)	1:577:A:LEU:HD23	1:625:A:TRP:HA	8	0.6
(1,1712)	1:577:A:LEU:HD21	1:625:A:TRP:HA	17	0.6
(1,1705)	1:622:A:PHE:HD1	1:577:A:LEU:HD23	8	0.6
(1,1705)	1:622:A:PHE:HD1	1:577:A:LEU:HD23	13	0.6
(1,1704)	1:622:A:PHE:HD2	1:618:A:LEU:HB3	9	0.6
(1,1704)	1:622:A:PHE:HD2	1:618:A:LEU:HB3	20	0.6
(1,1690)	1:564:A:TYR:HE1	1:567:A:GLN:HB2	2	0.6
(1,1690)	1:564:A:TYR:HE1	1:567:A:GLN:HB2	16	0.6
(1,1611)	1:616:A:GLN:H	1:612:A:ALA:HB3	7	0.6
(1,1611)	1:616:A:GLN:H	1:612:A:ALA:HB2	8	0.6
(1,1575)	1:621:A:ALA:H	1:622:A:PHE:HA	12	0.6
(1,1549)	1:567:A:GLN:H	1:568:A:ARG:HA	3	0.6
(1,1544)	1:569:A:GLU:H	1:566:A:LEU:HB3	1	0.6
(1,1532)	1:573:A:LEU:H	1:573:A:LEU:HD12	4	0.6
(1,1532)	1:573:A:LEU:H	1:573:A:LEU:HD13	11	0.6
(1,1513)	1:579:A:ASP:H	1:576:A:LEU:HG	3	0.6
(1,1513)	1:579:A:ASP:H	1:576:A:LEU:HG	8	0.6
(1,1513)	1:579:A:ASP:H	1:576:A:LEU:HG	13	0.6
(1,1506)	1:582:A:ALA:H	1:618:A:LEU:HD11	11	0.6
(1,1469)	1:592:A:ALA:H	1:591:A:VAL:HG11	10	0.6
(1,1468)	1:592:A:ALA:H	1:593:A:ASP:HB3	15	0.6
(1,1457)	1:597:A:PHE:H	1:598:A:SER:HB2	4	0.6
(1,1457)	1:597:A:PHE:H	1:598:A:SER:HB2	10	0.6
(1,1397)	1:587:A:LEU:HD13	1:583:A:LYS:HA	4	0.6
(1,1387)	1:577:A:LEU:HD23	1:574:A:PRO:HB2	17	0.6
(1,1333)	1:573:A:LEU:HD12	1:624:A:ARG:HD2	2	0.6
(1,1325)	1:628:A:LEU:HD11	1:569:A:GLU:HA	14	0.6
(1,1306)	1:589:A:THR:HG21	1:590:A:GLN:HB2	14	0.6
(1,1306)	1:589:A:THR:HG22	1:590:A:GLN:HB2	20	0.6
(1,1303)	1:581:A:GLU:HG3	1:618:A:LEU:HD12	6	0.6
(1,1164)	1:601:A:HIS:HB3	1:605:A:GLN:HG3	14	0.6
(1,1120)	1:588:A:GLN:HA	1:611:A:MET:HE2	10	0.6
(1,1120)	1:588:A:GLN:HA	1:611:A:MET:HE1	16	0.6
(1,1120)	1:588:A:GLN:HA	1:611:A:MET:HE2	18	0.6
(1,1019)	1:604:A:THR:HG22	1:599:A:GLN:HG2	15	0.6
(1,956)	1:605:A:GLN:HB3	1:608:A:LEU:HD11	15	0.6

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,630)	1:577:A:LEU:HD11	1:580:A:LEU:HG	9	0.6
(1,630)	1:577:A:LEU:HD13	1:580:A:LEU:HG	18	0.6
(1,630)	1:577:A:LEU:HD12	1:580:A:LEU:HG	19	0.6
(1,538)	1:635:A:GLY:H	1:631:A:LEU:HD12	7	0.6
(1,317)	1:563:A:SER:H	1:566:A:LEU:HD22	10	0.6
(1,308)	1:566:A:LEU:H	1:566:A:LEU:HD22	18	0.6
(1,300)	1:567:A:GLN:H	1:566:A:LEU:HD22	18	0.6
(1,2160)	1:630:A:ALA:HB3	1:627:A:TYR:HB2	1	0.59
(1,2117)	1:551:A:LYS:HG2	1:551:A:LYS:HD3	12	0.59
(1,2117)	1:556:A:LYS:HG2	1:556:A:LYS:HD3	20	0.59
(1,2103)	1:562:A:LEU:HG	1:562:A:LEU:HD22	13	0.59
(1,2103)	1:562:A:LEU:HG	1:562:A:LEU:HD21	17	0.59
(1,2093)	1:570:A:LEU:HD23	1:570:A:LEU:HD12	8	0.59
(1,2093)	1:570:A:LEU:HD22	1:570:A:LEU:HD12	20	0.59
(1,2078)	1:562:A:LEU:HB3	1:566:A:LEU:HD13	3	0.59
(1,2025)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	2	0.59
(1,2013)	1:565:A:LYS:HA	1:568:A:ARG:HB3	3	0.59
(1,2010)	1:551:A:LYS:HE2	1:551:A:LYS:HD2	11	0.59
(1,2010)	1:556:A:LYS:HE3	1:556:A:LYS:HD2	16	0.59
(1,1995)	1:557:A:ARG:HD2	1:555:A:VAL:HG12	10	0.59
(1,1991)	1:562:A:LEU:HB3	1:566:A:LEU:HD13	3	0.59
(1,1982)	1:632:A:LYS:HE2	1:632:A:LYS:HD3	7	0.59
(1,1982)	1:583:A:LYS:HE2	1:583:A:LYS:HD3	8	0.59
(1,1982)	1:583:A:LYS:HE2	1:583:A:LYS:HD3	15	0.59
(1,1982)	1:632:A:LYS:HE2	1:632:A:LYS:HD3	19	0.59
(1,1980)	1:565:A:LYS:HE2	1:565:A:LYS:HD3	7	0.59
(1,1917)	1:585:A:GLU:HB2	1:584:A:LEU:HD11	14	0.59
(1,1891)	1:562:A:LEU:HG	1:562:A:LEU:HD11	2	0.59
(1,1891)	1:562:A:LEU:HG	1:562:A:LEU:HD13	14	0.59
(1,1888)	1:568:A:ARG:HG2	1:571:A:GLU:HB3	4	0.59
(1,1880)	1:551:A:LYS:HG2	1:551:A:LYS:HD3	11	0.59
(1,1879)	1:565:A:LYS:HG2	1:565:A:LYS:HD3	15	0.59
(1,1865)	1:622:A:PHE:HA	1:623:A:GLU:HA	3	0.59
(1,1852)	1:604:A:THR:HB	1:599:A:GLN:HB2	4	0.59
(1,1812)	1:632:A:LYS:HA	1:631:A:LEU:HD22	5	0.59
(1,1758)	1:609:A:ALA:HB1	1:609:A:ALA:HA	1	0.59
(1,1758)	1:609:A:ALA:HB3	1:609:A:ALA:HA	2	0.59
(1,1758)	1:582:A:ALA:HB2	1:582:A:ALA:HA	6	0.59
(1,1758)	1:612:A:ALA:HB2	1:612:A:ALA:HA	8	0.59
(1,1758)	1:609:A:ALA:HB1	1:609:A:ALA:HA	14	0.59
(1,1758)	1:609:A:ALA:HB2	1:609:A:ALA:HA	16	0.59
(1,1758)	1:582:A:ALA:HB1	1:582:A:ALA:HA	18	0.59

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1758)	1:609:A:ALA:HB3	1:609:A:ALA:HA	19	0.59
(1,1705)	1:622:A:PHE:HE1	1:577:A:LEU:HD23	10	0.59
(1,1705)	1:622:A:PHE:HD1	1:577:A:LEU:HD21	18	0.59
(1,1704)	1:622:A:PHE:HD2	1:618:A:LEU:HB3	7	0.59
(1,1704)	1:622:A:PHE:HD2	1:618:A:LEU:HB3	19	0.59
(1,1690)	1:564:A:TYR:HE1	1:567:A:GLN:HB2	19	0.59
(1,1681)	1:625:A:TRP:HE3	1:577:A:LEU:HD21	5	0.59
(1,1552)	1:567:A:GLN:H	1:568:A:ARG:HB2	12	0.59
(1,1552)	1:567:A:GLN:H	1:566:A:LEU:HG	17	0.59
(1,1532)	1:573:A:LEU:H	1:573:A:LEU:HD11	15	0.59
(1,1513)	1:579:A:ASP:H	1:576:A:LEU:HG	4	0.59
(1,1513)	1:579:A:ASP:H	1:576:A:LEU:HG	18	0.59
(1,1480)	1:588:A:GLN:H	1:586:A:ALA:HB2	14	0.59
(1,1457)	1:597:A:PHE:H	1:598:A:SER:HB2	5	0.59
(1,1397)	1:587:A:LEU:HD13	1:583:A:LYS:HA	12	0.59
(1,1387)	1:577:A:LEU:HD22	1:574:A:PRO:HB2	11	0.59
(1,1325)	1:628:A:LEU:HD13	1:569:A:GLU:HA	2	0.59
(1,1306)	1:589:A:THR:HG22	1:590:A:GLN:HB2	12	0.59
(1,1306)	1:589:A:THR:HG22	1:590:A:GLN:HB2	18	0.59
(1,1288)	1:566:A:LEU:HD23	1:562:A:LEU:HD22	7	0.59
(1,1264)	1:568:A:ARG:HD2	1:564:A:TYR:HA	10	0.59
(1,1250)	1:626:A:GLU:HG2	1:623:A:GLU:HA	19	0.59
(1,1174)	1:623:A:GLU:HG2	1:622:A:PHE:HB2	17	0.59
(1,1164)	1:601:A:HIS:HB3	1:605:A:GLN:HG2	3	0.59
(1,1154)	1:603:A:GLN:HG2	1:600:A:PRO:HB3	10	0.59
(1,1120)	1:588:A:GLN:HA	1:611:A:MET:HE3	19	0.59
(1,1111)	1:631:A:LEU:HD21	1:562:A:LEU:HB3	6	0.59
(1,1019)	1:604:A:THR:HG23	1:599:A:GLN:HG2	19	0.59
(1,630)	1:577:A:LEU:HD12	1:580:A:LEU:HG	5	0.59
(1,586)	1:625:A:TRP:HD1	1:577:A:LEU:HD22	14	0.59
(1,538)	1:635:A:GLY:H	1:631:A:LEU:HD12	10	0.59
(1,2160)	1:630:A:ALA:HB2	1:627:A:TYR:HB2	18	0.58
(1,2120)	1:573:A:LEU:HD23	1:624:A:ARG:HB2	2	0.58
(1,2120)	1:573:A:LEU:HD23	1:624:A:ARG:HB2	7	0.58
(1,2117)	1:561:A:LYS:HG3	1:561:A:LYS:HD2	1	0.58
(1,2117)	1:551:A:LYS:HG3	1:551:A:LYS:HD2	2	0.58
(1,2117)	1:561:A:LYS:HG3	1:561:A:LYS:HD2	7	0.58
(1,2117)	1:561:A:LYS:HG3	1:561:A:LYS:HD2	10	0.58
(1,2117)	1:551:A:LYS:HG2	1:551:A:LYS:HD2	14	0.58
(1,2103)	1:562:A:LEU:HG	1:562:A:LEU:HD22	4	0.58
(1,2103)	1:562:A:LEU:HG	1:562:A:LEU:HD23	6	0.58
(1,2103)	1:562:A:LEU:HG	1:562:A:LEU:HD21	12	0.58

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2093)	1:570:A:LEU:HD23	1:570:A:LEU:HD12	11	0.58
(1,2042)	1:625:A:TRP:HA	1:573:A:LEU:HG	3	0.58
(1,2025)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	20	0.58
(1,2022)	1:599:A:GLN:HG3	1:600:A:PRO:HD2	10	0.58
(1,2014)	1:601:A:HIS:HB3	1:602:A:GLU:HB2	13	0.58
(1,2010)	1:551:A:LYS:HE2	1:551:A:LYS:HD3	8	0.58
(1,2010)	1:556:A:LYS:HE3	1:556:A:LYS:HD2	9	0.58
(1,2010)	1:561:A:LYS:HE2	1:561:A:LYS:HD2	19	0.58
(1,1982)	1:632:A:LYS:HE3	1:632:A:LYS:HD2	3	0.58
(1,1982)	1:583:A:LYS:HE2	1:583:A:LYS:HD3	6	0.58
(1,1980)	1:551:A:LYS:HE2	1:551:A:LYS:HD3	8	0.58
(1,1960)	1:622:A:PHE:HB3	1:619:A:GLU:HB2	7	0.58
(1,1959)	1:622:A:PHE:HB2	1:619:A:GLU:HB2	12	0.58
(1,1958)	1:622:A:PHE:HB3	1:619:A:GLU:HB2	7	0.58
(1,1891)	1:562:A:LEU:HG	1:562:A:LEU:HD23	6	0.58
(1,1891)	1:576:A:LEU:HG	1:580:A:LEU:HD12	10	0.58
(1,1891)	1:562:A:LEU:HG	1:562:A:LEU:HD23	11	0.58
(1,1880)	1:632:A:LYS:HG2	1:632:A:LYS:HD2	2	0.58
(1,1880)	1:551:A:LYS:HG2	1:551:A:LYS:HD2	14	0.58
(1,1880)	1:565:A:LYS:HG3	1:565:A:LYS:HD2	16	0.58
(1,1879)	1:561:A:LYS:HG3	1:561:A:LYS:HD2	1	0.58
(1,1879)	1:561:A:LYS:HG3	1:561:A:LYS:HD2	7	0.58
(1,1879)	1:561:A:LYS:HG3	1:561:A:LYS:HD2	10	0.58
(1,1879)	1:551:A:LYS:HG3	1:551:A:LYS:HD3	14	0.58
(1,1865)	1:622:A:PHE:HA	1:623:A:GLU:HA	10	0.58
(1,1853)	1:554:A:THR:HB	1:555:A:VAL:HG23	14	0.58
(1,1845)	1:554:A:THR:HA	1:555:A:VAL:HG23	19	0.58
(1,1836)	1:619:A:GLU:HA	1:618:A:LEU:HD12	11	0.58
(1,1836)	1:619:A:GLU:HA	1:618:A:LEU:HD12	12	0.58
(1,1758)	1:609:A:ALA:HB3	1:609:A:ALA:HA	20	0.58
(1,1723)	1:591:A:VAL:HG13	1:611:A:MET:HG3	7	0.58
(1,1723)	1:591:A:VAL:HG12	1:607:A:VAL:HB	8	0.58
(1,1665)	1:632:A:LYS:H	1:570:A:LEU:HD13	5	0.58
(1,1633)	1:622:A:PHE:H	1:619:A:GLU:HB3	14	0.58
(1,1621)	1:619:A:GLU:H	1:618:A:LEU:HD22	8	0.58
(1,1538)	1:571:A:GLU:H	1:628:A:LEU:HD13	2	0.58
(1,1538)	1:571:A:GLU:H	1:628:A:LEU:HD13	4	0.58
(1,1534)	1:572:A:GLN:H	1:572:A:GLN:HB3	1	0.58
(1,1532)	1:573:A:LEU:H	1:573:A:LEU:HD12	7	0.58
(1,1506)	1:582:A:ALA:H	1:618:A:LEU:HD13	4	0.58
(1,1480)	1:588:A:GLN:H	1:586:A:ALA:HB2	5	0.58
(1,1469)	1:592:A:ALA:H	1:591:A:VAL:HG11	19	0.58

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1467)	1:593:A:ASP:H	1:591:A:VAL:HG12	12	0.58
(1,1466)	1:606:A:LYS:H	1:609:A:ALA:HB2	12	0.58
(1,1397)	1:587:A:LEU:HD12	1:583:A:LYS:HA	7	0.58
(1,1390)	1:599:A:GLN:HG3	1:600:A:PRO:HD2	10	0.58
(1,1376)	1:566:A:LEU:HD22	1:563:A:SER:HB2	14	0.58
(1,1367)	1:570:A:LEU:HD21	1:628:A:LEU:HB3	3	0.58
(1,1367)	1:570:A:LEU:HD22	1:628:A:LEU:HB3	7	0.58
(1,1326)	1:566:A:LEU:HD22	1:563:A:SER:HB3	4	0.58
(1,1326)	1:566:A:LEU:HD23	1:563:A:SER:HB3	10	0.58
(1,1306)	1:589:A:THR:HG23	1:590:A:GLN:HB2	4	0.58
(1,1230)	1:612:A:ALA:HA	1:611:A:MET:HG3	14	0.58
(1,1120)	1:588:A:GLN:HA	1:611:A:MET:HE3	2	0.58
(1,1120)	1:588:A:GLN:HA	1:611:A:MET:HE2	4	0.58
(1,1095)	1:565:A:LYS:HE2	1:566:A:LEU:HD12	11	0.58
(1,1054)	1:604:A:THR:HG23	1:597:A:PHE:HB2	4	0.58
(1,1019)	1:604:A:THR:HG23	1:599:A:GLN:HG2	2	0.58
(1,840)	1:581:A:GLU:HA	1:618:A:LEU:HD12	14	0.58
(1,809)	1:605:A:GLN:HA	1:608:A:LEU:HD23	18	0.58
(1,630)	1:577:A:LEU:HD13	1:580:A:LEU:HG	12	0.58
(1,572)	1:625:A:TRP:HE3	1:625:A:TRP:HB2	1	0.58
(1,308)	1:566:A:LEU:H	1:566:A:LEU:HD21	13	0.58
(1,2171)	1:591:A:VAL:HG23	1:597:A:PHE:HZ	7	0.57
(1,2166)	1:562:A:LEU:HD13	1:561:A:LYS:HG3	15	0.57
(1,2165)	1:606:A:LYS:HA	1:610:A:ASP:HB2	11	0.57
(1,2120)	1:573:A:LEU:HD22	1:624:A:ARG:HB2	12	0.57
(1,2117)	1:561:A:LYS:HG3	1:561:A:LYS:HD2	8	0.57
(1,2117)	1:556:A:LYS:HG2	1:556:A:LYS:HD3	9	0.57
(1,2014)	1:601:A:HIS:HB3	1:602:A:GLU:HB2	9	0.57
(1,2010)	1:561:A:LYS:HE2	1:561:A:LYS:HD2	14	0.57
(1,2010)	1:551:A:LYS:HE3	1:551:A:LYS:HD2	17	0.57
(1,1982)	1:632:A:LYS:HE2	1:632:A:LYS:HD3	10	0.57
(1,1982)	1:632:A:LYS:HE2	1:632:A:LYS:HD2	11	0.57
(1,1982)	1:583:A:LYS:HE2	1:583:A:LYS:HD3	14	0.57
(1,1982)	1:632:A:LYS:HE2	1:632:A:LYS:HD3	17	0.57
(1,1980)	1:565:A:LYS:HE2	1:565:A:LYS:HD2	9	0.57
(1,1980)	1:561:A:LYS:HE2	1:561:A:LYS:HD2	14	0.57
(1,1980)	1:551:A:LYS:HE3	1:551:A:LYS:HD2	17	0.57
(1,1960)	1:622:A:PHE:HB3	1:619:A:GLU:HB2	4	0.57
(1,1958)	1:622:A:PHE:HB3	1:619:A:GLU:HB2	4	0.57
(1,1947)	1:581:A:GLU:HG2	1:584:A:LEU:HD11	19	0.57
(1,1947)	1:581:A:GLU:HG2	1:584:A:LEU:HD11	20	0.57
(1,1937)	1:616:A:GLN:HG3	1:613:A:ALA:HB1	5	0.57

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1924)	1:614:A:ALA:HB2	1:611:A:MET:HG2	16	0.57
(1,1891)	1:562:A:LEU:HG	1:562:A:LEU:HD11	18	0.57
(1,1886)	1:624:A:ARG:HG3	1:628:A:LEU:HD12	15	0.57
(1,1880)	1:565:A:LYS:HG3	1:565:A:LYS:HD2	6	0.57
(1,1880)	1:565:A:LYS:HG3	1:565:A:LYS:HD2	7	0.57
(1,1880)	1:632:A:LYS:HG2	1:632:A:LYS:HD2	8	0.57
(1,1880)	1:565:A:LYS:HG3	1:565:A:LYS:HD2	13	0.57
(1,1879)	1:565:A:LYS:HG2	1:565:A:LYS:HD3	2	0.57
(1,1879)	1:561:A:LYS:HG3	1:561:A:LYS:HD2	8	0.57
(1,1879)	1:556:A:LYS:HG2	1:556:A:LYS:HD3	9	0.57
(1,1879)	1:565:A:LYS:HG2	1:565:A:LYS:HD2	18	0.57
(1,1865)	1:622:A:PHE:HA	1:623:A:GLU:HA	2	0.57
(1,1853)	1:554:A:THR:HB	1:555:A:VAL:HG11	8	0.57
(1,1836)	1:619:A:GLU:HA	1:618:A:LEU:HD11	4	0.57
(1,1834)	1:583:A:LYS:HA	1:587:A:LEU:HD22	11	0.57
(1,1812)	1:632:A:LYS:HA	1:631:A:LEU:HD23	16	0.57
(1,1758)	1:609:A:ALA:HB1	1:609:A:ALA:HA	9	0.57
(1,1720)	1:604:A:THR:HG22	1:600:A:PRO:HD3	10	0.57
(1,1683)	1:622:A:PHE:HE2	1:618:A:LEU:HD23	15	0.57
(1,1683)	1:622:A:PHE:HE2	1:618:A:LEU:HD21	16	0.57
(1,1630)	1:621:A:ALA:H	1:618:A:LEU:HD21	14	0.57
(1,1611)	1:616:A:GLN:H	1:612:A:ALA:HB1	18	0.57
(1,1575)	1:621:A:ALA:H	1:622:A:PHE:HA	3	0.57
(1,1575)	1:621:A:ALA:H	1:622:A:PHE:HA	7	0.57
(1,1575)	1:621:A:ALA:H	1:622:A:PHE:HA	18	0.57
(1,1562)	1:604:A:THR:H	1:599:A:GLN:HB2	14	0.57
(1,1534)	1:572:A:GLN:H	1:572:A:GLN:HB3	8	0.57
(1,1532)	1:573:A:LEU:H	1:573:A:LEU:HD12	8	0.57
(1,1532)	1:573:A:LEU:H	1:573:A:LEU:HD12	17	0.57
(1,1513)	1:579:A:ASP:H	1:576:A:LEU:HG	12	0.57
(1,1480)	1:588:A:GLN:H	1:586:A:ALA:HB2	9	0.57
(1,1480)	1:588:A:GLN:H	1:586:A:ALA:HB1	15	0.57
(1,1397)	1:587:A:LEU:HD12	1:583:A:LYS:HA	19	0.57
(1,1387)	1:577:A:LEU:HD21	1:574:A:PRO:HB2	9	0.57
(1,1333)	1:573:A:LEU:HD12	1:624:A:ARG:HD2	13	0.57
(1,1333)	1:573:A:LEU:HD11	1:624:A:ARG:HD2	14	0.57
(1,1333)	1:573:A:LEU:HD13	1:624:A:ARG:HD2	17	0.57
(1,1326)	1:566:A:LEU:HD23	1:563:A:SER:HB3	8	0.57
(1,1306)	1:589:A:THR:HG23	1:590:A:GLN:HB2	10	0.57
(1,1306)	1:589:A:THR:HG22	1:590:A:GLN:HB2	17	0.57
(1,1293)	1:577:A:LEU:HD12	1:573:A:LEU:HD13	8	0.57
(1,1291)	1:608:A:LEU:HD12	1:604:A:THR:HG21	3	0.57

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1190)	1:562:A:LEU:HB2	1:632:A:LYS:HA	7	0.57
(1,1164)	1:601:A:HIS:HB3	1:605:A:GLN:HG3	11	0.57
(1,1054)	1:604:A:THR:HG22	1:597:A:PHE:HB2	20	0.57
(1,809)	1:605:A:GLN:HA	1:608:A:LEU:HD22	8	0.57
(1,631)	1:577:A:LEU:HD11	1:622:A:PHE:HB3	2	0.57
(1,572)	1:625:A:TRP:HE3	1:625:A:TRP:HB2	10	0.57
(1,572)	1:625:A:TRP:HE3	1:625:A:TRP:HB2	19	0.57
(1,572)	1:625:A:TRP:HE3	1:625:A:TRP:HB2	20	0.57
(1,308)	1:566:A:LEU:H	1:566:A:LEU:HD23	8	0.57
(1,308)	1:566:A:LEU:H	1:566:A:LEU:HD21	9	0.57
(1,308)	1:566:A:LEU:H	1:566:A:LEU:HD23	20	0.57
(1,238)	1:575:A:GLN:H	1:575:A:GLN:HB3	2	0.57
(1,238)	1:575:A:GLN:H	1:575:A:GLN:HB3	4	0.57
(1,238)	1:575:A:GLN:H	1:575:A:GLN:HB3	9	0.57
(1,238)	1:575:A:GLN:H	1:575:A:GLN:HB3	16	0.57
(1,238)	1:575:A:GLN:H	1:575:A:GLN:HB3	20	0.57
(1,146)	1:586:A:ALA:H	1:585:A:GLU:HB2	13	0.57
(1,92)	1:592:A:ALA:H	1:589:A:THR:HG23	2	0.57
(1,92)	1:592:A:ALA:H	1:589:A:THR:HG23	6	0.57
(1,92)	1:592:A:ALA:H	1:589:A:THR:HG21	11	0.57
(1,2171)	1:591:A:VAL:HG21	1:597:A:PHE:HZ	13	0.56
(1,2163)	1:567:A:GLN:HA	1:570:A:LEU:HD11	1	0.56
(1,2160)	1:630:A:ALA:HB1	1:627:A:TYR:HB2	6	0.56
(1,2135)	1:567:A:GLN:HA	1:570:A:LEU:HD11	1	0.56
(1,2117)	1:551:A:LYS:HG3	1:551:A:LYS:HD2	5	0.56
(1,2117)	1:556:A:LYS:HG2	1:556:A:LYS:HD3	11	0.56
(1,2117)	1:551:A:LYS:HG3	1:551:A:LYS:HD2	16	0.56
(1,2117)	1:556:A:LYS:HG2	1:556:A:LYS:HD3	19	0.56
(1,2109)	1:608:A:LEU:HD11	1:591:A:VAL:HG11	2	0.56
(1,2103)	1:562:A:LEU:HG	1:562:A:LEU:HD23	3	0.56
(1,2103)	1:562:A:LEU:HG	1:562:A:LEU:HD22	20	0.56
(1,2052)	1:603:A:GLN:HG3	1:599:A:GLN:HA	14	0.56
(1,2037)	1:603:A:GLN:HA	1:599:A:GLN:HB2	15	0.56
(1,2014)	1:601:A:HIS:HB3	1:602:A:GLU:HB2	15	0.56
(1,2010)	1:561:A:LYS:HE2	1:561:A:LYS:HD3	1	0.56
(1,2010)	1:561:A:LYS:HE3	1:561:A:LYS:HD2	10	0.56
(1,2010)	1:556:A:LYS:HE2	1:556:A:LYS:HD3	12	0.56
(1,2010)	1:561:A:LYS:HE3	1:561:A:LYS:HD2	13	0.56
(1,1982)	1:632:A:LYS:HE2	1:632:A:LYS:HD3	2	0.56
(1,1982)	1:583:A:LYS:HE2	1:583:A:LYS:HD3	9	0.56
(1,1982)	1:632:A:LYS:HE2	1:632:A:LYS:HD3	20	0.56
(1,1980)	1:561:A:LYS:HE2	1:561:A:LYS:HD3	1	0.56

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1980)	1:556:A:LYS:HE2	1:556:A:LYS:HD3	12	0.56
(1,1980)	1:561:A:LYS:HE3	1:561:A:LYS:HD2	13	0.56
(1,1980)	1:565:A:LYS:HE2	1:565:A:LYS:HD2	19	0.56
(1,1960)	1:622:A:PHE:HB3	1:623:A:GLU:HB2	8	0.56
(1,1958)	1:622:A:PHE:HB3	1:623:A:GLU:HB2	8	0.56
(1,1891)	1:562:A:LEU:HG	1:562:A:LEU:HD23	3	0.56
(1,1891)	1:562:A:LEU:HG	1:562:A:LEU:HD13	4	0.56
(1,1891)	1:562:A:LEU:HG	1:562:A:LEU:HD13	8	0.56
(1,1891)	1:576:A:LEU:HG	1:580:A:LEU:HD13	15	0.56
(1,1891)	1:562:A:LEU:HG	1:562:A:LEU:HD22	16	0.56
(1,1888)	1:568:A:ARG:HG3	1:571:A:GLU:HB3	20	0.56
(1,1880)	1:632:A:LYS:HG2	1:632:A:LYS:HD2	4	0.56
(1,1880)	1:565:A:LYS:HG3	1:565:A:LYS:HD2	5	0.56
(1,1880)	1:632:A:LYS:HG2	1:632:A:LYS:HD3	17	0.56
(1,1880)	1:632:A:LYS:HG2	1:632:A:LYS:HD3	19	0.56
(1,1880)	1:632:A:LYS:HG2	1:632:A:LYS:HD2	20	0.56
(1,1879)	1:551:A:LYS:HG3	1:551:A:LYS:HD2	5	0.56
(1,1879)	1:556:A:LYS:HG2	1:556:A:LYS:HD3	11	0.56
(1,1879)	1:551:A:LYS:HG3	1:551:A:LYS:HD2	16	0.56
(1,1879)	1:565:A:LYS:HG2	1:565:A:LYS:HD3	17	0.56
(1,1879)	1:556:A:LYS:HG2	1:556:A:LYS:HD3	19	0.56
(1,1865)	1:622:A:PHE:HA	1:623:A:GLU:HA	6	0.56
(1,1865)	1:622:A:PHE:HA	1:623:A:GLU:HA	8	0.56
(1,1836)	1:619:A:GLU:HA	1:618:A:LEU:HD11	1	0.56
(1,1836)	1:619:A:GLU:HA	1:618:A:LEU:HD12	19	0.56
(1,1834)	1:583:A:LYS:HA	1:587:A:LEU:HD21	3	0.56
(1,1812)	1:632:A:LYS:HA	1:631:A:LEU:HD22	9	0.56
(1,1779)	1:614:A:ALA:HA	1:580:A:LEU:HD13	14	0.56
(1,1712)	1:577:A:LEU:HD23	1:625:A:TRP:HA	1	0.56
(1,1712)	1:577:A:LEU:HD21	1:625:A:TRP:HA	5	0.56
(1,1712)	1:577:A:LEU:HD23	1:625:A:TRP:HA	11	0.56
(1,1712)	1:577:A:LEU:HD21	1:625:A:TRP:HA	16	0.56
(1,1704)	1:622:A:PHE:HD2	1:618:A:LEU:HB3	8	0.56
(1,1691)	1:627:A:TYR:HE1	1:627:A:TYR:HA	9	0.56
(1,1690)	1:564:A:TYR:HE1	1:567:A:GLN:HB3	17	0.56
(1,1621)	1:619:A:GLU:H	1:618:A:LEU:HD22	2	0.56
(1,1611)	1:616:A:GLN:H	1:612:A:ALA:HB1	10	0.56
(1,1611)	1:616:A:GLN:H	1:612:A:ALA:HB3	19	0.56
(1,1575)	1:621:A:ALA:H	1:622:A:PHE:HA	8	0.56
(1,1575)	1:621:A:ALA:H	1:622:A:PHE:HA	11	0.56
(1,1575)	1:621:A:ALA:H	1:622:A:PHE:HA	17	0.56
(1,1532)	1:573:A:LEU:H	1:573:A:LEU:HD11	2	0.56

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1510)	1:581:A:GLU:H	1:582:A:ALA:HB1	12	0.56
(1,1480)	1:588:A:GLN:H	1:586:A:ALA:HB3	6	0.56
(1,1480)	1:588:A:GLN:H	1:586:A:ALA:HB1	8	0.56
(1,1480)	1:588:A:GLN:H	1:586:A:ALA:HB3	11	0.56
(1,1457)	1:597:A:PHE:H	1:598:A:SER:HB2	8	0.56
(1,1457)	1:597:A:PHE:H	1:598:A:SER:HB2	11	0.56
(1,1451)	1:599:A:GLN:H	1:597:A:PHE:HB2	15	0.56
(1,1431)	1:622:A:PHE:HE2	1:618:A:LEU:HD23	15	0.56
(1,1431)	1:622:A:PHE:HE2	1:618:A:LEU:HD21	16	0.56
(1,1405)	1:606:A:LYS:HD2	1:607:A:VAL:HG21	5	0.56
(1,1397)	1:587:A:LEU:HD11	1:583:A:LYS:HA	15	0.56
(1,1396)	1:632:A:LYS:HG3	1:562:A:LEU:HB3	2	0.56
(1,1376)	1:566:A:LEU:HD21	1:563:A:SER:HB2	13	0.56
(1,1335)	1:566:A:LEU:HG	1:562:A:LEU:HD23	16	0.56
(1,1325)	1:628:A:LEU:HD12	1:569:A:GLU:HA	15	0.56
(1,1306)	1:589:A:THR:HG23	1:590:A:GLN:HB2	9	0.56
(1,1306)	1:589:A:THR:HG21	1:590:A:GLN:HB2	11	0.56
(1,1293)	1:577:A:LEU:HD12	1:573:A:LEU:HD11	14	0.56
(1,1120)	1:588:A:GLN:HA	1:611:A:MET:HE1	17	0.56
(1,1019)	1:604:A:THR:HG23	1:599:A:GLN:HG2	5	0.56
(1,1019)	1:604:A:THR:HG22	1:599:A:GLN:HG2	10	0.56
(1,1019)	1:604:A:THR:HG23	1:599:A:GLN:HG2	12	0.56
(1,968)	1:604:A:THR:HG21	1:603:A:GLN:HB3	7	0.56
(1,838)	1:623:A:GLU:HA	1:626:A:GLU:HB3	5	0.56
(1,809)	1:605:A:GLN:HA	1:608:A:LEU:HD22	14	0.56
(1,631)	1:577:A:LEU:HD12	1:622:A:PHE:HB3	8	0.56
(1,631)	1:577:A:LEU:HD12	1:622:A:PHE:HB3	20	0.56
(1,308)	1:566:A:LEU:H	1:566:A:LEU:HD22	12	0.56
(1,238)	1:575:A:GLN:H	1:575:A:GLN:HB3	7	0.56
(1,238)	1:575:A:GLN:H	1:575:A:GLN:HB3	11	0.56
(1,238)	1:575:A:GLN:H	1:575:A:GLN:HB3	15	0.56
(1,238)	1:575:A:GLN:H	1:575:A:GLN:HB3	17	0.56
(1,92)	1:592:A:ALA:H	1:589:A:THR:HG22	1	0.56
(1,35)	1:598:A:SER:H	1:599:A:GLN:HB3	6	0.56
(1,2163)	1:567:A:GLN:HA	1:570:A:LEU:HD13	3	0.55
(1,2163)	1:567:A:GLN:HA	1:570:A:LEU:HD12	5	0.55
(1,2135)	1:567:A:GLN:HA	1:570:A:LEU:HD13	3	0.55
(1,2135)	1:567:A:GLN:HA	1:570:A:LEU:HD12	5	0.55
(1,2120)	1:573:A:LEU:HD22	1:624:A:ARG:HB2	14	0.55
(1,2103)	1:562:A:LEU:HB3	1:562:A:LEU:HD23	11	0.55
(1,2093)	1:570:A:LEU:HD21	1:570:A:LEU:HD11	2	0.55
(1,2025)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	1	0.55

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2010)	1:561:A:LYS:HE2	1:561:A:LYS:HD3	2	0.55
(1,2010)	1:561:A:LYS:HE2	1:561:A:LYS:HD3	3	0.55
(1,2010)	1:556:A:LYS:HE3	1:556:A:LYS:HD3	5	0.55
(1,2010)	1:551:A:LYS:HE3	1:551:A:LYS:HD2	18	0.55
(1,1982)	1:583:A:LYS:HE2	1:583:A:LYS:HD3	4	0.55
(1,1982)	1:583:A:LYS:HE2	1:583:A:LYS:HD3	13	0.55
(1,1980)	1:561:A:LYS:HE2	1:561:A:LYS:HD3	2	0.55
(1,1980)	1:561:A:LYS:HE2	1:561:A:LYS:HD3	3	0.55
(1,1980)	1:556:A:LYS:HE3	1:556:A:LYS:HD3	5	0.55
(1,1980)	1:565:A:LYS:HE2	1:565:A:LYS:HD3	11	0.55
(1,1980)	1:565:A:LYS:HE3	1:565:A:LYS:HD2	16	0.55
(1,1980)	1:551:A:LYS:HE3	1:551:A:LYS:HD2	18	0.55
(1,1965)	1:579:A:ASP:HB2	1:576:A:LEU:HG	7	0.55
(1,1965)	1:579:A:ASP:HB2	1:576:A:LEU:HG	18	0.55
(1,1960)	1:622:A:PHE:HB3	1:619:A:GLU:HB2	2	0.55
(1,1958)	1:622:A:PHE:HB3	1:619:A:GLU:HB2	2	0.55
(1,1902)	1:567:A:GLN:HB2	1:562:A:LEU:HB2	10	0.55
(1,1891)	1:562:A:LEU:HG	1:562:A:LEU:HD12	12	0.55
(1,1891)	1:562:A:LEU:HG	1:562:A:LEU:HD13	17	0.55
(1,1880)	1:556:A:LYS:HG3	1:556:A:LYS:HD2	12	0.55
(1,1865)	1:622:A:PHE:HA	1:623:A:GLU:HA	18	0.55
(1,1853)	1:554:A:THR:HB	1:555:A:VAL:HG21	2	0.55
(1,1853)	1:554:A:THR:HB	1:555:A:VAL:HG11	13	0.55
(1,1853)	1:554:A:THR:HB	1:555:A:VAL:HG22	20	0.55
(1,1852)	1:604:A:THR:HB	1:599:A:GLN:HB2	13	0.55
(1,1846)	1:622:A:PHE:HA	1:618:A:LEU:HD21	14	0.55
(1,1812)	1:632:A:LYS:HA	1:631:A:LEU:HD21	4	0.55
(1,1730)	1:607:A:VAL:HG21	1:587:A:LEU:HD22	13	0.55
(1,1723)	1:591:A:VAL:HG12	1:611:A:MET:HG3	10	0.55
(1,1717)	1:604:A:THR:HG22	1:603:A:GLN:HB3	13	0.55
(1,1705)	1:622:A:PHE:HD1	1:577:A:LEU:HD21	17	0.55
(1,1665)	1:632:A:LYS:H	1:562:A:LEU:HD22	19	0.55
(1,1611)	1:616:A:GLN:H	1:612:A:ALA:HB3	12	0.55
(1,1611)	1:616:A:GLN:H	1:612:A:ALA:HB2	16	0.55
(1,1588)	1:613:A:ALA:H	1:611:A:MET:HB2	7	0.55
(1,1575)	1:621:A:ALA:H	1:622:A:PHE:HA	6	0.55
(1,1575)	1:621:A:ALA:H	1:622:A:PHE:HA	14	0.55
(1,1569)	1:607:A:VAL:H	1:608:A:LEU:HD23	12	0.55
(1,1562)	1:604:A:THR:H	1:599:A:GLN:HB2	5	0.55
(1,1553)	1:566:A:LEU:H	1:566:A:LEU:HG	1	0.55
(1,1535)	1:572:A:GLN:H	1:573:A:LEU:HD12	20	0.55
(1,1532)	1:573:A:LEU:H	1:573:A:LEU:HD11	12	0.55

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1515)	1:579:A:ASP:H	1:576:A:LEU:HD13	10	0.55
(1,1510)	1:581:A:GLU:H	1:582:A:ALA:HB2	11	0.55
(1,1506)	1:582:A:ALA:H	1:618:A:LEU:HD13	1	0.55
(1,1469)	1:592:A:ALA:H	1:591:A:VAL:HG12	3	0.55
(1,1469)	1:592:A:ALA:H	1:591:A:VAL:HG12	9	0.55
(1,1467)	1:593:A:ASP:H	1:591:A:VAL:HG13	15	0.55
(1,1457)	1:597:A:PHE:H	1:598:A:SER:HB2	15	0.55
(1,1457)	1:597:A:PHE:H	1:598:A:SER:HB2	17	0.55
(1,1449)	1:603:A:GLN:H	1:605:A:GLN:HB2	20	0.55
(1,1412)	1:584:A:LEU:HD23	1:615:A:GLU:HB2	7	0.55
(1,1397)	1:587:A:LEU:HD11	1:583:A:LYS:HA	8	0.55
(1,1387)	1:577:A:LEU:HD22	1:574:A:PRO:HB2	8	0.55
(1,1378)	1:624:A:ARG:HD3	1:573:A:LEU:HD13	8	0.55
(1,1376)	1:566:A:LEU:HD22	1:563:A:SER:HB2	19	0.55
(1,1325)	1:628:A:LEU:HD13	1:569:A:GLU:HA	17	0.55
(1,1291)	1:608:A:LEU:HD12	1:604:A:THR:HG22	17	0.55
(1,1164)	1:601:A:HIS:HB3	1:605:A:GLN:HG2	19	0.55
(1,1111)	1:631:A:LEU:HD23	1:562:A:LEU:HB2	18	0.55
(1,1062)	1:610:A:ASP:HB2	1:587:A:LEU:HD21	6	0.55
(1,1054)	1:604:A:THR:HG21	1:597:A:PHE:HB2	16	0.55
(1,1054)	1:604:A:THR:HG21	1:597:A:PHE:HB2	19	0.55
(1,1019)	1:604:A:THR:HG22	1:599:A:GLN:HG2	1	0.55
(1,1019)	1:604:A:THR:HG21	1:599:A:GLN:HG2	14	0.55
(1,970)	1:632:A:LYS:HD3	1:570:A:LEU:HD13	8	0.55
(1,968)	1:604:A:THR:HG22	1:603:A:GLN:HB3	13	0.55
(1,809)	1:605:A:GLN:HA	1:608:A:LEU:HD21	3	0.55
(1,809)	1:605:A:GLN:HA	1:608:A:LEU:HD23	4	0.55
(1,755)	1:621:A:ALA:HA	1:576:A:LEU:HD23	1	0.55
(1,631)	1:577:A:LEU:HD11	1:622:A:PHE:HB3	3	0.55
(1,630)	1:577:A:LEU:HD11	1:580:A:LEU:HG	6	0.55
(1,630)	1:577:A:LEU:HD11	1:580:A:LEU:HG	13	0.55
(1,586)	1:625:A:TRP:HD1	1:577:A:LEU:HD23	7	0.55
(1,572)	1:625:A:TRP:HE3	1:625:A:TRP:HB2	4	0.55
(1,572)	1:625:A:TRP:HE3	1:625:A:TRP:HB2	9	0.55
(1,572)	1:625:A:TRP:HE3	1:625:A:TRP:HB2	17	0.55
(1,538)	1:635:A:GLY:H	1:631:A:LEU:HD13	9	0.55
(1,348)	1:607:A:VAL:H	1:607:A:VAL:HG13	6	0.55
(1,348)	1:607:A:VAL:H	1:607:A:VAL:HG11	10	0.55
(1,348)	1:607:A:VAL:H	1:607:A:VAL:HG12	12	0.55
(1,348)	1:607:A:VAL:H	1:607:A:VAL:HG11	16	0.55
(1,300)	1:567:A:GLN:H	1:566:A:LEU:HD21	1	0.55
(1,300)	1:567:A:GLN:H	1:566:A:LEU:HD23	8	0.55

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,262)	1:571:A:GLU:H	1:571:A:GLU:HG2	12	0.55
(1,248)	1:573:A:LEU:H	1:572:A:GLN:HB2	5	0.55
(1,238)	1:575:A:GLN:H	1:575:A:GLN:HB3	3	0.55
(1,238)	1:575:A:GLN:H	1:575:A:GLN:HB3	10	0.55
(1,238)	1:575:A:GLN:H	1:575:A:GLN:HB3	18	0.55
(1,125)	1:589:A:THR:H	1:586:A:ALA:HB3	3	0.55
(1,92)	1:592:A:ALA:H	1:589:A:THR:HG23	13	0.55
(1,24)	1:599:A:GLN:H	1:599:A:GLN:HG2	3	0.55
(1,2117)	1:561:A:LYS:HG3	1:561:A:LYS:HD2	6	0.54
(1,2117)	1:561:A:LYS:HG3	1:561:A:LYS:HD2	13	0.54
(1,2109)	1:608:A:LEU:HD12	1:591:A:VAL:HG11	5	0.54
(1,2109)	1:608:A:LEU:HD12	1:591:A:VAL:HG12	15	0.54
(1,2042)	1:573:A:LEU:HG	1:570:A:LEU:HA	7	0.54
(1,2042)	1:573:A:LEU:HG	1:570:A:LEU:HA	14	0.54
(1,2042)	1:573:A:LEU:HG	1:570:A:LEU:HA	20	0.54
(1,2034)	1:618:A:LEU:HG	1:615:A:GLU:HA	8	0.54
(1,2034)	1:618:A:LEU:HG	1:615:A:GLU:HA	16	0.54
(1,2013)	1:565:A:LYS:HA	1:568:A:ARG:HB3	11	0.54
(1,2013)	1:565:A:LYS:HA	1:568:A:ARG:HB3	19	0.54
(1,2010)	1:556:A:LYS:HE3	1:556:A:LYS:HD2	6	0.54
(1,2010)	1:556:A:LYS:HE3	1:556:A:LYS:HD2	15	0.54
(1,1982)	1:632:A:LYS:HE2	1:632:A:LYS:HD3	5	0.54
(1,1982)	1:632:A:LYS:HE2	1:632:A:LYS:HD3	18	0.54
(1,1980)	1:556:A:LYS:HE3	1:556:A:LYS:HD2	6	0.54
(1,1965)	1:579:A:ASP:HB2	1:576:A:LEU:HG	1	0.54
(1,1965)	1:579:A:ASP:HB2	1:576:A:LEU:HG	16	0.54
(1,1937)	1:616:A:GLN:HG3	1:613:A:ALA:HB3	7	0.54
(1,1924)	1:614:A:ALA:HB2	1:611:A:MET:HG2	3	0.54
(1,1902)	1:567:A:GLN:HB2	1:562:A:LEU:HB3	3	0.54
(1,1902)	1:567:A:GLN:HB2	1:562:A:LEU:HB2	15	0.54
(1,1891)	1:562:A:LEU:HG	1:562:A:LEU:HD12	13	0.54
(1,1891)	1:562:A:LEU:HG	1:562:A:LEU:HD11	20	0.54
(1,1879)	1:561:A:LYS:HG3	1:561:A:LYS:HD2	6	0.54
(1,1879)	1:561:A:LYS:HG3	1:561:A:LYS:HD2	13	0.54
(1,1865)	1:622:A:PHE:HA	1:623:A:GLU:HA	12	0.54
(1,1865)	1:622:A:PHE:HA	1:619:A:GLU:HA	16	0.54
(1,1852)	1:604:A:THR:HB	1:608:A:LEU:HB2	8	0.54
(1,1834)	1:583:A:LYS:HA	1:587:A:LEU:HD22	12	0.54
(1,1812)	1:632:A:LYS:HA	1:631:A:LEU:HD21	13	0.54
(1,1763)	1:621:A:ALA:HB2	1:617:A:GLU:HG2	1	0.54
(1,1741)	1:628:A:LEU:HD21	1:624:A:ARG:HA	20	0.54
(1,1730)	1:607:A:VAL:HG21	1:587:A:LEU:HD23	9	0.54

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1712)	1:577:A:LEU:HD23	1:625:A:TRP:HA	13	0.54
(1,1705)	1:622:A:PHE:HE1	1:577:A:LEU:HD22	6	0.54
(1,1705)	1:622:A:PHE:HD1	1:577:A:LEU:HD22	9	0.54
(1,1704)	1:622:A:PHE:HD2	1:618:A:LEU:HB3	17	0.54
(1,1575)	1:621:A:ALA:H	1:622:A:PHE:HA	9	0.54
(1,1575)	1:621:A:ALA:H	1:622:A:PHE:HA	13	0.54
(1,1575)	1:621:A:ALA:H	1:622:A:PHE:HA	15	0.54
(1,1545)	1:569:A:GLU:H	1:628:A:LEU:HD13	9	0.54
(1,1533)	1:572:A:GLN:H	1:572:A:GLN:HB2	4	0.54
(1,1532)	1:573:A:LEU:H	1:573:A:LEU:HD12	20	0.54
(1,1506)	1:582:A:ALA:H	1:618:A:LEU:HD13	5	0.54
(1,1506)	1:582:A:ALA:H	1:618:A:LEU:HD12	10	0.54
(1,1480)	1:588:A:GLN:H	1:586:A:ALA:HB3	4	0.54
(1,1468)	1:592:A:ALA:H	1:593:A:ASP:HB3	2	0.54
(1,1468)	1:592:A:ALA:H	1:593:A:ASP:HB2	6	0.54
(1,1468)	1:592:A:ALA:H	1:593:A:ASP:HB3	11	0.54
(1,1457)	1:597:A:PHE:H	1:598:A:SER:HB2	14	0.54
(1,1376)	1:566:A:LEU:HD23	1:563:A:SER:HB2	8	0.54
(1,1306)	1:589:A:THR:HG22	1:590:A:GLN:HB2	1	0.54
(1,1291)	1:608:A:LEU:HD11	1:604:A:THR:HG23	14	0.54
(1,1264)	1:568:A:ARG:HD2	1:564:A:TYR:HA	12	0.54
(1,1165)	1:601:A:HIS:HB2	1:605:A:GLN:HG2	14	0.54
(1,1164)	1:601:A:HIS:HB3	1:605:A:GLN:HG2	15	0.54
(1,975)	1:615:A:GLU:HB2	1:584:A:LEU:HD12	15	0.54
(1,572)	1:625:A:TRP:HE3	1:625:A:TRP:HB2	3	0.54
(1,572)	1:625:A:TRP:HE3	1:625:A:TRP:HB2	18	0.54
(1,348)	1:607:A:VAL:H	1:607:A:VAL:HG13	1	0.54
(1,348)	1:607:A:VAL:H	1:607:A:VAL:HG13	5	0.54
(1,348)	1:607:A:VAL:H	1:607:A:VAL:HG13	7	0.54
(1,348)	1:607:A:VAL:H	1:607:A:VAL:HG12	13	0.54
(1,348)	1:607:A:VAL:H	1:607:A:VAL:HG12	18	0.54
(1,300)	1:567:A:GLN:H	1:566:A:LEU:HD23	17	0.54
(1,300)	1:567:A:GLN:H	1:566:A:LEU:HD22	19	0.54
(1,238)	1:575:A:GLN:H	1:575:A:GLN:HB3	6	0.54
(1,238)	1:575:A:GLN:H	1:575:A:GLN:HB3	8	0.54
(1,154)	1:585:A:GLU:H	1:584:A:LEU:HB2	14	0.54
(1,146)	1:586:A:ALA:H	1:585:A:GLU:HB2	1	0.54
(1,146)	1:586:A:ALA:H	1:585:A:GLU:HB2	8	0.54
(1,92)	1:592:A:ALA:H	1:589:A:THR:HG22	4	0.54
(1,24)	1:599:A:GLN:H	1:599:A:GLN:HG2	2	0.54
(1,24)	1:599:A:GLN:H	1:599:A:GLN:HG2	13	0.54
(1,2118)	1:583:A:LYS:HE2	1:580:A:LEU:HD23	16	0.53

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2109)	1:608:A:LEU:HD12	1:591:A:VAL:HG11	3	0.53
(1,2103)	1:562:A:LEU:HB3	1:562:A:LEU:HD22	16	0.53
(1,2103)	1:562:A:LEU:HB3	1:562:A:LEU:HD21	19	0.53
(1,2025)	1:602:A:GLU:HG2	1:601:A:HIS:HB2	8	0.53
(1,1982)	1:632:A:LYS:HE3	1:632:A:LYS:HD2	1	0.53
(1,1958)	1:622:A:PHE:HB3	1:619:A:GLU:HB2	11	0.53
(1,1901)	1:613:A:ALA:HB2	1:616:A:GLN:HB2	14	0.53
(1,1895)	1:570:A:LEU:HG	1:573:A:LEU:HB2	12	0.53
(1,1894)	1:562:A:LEU:HG	1:567:A:GLN:HG3	11	0.53
(1,1879)	1:565:A:LYS:HG2	1:565:A:LYS:HD3	20	0.53
(1,1853)	1:554:A:THR:HB	1:555:A:VAL:HG21	1	0.53
(1,1836)	1:619:A:GLU:HA	1:618:A:LEU:HD11	5	0.53
(1,1812)	1:632:A:LYS:HA	1:631:A:LEU:HD21	3	0.53
(1,1807)	1:587:A:LEU:HA	1:590:A:GLN:HB2	15	0.53
(1,1794)	1:566:A:LEU:HA	1:562:A:LEU:HG	14	0.53
(1,1778)	1:612:A:ALA:HA	1:584:A:LEU:HD22	4	0.53
(1,1741)	1:628:A:LEU:HD23	1:624:A:ARG:HA	17	0.53
(1,1705)	1:622:A:PHE:HE1	1:577:A:LEU:HD21	14	0.53
(1,1691)	1:627:A:TYR:HE1	1:627:A:TYR:HA	7	0.53
(1,1691)	1:627:A:TYR:HE1	1:627:A:TYR:HA	12	0.53
(1,1690)	1:564:A:TYR:HE1	1:567:A:GLN:HB3	18	0.53
(1,1678)	1:627:A:TYR:HE1	1:631:A:LEU:HG	12	0.53
(1,1621)	1:619:A:GLU:H	1:618:A:LEU:HD23	6	0.53
(1,1621)	1:619:A:GLU:H	1:618:A:LEU:HD21	20	0.53
(1,1588)	1:583:A:LYS:H	1:581:A:GLU:HG2	19	0.53
(1,1575)	1:621:A:ALA:H	1:622:A:PHE:HA	2	0.53
(1,1575)	1:621:A:ALA:H	1:622:A:PHE:HA	10	0.53
(1,1538)	1:571:A:GLU:H	1:570:A:LEU:HD12	19	0.53
(1,1532)	1:573:A:LEU:H	1:573:A:LEU:HD13	3	0.53
(1,1513)	1:579:A:ASP:H	1:576:A:LEU:HG	15	0.53
(1,1506)	1:582:A:ALA:H	1:618:A:LEU:HD12	13	0.53
(1,1469)	1:592:A:ALA:H	1:591:A:VAL:HG12	5	0.53
(1,1468)	1:592:A:ALA:H	1:593:A:ASP:HB2	1	0.53
(1,1465)	1:606:A:LYS:H	1:606:A:LYS:HG2	9	0.53
(1,1465)	1:606:A:LYS:H	1:606:A:LYS:HG2	11	0.53
(1,1397)	1:587:A:LEU:HD11	1:583:A:LYS:HA	11	0.53
(1,1387)	1:577:A:LEU:HD21	1:574:A:PRO:HB2	19	0.53
(1,1376)	1:566:A:LEU:HD22	1:563:A:SER:HB2	12	0.53
(1,1333)	1:573:A:LEU:HD13	1:624:A:ARG:HD2	18	0.53
(1,1325)	1:628:A:LEU:HD13	1:569:A:GLU:HA	4	0.53
(1,1291)	1:608:A:LEU:HD12	1:604:A:THR:HG21	8	0.53
(1,1165)	1:601:A:HIS:HB2	1:605:A:GLN:HG2	20	0.53

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1111)	1:631:A:LEU:HD21	1:562:A:LEU:HB2	17	0.53
(1,1019)	1:604:A:THR:HG22	1:599:A:GLN:HG2	3	0.53
(1,1019)	1:604:A:THR:HG21	1:599:A:GLN:HG2	18	0.53
(1,1019)	1:604:A:THR:HG23	1:599:A:GLN:HG2	20	0.53
(1,809)	1:605:A:GLN:HA	1:608:A:LEU:HD21	11	0.53
(1,755)	1:621:A:ALA:HA	1:576:A:LEU:HD23	4	0.53
(1,755)	1:621:A:ALA:HA	1:576:A:LEU:HD22	18	0.53
(1,630)	1:577:A:LEU:HD11	1:580:A:LEU:HG	17	0.53
(1,572)	1:625:A:TRP:HE3	1:625:A:TRP:HB2	12	0.53
(1,572)	1:625:A:TRP:HE3	1:625:A:TRP:HB2	13	0.53
(1,572)	1:625:A:TRP:HE3	1:625:A:TRP:HB2	15	0.53
(1,348)	1:607:A:VAL:H	1:607:A:VAL:HG12	14	0.53
(1,348)	1:607:A:VAL:H	1:607:A:VAL:HG12	17	0.53
(1,238)	1:575:A:GLN:H	1:575:A:GLN:HB3	1	0.53
(1,92)	1:592:A:ALA:H	1:589:A:THR:HG21	14	0.53
(1,44)	1:597:A:PHE:H	1:597:A:PHE:HB3	1	0.53
(1,44)	1:597:A:PHE:H	1:597:A:PHE:HB3	8	0.53
(1,44)	1:597:A:PHE:H	1:597:A:PHE:HB3	15	0.53
(1,24)	1:599:A:GLN:H	1:599:A:GLN:HG2	11	0.53
(1,2166)	1:562:A:LEU:HD13	1:561:A:LYS:HG3	7	0.52
(1,2103)	1:562:A:LEU:HB3	1:562:A:LEU:HD21	14	0.52
(1,2103)	1:562:A:LEU:HB3	1:562:A:LEU:HD23	15	0.52
(1,2052)	1:603:A:GLN:HG3	1:600:A:PRO:HA	5	0.52
(1,2034)	1:618:A:LEU:HG	1:581:A:GLU:HA	12	0.52
(1,2025)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	16	0.52
(1,1982)	1:583:A:LYS:HE2	1:583:A:LYS:HD3	16	0.52
(1,1980)	1:565:A:LYS:HE3	1:565:A:LYS:HD2	10	0.52
(1,1980)	1:565:A:LYS:HE3	1:565:A:LYS:HD2	15	0.52
(1,1961)	1:610:A:ASP:HB3	1:587:A:LEU:HB3	6	0.52
(1,1958)	1:622:A:PHE:HB3	1:623:A:GLU:HB2	17	0.52
(1,1944)	1:585:A:GLU:HG3	1:586:A:ALA:HB1	20	0.52
(1,1939)	1:572:A:GLN:HG3	1:568:A:ARG:HG3	10	0.52
(1,1924)	1:614:A:ALA:HB1	1:611:A:MET:HG2	19	0.52
(1,1880)	1:556:A:LYS:HG3	1:556:A:LYS:HD2	15	0.52
(1,1845)	1:554:A:THR:HA	1:555:A:VAL:HG11	17	0.52
(1,1741)	1:628:A:LEU:HD22	1:624:A:ARG:HA	13	0.52
(1,1705)	1:622:A:PHE:HD1	1:577:A:LEU:HD22	19	0.52
(1,1704)	1:622:A:PHE:HD2	1:618:A:LEU:HB3	11	0.52
(1,1691)	1:627:A:TYR:HE1	1:627:A:TYR:HA	13	0.52
(1,1633)	1:622:A:PHE:H	1:623:A:GLU:HB3	20	0.52
(1,1592)	1:613:A:ALA:H	1:616:A:GLN:HB2	18	0.52
(1,1575)	1:621:A:ALA:H	1:622:A:PHE:HA	1	0.52

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1569)	1:607:A:VAL:H	1:608:A:LEU:HD21	17	0.52
(1,1549)	1:567:A:GLN:H	1:568:A:ARG:HA	10	0.52
(1,1532)	1:573:A:LEU:H	1:573:A:LEU:HD13	9	0.52
(1,1526)	1:576:A:LEU:H	1:576:A:LEU:HD23	3	0.52
(1,1513)	1:579:A:ASP:H	1:576:A:LEU:HG	11	0.52
(1,1510)	1:581:A:GLU:H	1:582:A:ALA:HB2	14	0.52
(1,1480)	1:588:A:GLN:H	1:586:A:ALA:HB1	16	0.52
(1,1480)	1:588:A:GLN:H	1:586:A:ALA:HB1	17	0.52
(1,1468)	1:592:A:ALA:H	1:593:A:ASP:HB3	18	0.52
(1,1465)	1:606:A:LYS:H	1:606:A:LYS:HG2	13	0.52
(1,1465)	1:606:A:LYS:H	1:606:A:LYS:HG2	14	0.52
(1,1465)	1:606:A:LYS:H	1:606:A:LYS:HG2	18	0.52
(1,1399)	1:583:A:LYS:HG2	1:580:A:LEU:HD22	18	0.52
(1,1387)	1:577:A:LEU:HD23	1:574:A:PRO:HB2	18	0.52
(1,1369)	1:591:A:VAL:HG21	1:596:A:PHE:HB2	4	0.52
(1,1369)	1:591:A:VAL:HG23	1:596:A:PHE:HB2	7	0.52
(1,1326)	1:566:A:LEU:HD22	1:563:A:SER:HB3	12	0.52
(1,1265)	1:593:A:ASP:HB3	1:595:A:SER:HB2	3	0.52
(1,1163)	1:599:A:GLN:HG3	1:600:A:PRO:HD3	11	0.52
(1,1154)	1:603:A:GLN:HG2	1:600:A:PRO:HB3	7	0.52
(1,1147)	1:565:A:LYS:HA	1:565:A:LYS:HD3	18	0.52
(1,1111)	1:631:A:LEU:HD21	1:562:A:LEU:HB2	12	0.52
(1,1019)	1:604:A:THR:HG22	1:599:A:GLN:HG2	6	0.52
(1,755)	1:621:A:ALA:HA	1:576:A:LEU:HD22	5	0.52
(1,725)	1:600:A:PRO:HD3	1:599:A:GLN:HB2	7	0.52
(1,572)	1:625:A:TRP:HE3	1:625:A:TRP:HB2	7	0.52
(1,572)	1:625:A:TRP:HE3	1:625:A:TRP:HB2	11	0.52
(1,572)	1:625:A:TRP:HE3	1:625:A:TRP:HB2	16	0.52
(1,348)	1:607:A:VAL:H	1:607:A:VAL:HG11	2	0.52
(1,348)	1:607:A:VAL:H	1:607:A:VAL:HG12	3	0.52
(1,348)	1:607:A:VAL:H	1:607:A:VAL:HG12	8	0.52
(1,348)	1:607:A:VAL:H	1:607:A:VAL:HG12	9	0.52
(1,348)	1:607:A:VAL:H	1:607:A:VAL:HG13	11	0.52
(1,348)	1:607:A:VAL:H	1:607:A:VAL:HG11	20	0.52
(1,308)	1:566:A:LEU:H	1:566:A:LEU:HD22	4	0.52
(1,238)	1:575:A:GLN:H	1:575:A:GLN:HB3	14	0.52
(1,92)	1:592:A:ALA:H	1:589:A:THR:HG22	8	0.52
(1,92)	1:592:A:ALA:H	1:589:A:THR:HG23	16	0.52
(1,44)	1:597:A:PHE:H	1:597:A:PHE:HB3	3	0.52
(1,44)	1:597:A:PHE:H	1:597:A:PHE:HB3	4	0.52
(1,44)	1:597:A:PHE:H	1:597:A:PHE:HB3	6	0.52
(1,44)	1:597:A:PHE:H	1:597:A:PHE:HB3	9	0.52

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,44)	1:597:A:PHE:H	1:597:A:PHE:HB3	13	0.52
(1,44)	1:597:A:PHE:H	1:597:A:PHE:HB3	16	0.52
(1,44)	1:597:A:PHE:H	1:597:A:PHE:HB3	17	0.52
(1,44)	1:597:A:PHE:H	1:597:A:PHE:HB3	18	0.52
(1,44)	1:597:A:PHE:H	1:597:A:PHE:HB3	19	0.52
(1,24)	1:599:A:GLN:H	1:599:A:GLN:HG2	12	0.52
(1,2171)	1:591:A:VAL:HG21	1:597:A:PHE:HZ	16	0.51
(1,2168)	1:626:A:GLU:HA	1:625:A:TRP:HA	15	0.51
(1,2168)	1:626:A:GLU:HA	1:627:A:TYR:HA	17	0.51
(1,2165)	1:606:A:LYS:HA	1:606:A:LYS:HE3	2	0.51
(1,2159)	1:627:A:TYR:HB3	1:628:A:LEU:HA	4	0.51
(1,2117)	1:551:A:LYS:HG2	1:551:A:LYS:HD3	18	0.51
(1,2109)	1:608:A:LEU:HD13	1:591:A:VAL:HG13	13	0.51
(1,2103)	1:562:A:LEU:HB3	1:562:A:LEU:HD23	2	0.51
(1,2103)	1:562:A:LEU:HB3	1:562:A:LEU:HD21	5	0.51
(1,2059)	1:615:A:GLU:HA	1:619:A:GLU:HG2	16	0.51
(1,2034)	1:618:A:LEU:HG	1:615:A:GLU:HA	3	0.51
(1,2025)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	3	0.51
(1,2010)	1:561:A:LYS:HE3	1:561:A:LYS:HD2	4	0.51
(1,1980)	1:565:A:LYS:HE2	1:565:A:LYS:HD3	4	0.51
(1,1924)	1:614:A:ALA:HB1	1:611:A:MET:HG2	1	0.51
(1,1924)	1:614:A:ALA:HB2	1:611:A:MET:HG2	17	0.51
(1,1891)	1:576:A:LEU:HG	1:580:A:LEU:HD13	7	0.51
(1,1880)	1:565:A:LYS:HG3	1:565:A:LYS:HD2	10	0.51
(1,1880)	1:551:A:LYS:HG2	1:551:A:LYS:HD3	18	0.51
(1,1865)	1:622:A:PHE:HA	1:623:A:GLU:HA	14	0.51
(1,1774)	1:592:A:ALA:HA	1:589:A:THR:HA	5	0.51
(1,1733)	1:607:A:VAL:HG21	1:610:A:ASP:HB3	1	0.51
(1,1701)	1:622:A:PHE:HE2	1:577:A:LEU:HA	16	0.51
(1,1691)	1:627:A:TYR:HE1	1:627:A:TYR:HA	17	0.51
(1,1678)	1:627:A:TYR:HE1	1:631:A:LEU:HG	5	0.51
(1,1575)	1:621:A:ALA:H	1:622:A:PHE:HA	16	0.51
(1,1575)	1:621:A:ALA:H	1:622:A:PHE:HA	20	0.51
(1,1546)	1:568:A:ARG:H	1:567:A:GLN:HG3	18	0.51
(1,1535)	1:572:A:GLN:H	1:573:A:LEU:HD22	1	0.51
(1,1510)	1:581:A:GLU:H	1:582:A:ALA:HB3	13	0.51
(1,1480)	1:588:A:GLN:H	1:586:A:ALA:HB2	2	0.51
(1,1480)	1:588:A:GLN:H	1:586:A:ALA:HB2	10	0.51
(1,1480)	1:588:A:GLN:H	1:586:A:ALA:HB2	19	0.51
(1,1468)	1:592:A:ALA:H	1:593:A:ASP:HB3	12	0.51
(1,1465)	1:606:A:LYS:H	1:606:A:LYS:HG2	6	0.51
(1,1465)	1:606:A:LYS:H	1:606:A:LYS:HG2	10	0.51

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1465)	1:606:A:LYS:H	1:606:A:LYS:HG2	12	0.51
(1,1420)	1:627:A:TYR:HE1	1:631:A:LEU:HD23	5	0.51
(1,1397)	1:587:A:LEU:HD11	1:583:A:LYS:HA	18	0.51
(1,1220)	1:551:A:LYS:HD2	1:551:A:LYS:HA	12	0.51
(1,1177)	1:623:A:GLU:HG2	1:622:A:PHE:HB3	13	0.51
(1,1165)	1:601:A:HIS:HB2	1:605:A:GLN:HG2	11	0.51
(1,1165)	1:601:A:HIS:HB2	1:605:A:GLN:HG2	19	0.51
(1,1164)	1:601:A:HIS:HB3	1:605:A:GLN:HG2	2	0.51
(1,1120)	1:588:A:GLN:HA	1:611:A:MET:HE3	5	0.51
(1,1062)	1:610:A:ASP:HB2	1:587:A:LEU:HD21	2	0.51
(1,1062)	1:610:A:ASP:HB2	1:587:A:LEU:HD21	19	0.51
(1,1054)	1:604:A:THR:HG22	1:597:A:PHE:HB2	2	0.51
(1,1054)	1:604:A:THR:HG22	1:597:A:PHE:HB2	5	0.51
(1,1054)	1:604:A:THR:HG22	1:597:A:PHE:HB2	12	0.51
(1,1054)	1:604:A:THR:HG21	1:597:A:PHE:HB2	15	0.51
(1,1024)	1:590:A:GLN:HG3	1:589:A:THR:HG22	18	0.51
(1,906)	1:596:A:PHE:HA	1:599:A:GLN:HG2	15	0.51
(1,906)	1:596:A:PHE:HA	1:599:A:GLN:HG2	20	0.51
(1,893)	1:583:A:LYS:HA	1:583:A:LYS:HE3	2	0.51
(1,870)	1:556:A:LYS:HA	1:556:A:LYS:HE2	3	0.51
(1,755)	1:621:A:ALA:HA	1:576:A:LEU:HD22	16	0.51
(1,634)	1:577:A:LEU:HD12	1:574:A:PRO:HA	1	0.51
(1,572)	1:625:A:TRP:HE3	1:625:A:TRP:HB2	2	0.51
(1,572)	1:625:A:TRP:HE3	1:625:A:TRP:HB2	6	0.51
(1,572)	1:625:A:TRP:HE3	1:625:A:TRP:HB2	14	0.51
(1,559)	1:596:A:PHE:HE1	1:604:A:THR:HG23	1	0.51
(1,559)	1:596:A:PHE:HE1	1:604:A:THR:HG21	17	0.51
(1,348)	1:607:A:VAL:H	1:607:A:VAL:HG11	4	0.51
(1,348)	1:607:A:VAL:H	1:607:A:VAL:HG11	15	0.51
(1,317)	1:563:A:SER:H	1:566:A:LEU:HD22	7	0.51
(1,300)	1:567:A:GLN:H	1:566:A:LEU:HD23	20	0.51
(1,299)	1:567:A:GLN:H	1:566:A:LEU:HD12	7	0.51
(1,44)	1:597:A:PHE:H	1:597:A:PHE:HB3	2	0.51
(1,44)	1:597:A:PHE:H	1:597:A:PHE:HB3	5	0.51
(1,44)	1:597:A:PHE:H	1:597:A:PHE:HB3	7	0.51
(1,44)	1:597:A:PHE:H	1:597:A:PHE:HB3	10	0.51
(1,44)	1:597:A:PHE:H	1:597:A:PHE:HB3	11	0.51
(1,44)	1:597:A:PHE:H	1:597:A:PHE:HB3	12	0.51
(1,44)	1:597:A:PHE:H	1:597:A:PHE:HB3	14	0.51
(1,44)	1:597:A:PHE:H	1:597:A:PHE:HB3	20	0.51
(1,2168)	1:626:A:GLU:HA	1:625:A:TRP:HA	4	0.5
(1,2165)	1:606:A:LYS:HA	1:606:A:LYS:HE2	15	0.5

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2160)	1:630:A:ALA:HB1	1:627:A:TYR:HB2	7	0.5
(1,2159)	1:627:A:TYR:HB3	1:628:A:LEU:HA	15	0.5
(1,2149)	1:631:A:LEU:HD11	1:566:A:LEU:HD13	7	0.5
(1,2109)	1:608:A:LEU:HD12	1:591:A:VAL:HG13	17	0.5
(1,2103)	1:562:A:LEU:HB3	1:562:A:LEU:HD22	7	0.5
(1,2046)	1:626:A:GLU:HB3	1:627:A:TYR:HA	5	0.5
(1,2042)	1:573:A:LEU:HG	1:570:A:LEU:HA	15	0.5
(1,2034)	1:618:A:LEU:HG	1:615:A:GLU:HA	10	0.5
(1,2034)	1:618:A:LEU:HG	1:581:A:GLU:HA	15	0.5
(1,2025)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	7	0.5
(1,2014)	1:601:A:HIS:HB3	1:602:A:GLU:HB2	8	0.5
(1,1965)	1:579:A:ASP:HB2	1:576:A:LEU:HG	6	0.5
(1,1941)	1:616:A:GLN:HG2	1:613:A:ALA:HB1	5	0.5
(1,1924)	1:614:A:ALA:HB2	1:611:A:MET:HG2	6	0.5
(1,1924)	1:614:A:ALA:HB1	1:611:A:MET:HG2	7	0.5
(1,1924)	1:614:A:ALA:HB2	1:611:A:MET:HG2	8	0.5
(1,1924)	1:614:A:ALA:HB3	1:611:A:MET:HG2	11	0.5
(1,1895)	1:618:A:LEU:HG	1:581:A:GLU:HB2	9	0.5
(1,1880)	1:565:A:LYS:HG3	1:565:A:LYS:HD2	3	0.5
(1,1812)	1:632:A:LYS:HA	1:631:A:LEU:HD21	6	0.5
(1,1812)	1:632:A:LYS:HA	1:631:A:LEU:HD23	7	0.5
(1,1779)	1:614:A:ALA:HA	1:587:A:LEU:HD13	9	0.5
(1,1761)	1:621:A:ALA:HB3	1:624:A:ARG:HG2	1	0.5
(1,1761)	1:621:A:ALA:HB2	1:624:A:ARG:HG2	20	0.5
(1,1717)	1:604:A:THR:HG22	1:608:A:LEU:HG	7	0.5
(1,1712)	1:577:A:LEU:HD21	1:625:A:TRP:HA	7	0.5
(1,1708)	1:625:A:TRP:HD1	1:628:A:LEU:HD13	5	0.5
(1,1705)	1:622:A:PHE:HD1	1:577:A:LEU:HD21	20	0.5
(1,1704)	1:622:A:PHE:HD2	1:618:A:LEU:HB3	5	0.5
(1,1704)	1:622:A:PHE:HD2	1:618:A:LEU:HB3	12	0.5
(1,1701)	1:622:A:PHE:HE2	1:577:A:LEU:HA	17	0.5
(1,1694)	1:564:A:TYR:HD2	1:568:A:ARG:HG2	18	0.5
(1,1691)	1:627:A:TYR:HE1	1:627:A:TYR:HA	5	0.5
(1,1633)	1:622:A:PHE:H	1:620:A:GLN:HB2	13	0.5
(1,1588)	1:583:A:LYS:H	1:581:A:GLU:HG2	20	0.5
(1,1575)	1:621:A:ALA:H	1:622:A:PHE:HA	5	0.5
(1,1469)	1:592:A:ALA:H	1:591:A:VAL:HG12	12	0.5
(1,1465)	1:606:A:LYS:H	1:606:A:LYS:HG2	1	0.5
(1,1465)	1:606:A:LYS:H	1:606:A:LYS:HG2	5	0.5
(1,1465)	1:606:A:LYS:H	1:606:A:LYS:HG2	8	0.5
(1,1437)	1:564:A:TYR:HD2	1:568:A:ARG:HG2	18	0.5
(1,1397)	1:587:A:LEU:HD12	1:583:A:LYS:HA	2	0.5

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1397)	1:587:A:LEU:HD12	1:583:A:LYS:HA	6	0.5
(1,1397)	1:587:A:LEU:HD11	1:583:A:LYS:HA	9	0.5
(1,1397)	1:587:A:LEU:HD13	1:583:A:LYS:HA	13	0.5
(1,1397)	1:587:A:LEU:HD12	1:583:A:LYS:HA	20	0.5
(1,1396)	1:632:A:LYS:HG3	1:562:A:LEU:HB2	10	0.5
(1,1378)	1:624:A:ARG:HD3	1:573:A:LEU:HD13	19	0.5
(1,1333)	1:573:A:LEU:HD11	1:624:A:ARG:HD2	9	0.5
(1,1164)	1:601:A:HIS:HB3	1:605:A:GLN:HG2	7	0.5
(1,1164)	1:601:A:HIS:HB3	1:605:A:GLN:HG2	12	0.5
(1,1120)	1:588:A:GLN:HA	1:611:A:MET:HE2	7	0.5
(1,1111)	1:631:A:LEU:HD22	1:562:A:LEU:HB2	8	0.5
(1,1062)	1:610:A:ASP:HB2	1:587:A:LEU:HD23	17	0.5
(1,1054)	1:604:A:THR:HG21	1:597:A:PHE:HB2	6	0.5
(1,1054)	1:604:A:THR:HG22	1:597:A:PHE:HB2	9	0.5
(1,956)	1:605:A:GLN:HB3	1:608:A:LEU:HD11	5	0.5
(1,755)	1:621:A:ALA:HA	1:576:A:LEU:HD23	20	0.5
(1,630)	1:577:A:LEU:HD11	1:580:A:LEU:HG	14	0.5
(1,572)	1:625:A:TRP:HE3	1:625:A:TRP:HB2	8	0.5
(1,559)	1:596:A:PHE:HE1	1:604:A:THR:HG21	8	0.5
(1,538)	1:635:A:GLY:H	1:631:A:LEU:HD11	19	0.5
(1,299)	1:567:A:GLN:H	1:566:A:LEU:HD11	15	0.5
(1,154)	1:585:A:GLU:H	1:584:A:LEU:HB2	5	0.5
(1,110)	1:590:A:GLN:H	1:590:A:GLN:HG3	18	0.5
(1,92)	1:592:A:ALA:H	1:589:A:THR:HG22	19	0.5
(1,2168)	1:626:A:GLU:HA	1:625:A:TRP:HA	9	0.49
(1,2168)	1:626:A:GLU:HA	1:627:A:TYR:HA	13	0.49
(1,2168)	1:626:A:GLU:HA	1:625:A:TRP:HA	19	0.49
(1,2168)	1:626:A:GLU:HA	1:627:A:TYR:HA	20	0.49
(1,2160)	1:630:A:ALA:HB3	1:627:A:TYR:HB2	20	0.49
(1,2159)	1:627:A:TYR:HB3	1:628:A:LEU:HA	16	0.49
(1,2109)	1:608:A:LEU:HD13	1:591:A:VAL:HG13	19	0.49
(1,2103)	1:562:A:LEU:HB3	1:562:A:LEU:HD21	10	0.49
(1,2042)	1:573:A:LEU:HG	1:570:A:LEU:HA	11	0.49
(1,2042)	1:573:A:LEU:HG	1:570:A:LEU:HA	16	0.49
(1,2037)	1:603:A:GLN:HA	1:605:A:GLN:HB2	14	0.49
(1,2034)	1:618:A:LEU:HG	1:615:A:GLU:HA	1	0.49
(1,2025)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	4	0.49
(1,1965)	1:579:A:ASP:HB2	1:576:A:LEU:HG	15	0.49
(1,1946)	1:581:A:GLU:HG2	1:618:A:LEU:HD22	12	0.49
(1,1924)	1:614:A:ALA:HB1	1:611:A:MET:HG2	18	0.49
(1,1907)	1:591:A:VAL:HA	1:608:A:LEU:HD22	9	0.49
(1,1901)	1:613:A:ALA:HB1	1:616:A:GLN:HB2	1	0.49

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1886)	1:624:A:ARG:HG3	1:628:A:LEU:HD11	8	0.49
(1,1852)	1:604:A:THR:HB	1:599:A:GLN:HB2	9	0.49
(1,1812)	1:632:A:LYS:HA	1:631:A:LEU:HD21	12	0.49
(1,1790)	1:557:A:ARG:HA	1:555:A:VAL:HG22	13	0.49
(1,1790)	1:557:A:ARG:HA	1:555:A:VAL:HG21	17	0.49
(1,1779)	1:614:A:ALA:HA	1:580:A:LEU:HD12	4	0.49
(1,1778)	1:612:A:ALA:HA	1:584:A:LEU:HD22	8	0.49
(1,1723)	1:591:A:VAL:HG11	1:611:A:MET:HG3	20	0.49
(1,1709)	1:625:A:TRP:HD1	1:574:A:PRO:HG2	10	0.49
(1,1709)	1:625:A:TRP:HD1	1:573:A:LEU:HB2	15	0.49
(1,1708)	1:625:A:TRP:HD1	1:628:A:LEU:HD13	8	0.49
(1,1701)	1:622:A:PHE:HE2	1:577:A:LEU:HA	8	0.49
(1,1691)	1:627:A:TYR:HE2	1:624:A:ARG:HA	15	0.49
(1,1621)	1:619:A:GLU:H	1:618:A:LEU:HD21	13	0.49
(1,1611)	1:616:A:GLN:H	1:612:A:ALA:HB3	20	0.49
(1,1553)	1:566:A:LEU:H	1:566:A:LEU:HG	6	0.49
(1,1526)	1:576:A:LEU:H	1:576:A:LEU:HD21	12	0.49
(1,1510)	1:581:A:GLU:H	1:582:A:ALA:HB2	3	0.49
(1,1510)	1:581:A:GLU:H	1:582:A:ALA:HB3	15	0.49
(1,1506)	1:582:A:ALA:H	1:618:A:LEU:HD11	19	0.49
(1,1465)	1:606:A:LYS:H	1:606:A:LYS:HG2	2	0.49
(1,1457)	1:597:A:PHE:H	1:598:A:SER:HB2	12	0.49
(1,1451)	1:599:A:GLN:H	1:597:A:PHE:HB2	7	0.49
(1,1449)	1:603:A:GLN:H	1:605:A:GLN:HB2	19	0.49
(1,1402)	1:606:A:LYS:HB2	1:606:A:LYS:HE3	13	0.49
(1,1363)	1:562:A:LEU:HD21	1:631:A:LEU:HB2	8	0.49
(1,1288)	1:566:A:LEU:HD23	1:562:A:LEU:HD23	15	0.49
(1,1054)	1:604:A:THR:HG21	1:597:A:PHE:HB2	1	0.49
(1,1054)	1:604:A:THR:HG21	1:597:A:PHE:HB2	3	0.49
(1,1054)	1:604:A:THR:HG23	1:597:A:PHE:HB2	11	0.49
(1,938)	1:631:A:LEU:HG	1:562:A:LEU:HD23	4	0.49
(1,893)	1:583:A:LYS:HA	1:583:A:LYS:HE3	7	0.49
(1,809)	1:605:A:GLN:HA	1:608:A:LEU:HD23	10	0.49
(1,755)	1:621:A:ALA:HA	1:576:A:LEU:HD21	6	0.49
(1,755)	1:621:A:ALA:HA	1:576:A:LEU:HD22	14	0.49
(1,755)	1:621:A:ALA:HA	1:576:A:LEU:HD22	17	0.49
(1,631)	1:577:A:LEU:HD11	1:622:A:PHE:HB3	4	0.49
(1,631)	1:577:A:LEU:HD11	1:622:A:PHE:HB3	7	0.49
(1,631)	1:577:A:LEU:HD11	1:622:A:PHE:HB3	15	0.49
(1,631)	1:577:A:LEU:HD11	1:622:A:PHE:HB3	19	0.49
(1,630)	1:577:A:LEU:HD12	1:580:A:LEU:HG	4	0.49
(1,586)	1:625:A:TRP:HD1	1:577:A:LEU:HD23	6	0.49

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,550)	1:596:A:PHE:HD2	1:604:A:THR:HG23	16	0.49
(1,416)	1:616:A:GLN:H	1:615:A:GLU:HB3	13	0.49
(1,348)	1:607:A:VAL:H	1:607:A:VAL:HG11	19	0.49
(1,238)	1:575:A:GLN:H	1:575:A:GLN:HB3	19	0.49
(1,154)	1:585:A:GLU:H	1:584:A:LEU:HB2	7	0.49
(1,154)	1:585:A:GLU:H	1:584:A:LEU:HB2	15	0.49
(1,146)	1:586:A:ALA:H	1:585:A:GLU:HB2	4	0.49
(1,125)	1:589:A:THR:H	1:586:A:ALA:HB2	5	0.49
(1,92)	1:592:A:ALA:H	1:589:A:THR:HG22	20	0.49
(1,2168)	1:626:A:GLU:HA	1:625:A:TRP:HA	16	0.48
(1,2165)	1:606:A:LYS:HA	1:606:A:LYS:HE2	20	0.48
(1,2163)	1:567:A:GLN:HA	1:570:A:LEU:HD12	6	0.48
(1,2159)	1:627:A:TYR:HB3	1:628:A:LEU:HA	1	0.48
(1,2135)	1:567:A:GLN:HA	1:570:A:LEU:HD12	6	0.48
(1,2105)	1:566:A:LEU:HD22	1:628:A:LEU:HG	11	0.48
(1,2042)	1:573:A:LEU:HG	1:570:A:LEU:HA	18	0.48
(1,2034)	1:618:A:LEU:HG	1:615:A:GLU:HA	17	0.48
(1,1939)	1:572:A:GLN:HG3	1:573:A:LEU:HB3	3	0.48
(1,1939)	1:572:A:GLN:HG3	1:573:A:LEU:HB3	7	0.48
(1,1924)	1:614:A:ALA:HB2	1:611:A:MET:HG2	12	0.48
(1,1901)	1:612:A:ALA:HB1	1:616:A:GLN:HB3	10	0.48
(1,1865)	1:622:A:PHE:HA	1:623:A:GLU:HA	19	0.48
(1,1852)	1:604:A:THR:HB	1:608:A:LEU:HB2	16	0.48
(1,1779)	1:614:A:ALA:HA	1:580:A:LEU:HD11	7	0.48
(1,1763)	1:621:A:ALA:HB3	1:617:A:GLU:HG2	12	0.48
(1,1741)	1:628:A:LEU:HD23	1:624:A:ARG:HA	10	0.48
(1,1730)	1:607:A:VAL:HG22	1:587:A:LEU:HD21	15	0.48
(1,1729)	1:631:A:LEU:HD21	1:561:A:LYS:HA	9	0.48
(1,1701)	1:622:A:PHE:HE2	1:577:A:LEU:HA	7	0.48
(1,1611)	1:616:A:GLN:H	1:612:A:ALA:HB1	17	0.48
(1,1575)	1:621:A:ALA:H	1:622:A:PHE:HA	4	0.48
(1,1538)	1:571:A:GLU:H	1:628:A:LEU:HD12	3	0.48
(1,1535)	1:572:A:GLN:H	1:573:A:LEU:HD11	13	0.48
(1,1532)	1:573:A:LEU:H	1:573:A:LEU:HD12	18	0.48
(1,1526)	1:576:A:LEU:H	1:576:A:LEU:HD22	9	0.48
(1,1510)	1:581:A:GLU:H	1:582:A:ALA:HB1	2	0.48
(1,1510)	1:581:A:GLU:H	1:582:A:ALA:HB3	4	0.48
(1,1480)	1:588:A:GLN:H	1:586:A:ALA:HB1	13	0.48
(1,1480)	1:588:A:GLN:H	1:586:A:ALA:HB3	20	0.48
(1,1469)	1:592:A:ALA:H	1:591:A:VAL:HG11	13	0.48
(1,1465)	1:606:A:LYS:H	1:606:A:LYS:HG2	4	0.48
(1,1465)	1:606:A:LYS:H	1:606:A:LYS:HG2	15	0.48

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1465)	1:606:A:LYS:H	1:606:A:LYS:HG2	17	0.48
(1,1402)	1:606:A:LYS:HB2	1:606:A:LYS:HE3	2	0.48
(1,1402)	1:606:A:LYS:HB2	1:606:A:LYS:HE3	4	0.48
(1,1369)	1:591:A:VAL:HG21	1:596:A:PHE:HB2	17	0.48
(1,1335)	1:566:A:LEU:HG	1:562:A:LEU:HD21	18	0.48
(1,1326)	1:566:A:LEU:HD21	1:563:A:SER:HB3	13	0.48
(1,1287)	1:566:A:LEU:HD21	1:631:A:LEU:HD21	7	0.48
(1,1230)	1:612:A:ALA:HA	1:611:A:MET:HG3	6	0.48
(1,1230)	1:612:A:ALA:HA	1:611:A:MET:HG3	15	0.48
(1,1230)	1:612:A:ALA:HA	1:611:A:MET:HG3	17	0.48
(1,1165)	1:601:A:HIS:HB2	1:605:A:GLN:HG2	13	0.48
(1,1062)	1:610:A:ASP:HB2	1:587:A:LEU:HD22	16	0.48
(1,1054)	1:604:A:THR:HG21	1:597:A:PHE:HB2	10	0.48
(1,1053)	1:577:A:LEU:HD11	1:617:A:GLU:HG3	16	0.48
(1,956)	1:605:A:GLN:HB3	1:608:A:LEU:HD12	20	0.48
(1,926)	1:583:A:LYS:HG3	1:580:A:LEU:HD22	16	0.48
(1,893)	1:583:A:LYS:HA	1:583:A:LYS:HE3	4	0.48
(1,893)	1:583:A:LYS:HA	1:583:A:LYS:HE3	12	0.48
(1,630)	1:577:A:LEU:HD11	1:580:A:LEU:HG	10	0.48
(1,625)	1:577:A:LEU:HD13	1:573:A:LEU:HD23	10	0.48
(1,550)	1:596:A:PHE:HD1	1:604:A:THR:HG23	1	0.48
(1,550)	1:596:A:PHE:HD1	1:604:A:THR:HG21	17	0.48
(1,550)	1:596:A:PHE:HD2	1:604:A:THR:HG21	20	0.48
(1,300)	1:567:A:GLN:H	1:566:A:LEU:HD21	13	0.48
(1,238)	1:575:A:GLN:H	1:575:A:GLN:HB3	13	0.48
(1,154)	1:585:A:GLU:H	1:584:A:LEU:HB2	3	0.48
(1,92)	1:592:A:ALA:H	1:589:A:THR:HG22	12	0.48
(1,2171)	1:591:A:VAL:HG21	1:597:A:PHE:HZ	5	0.47
(1,2165)	1:606:A:LYS:HA	1:610:A:ASP:HB2	8	0.47
(1,2111)	1:584:A:LEU:HB2	1:618:A:LEU:HD23	14	0.47
(1,2059)	1:615:A:GLU:HA	1:619:A:GLU:HG2	11	0.47
(1,2052)	1:603:A:GLN:HG3	1:599:A:GLN:HA	10	0.47
(1,2042)	1:573:A:LEU:HG	1:570:A:LEU:HA	2	0.47
(1,2042)	1:573:A:LEU:HG	1:570:A:LEU:HA	12	0.47
(1,2034)	1:618:A:LEU:HG	1:581:A:GLU:HA	11	0.47
(1,2014)	1:601:A:HIS:HB3	1:602:A:GLU:HB2	12	0.47
(1,1978)	1:583:A:LYS:HE2	1:587:A:LEU:HD21	1	0.47
(1,1944)	1:585:A:GLU:HG3	1:586:A:ALA:HB2	13	0.47
(1,1924)	1:614:A:ALA:HB3	1:611:A:MET:HG2	4	0.47
(1,1924)	1:614:A:ALA:HB1	1:611:A:MET:HG2	15	0.47
(1,1913)	1:585:A:GLU:HB3	1:586:A:ALA:HB3	5	0.47
(1,1907)	1:591:A:VAL:HA	1:608:A:LEU:HD22	12	0.47

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1907)	1:591:A:VAL:HA	1:608:A:LEU:HD21	13	0.47
(1,1888)	1:568:A:ARG:HG2	1:571:A:GLU:HB3	9	0.47
(1,1865)	1:622:A:PHE:HA	1:619:A:GLU:HA	5	0.47
(1,1865)	1:622:A:PHE:HA	1:623:A:GLU:HA	11	0.47
(1,1854)	1:612:A:ALA:HA	1:611:A:MET:HA	12	0.47
(1,1852)	1:604:A:THR:HB	1:608:A:LEU:HB2	14	0.47
(1,1812)	1:632:A:LYS:HA	1:631:A:LEU:HD23	1	0.47
(1,1731)	1:607:A:VAL:HG21	1:603:A:GLN:HB2	5	0.47
(1,1717)	1:604:A:THR:HG23	1:608:A:LEU:HG	10	0.47
(1,1717)	1:604:A:THR:HG22	1:608:A:LEU:HG	14	0.47
(1,1711)	1:577:A:LEU:HD23	1:626:A:GLU:HG3	1	0.47
(1,1709)	1:625:A:TRP:HD1	1:573:A:LEU:HB2	7	0.47
(1,1705)	1:622:A:PHE:HD1	1:577:A:LEU:HD21	12	0.47
(1,1701)	1:622:A:PHE:HE2	1:577:A:LEU:HA	2	0.47
(1,1701)	1:622:A:PHE:HE2	1:577:A:LEU:HA	4	0.47
(1,1701)	1:622:A:PHE:HE2	1:577:A:LEU:HA	12	0.47
(1,1701)	1:622:A:PHE:HE2	1:577:A:LEU:HA	14	0.47
(1,1701)	1:622:A:PHE:HE2	1:577:A:LEU:HA	19	0.47
(1,1691)	1:627:A:TYR:HE1	1:627:A:TYR:HA	20	0.47
(1,1621)	1:619:A:GLU:H	1:618:A:LEU:HD21	11	0.47
(1,1575)	1:621:A:ALA:H	1:622:A:PHE:HA	19	0.47
(1,1549)	1:567:A:GLN:H	1:563:A:SER:HB3	2	0.47
(1,1549)	1:567:A:GLN:H	1:563:A:SER:HB3	5	0.47
(1,1538)	1:571:A:GLU:H	1:628:A:LEU:HD13	9	0.47
(1,1535)	1:572:A:GLN:H	1:573:A:LEU:HD13	3	0.47
(1,1526)	1:576:A:LEU:H	1:576:A:LEU:HD23	4	0.47
(1,1526)	1:576:A:LEU:H	1:576:A:LEU:HD21	6	0.47
(1,1526)	1:576:A:LEU:H	1:576:A:LEU:HD22	14	0.47
(1,1510)	1:581:A:GLU:H	1:582:A:ALA:HB2	5	0.47
(1,1510)	1:581:A:GLU:H	1:582:A:ALA:HB1	8	0.47
(1,1510)	1:581:A:GLU:H	1:582:A:ALA:HB3	10	0.47
(1,1480)	1:588:A:GLN:H	1:586:A:ALA:HB1	3	0.47
(1,1469)	1:592:A:ALA:H	1:591:A:VAL:HG12	2	0.47
(1,1467)	1:593:A:ASP:H	1:591:A:VAL:HG11	13	0.47
(1,1465)	1:606:A:LYS:H	1:606:A:LYS:HG2	20	0.47
(1,1402)	1:606:A:LYS:HB2	1:606:A:LYS:HE3	5	0.47
(1,1399)	1:583:A:LYS:HG2	1:580:A:LEU:HD22	8	0.47
(1,1399)	1:583:A:LYS:HG2	1:580:A:LEU:HD21	9	0.47
(1,1399)	1:583:A:LYS:HG2	1:580:A:LEU:HD22	17	0.47
(1,1397)	1:587:A:LEU:HD11	1:583:A:LYS:HA	5	0.47
(1,1387)	1:577:A:LEU:HD23	1:574:A:PRO:HB2	6	0.47
(1,1369)	1:591:A:VAL:HG23	1:596:A:PHE:HB2	11	0.47

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1309)	1:573:A:LEU:HD22	1:576:A:LEU:HB2	18	0.47
(1,1230)	1:612:A:ALA:HA	1:611:A:MET:HG3	1	0.47
(1,1230)	1:612:A:ALA:HA	1:611:A:MET:HG3	3	0.47
(1,1230)	1:612:A:ALA:HA	1:611:A:MET:HG3	4	0.47
(1,1230)	1:612:A:ALA:HA	1:611:A:MET:HG3	7	0.47
(1,1230)	1:612:A:ALA:HA	1:611:A:MET:HG3	16	0.47
(1,1230)	1:612:A:ALA:HA	1:611:A:MET:HG3	20	0.47
(1,1222)	1:565:A:LYS:HD3	1:563:A:SER:HB3	2	0.47
(1,1163)	1:599:A:GLN:HG3	1:600:A:PRO:HD3	3	0.47
(1,1147)	1:565:A:LYS:HA	1:565:A:LYS:HD3	6	0.47
(1,1095)	1:565:A:LYS:HE2	1:566:A:LEU:HD13	9	0.47
(1,1062)	1:610:A:ASP:HB2	1:587:A:LEU:HD21	15	0.47
(1,1062)	1:610:A:ASP:HB2	1:587:A:LEU:HD23	20	0.47
(1,926)	1:583:A:LYS:HG3	1:580:A:LEU:HD22	3	0.47
(1,926)	1:583:A:LYS:HG3	1:580:A:LEU:HD22	8	0.47
(1,926)	1:583:A:LYS:HG3	1:580:A:LEU:HD22	17	0.47
(1,926)	1:583:A:LYS:HG3	1:580:A:LEU:HD22	20	0.47
(1,893)	1:583:A:LYS:HA	1:583:A:LYS:HE3	9	0.47
(1,893)	1:583:A:LYS:HA	1:583:A:LYS:HE3	18	0.47
(1,755)	1:621:A:ALA:HA	1:576:A:LEU:HD21	2	0.47
(1,755)	1:621:A:ALA:HA	1:576:A:LEU:HD21	8	0.47
(1,755)	1:621:A:ALA:HA	1:576:A:LEU:HD22	11	0.47
(1,572)	1:625:A:TRP:HE3	1:625:A:TRP:HB2	5	0.47
(1,538)	1:635:A:GLY:H	1:631:A:LEU:HD13	3	0.47
(1,538)	1:635:A:GLY:H	1:631:A:LEU:HD12	20	0.47
(1,416)	1:616:A:GLN:H	1:615:A:GLU:HB3	8	0.47
(1,299)	1:567:A:GLN:H	1:566:A:LEU:HD13	5	0.47
(1,238)	1:575:A:GLN:H	1:575:A:GLN:HB3	12	0.47
(1,154)	1:585:A:GLU:H	1:584:A:LEU:HB2	11	0.47
(1,124)	1:589:A:THR:H	1:589:A:THR:HG22	5	0.47
(1,92)	1:592:A:ALA:H	1:589:A:THR:HG21	17	0.47
(1,92)	1:592:A:ALA:H	1:589:A:THR:HG21	18	0.47
(1,2168)	1:626:A:GLU:HA	1:625:A:TRP:HA	3	0.46
(1,2168)	1:626:A:GLU:HA	1:625:A:TRP:HA	10	0.46
(1,2168)	1:626:A:GLU:HA	1:625:A:TRP:HA	12	0.46
(1,2159)	1:627:A:TYR:HB3	1:628:A:LEU:HA	2	0.46
(1,2159)	1:627:A:TYR:HB3	1:628:A:LEU:HA	19	0.46
(1,2124)	1:612:A:ALA:HA	1:611:A:MET:HE3	4	0.46
(1,2104)	1:566:A:LEU:HD21	1:631:A:LEU:HB2	12	0.46
(1,2056)	1:572:A:GLN:HG3	1:569:A:GLU:HA	15	0.46
(1,2051)	1:603:A:GLN:HG2	1:600:A:PRO:HA	4	0.46
(1,1961)	1:610:A:ASP:HB3	1:587:A:LEU:HB3	19	0.46

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1901)	1:612:A:ALA:HB3	1:616:A:GLN:HB3	19	0.46
(1,1854)	1:612:A:ALA:HA	1:611:A:MET:HA	4	0.46
(1,1854)	1:614:A:ALA:HA	1:615:A:GLU:HA	18	0.46
(1,1852)	1:604:A:THR:HB	1:599:A:GLN:HB2	10	0.46
(1,1790)	1:557:A:ARG:HA	1:555:A:VAL:HG21	6	0.46
(1,1723)	1:591:A:VAL:HG13	1:611:A:MET:HG3	2	0.46
(1,1723)	1:591:A:VAL:HG12	1:611:A:MET:HG3	19	0.46
(1,1717)	1:604:A:THR:HG23	1:608:A:LEU:HG	16	0.46
(1,1711)	1:577:A:LEU:HD22	1:626:A:GLU:HG3	3	0.46
(1,1708)	1:625:A:TRP:HD1	1:628:A:LEU:HD11	17	0.46
(1,1701)	1:622:A:PHE:HE2	1:577:A:LEU:HA	3	0.46
(1,1701)	1:622:A:PHE:HE2	1:577:A:LEU:HA	9	0.46
(1,1701)	1:622:A:PHE:HE2	1:577:A:LEU:HA	15	0.46
(1,1621)	1:619:A:GLU:H	1:618:A:LEU:HD21	15	0.46
(1,1565)	1:607:A:VAL:H	1:610:A:ASP:HB2	2	0.46
(1,1545)	1:569:A:GLU:H	1:628:A:LEU:HD12	3	0.46
(1,1538)	1:571:A:GLU:H	1:628:A:LEU:HD11	18	0.46
(1,1526)	1:576:A:LEU:H	1:576:A:LEU:HD21	2	0.46
(1,1526)	1:576:A:LEU:H	1:576:A:LEU:HD21	8	0.46
(1,1526)	1:576:A:LEU:H	1:576:A:LEU:HD22	13	0.46
(1,1517)	1:578:A:GLU:H	1:577:A:LEU:HG	16	0.46
(1,1515)	1:579:A:ASP:H	1:576:A:LEU:HD13	1	0.46
(1,1510)	1:581:A:GLU:H	1:582:A:ALA:HB3	18	0.46
(1,1468)	1:592:A:ALA:H	1:593:A:ASP:HB3	20	0.46
(1,1465)	1:606:A:LYS:H	1:606:A:LYS:HG2	3	0.46
(1,1465)	1:606:A:LYS:H	1:606:A:LYS:HG2	7	0.46
(1,1402)	1:606:A:LYS:HB2	1:606:A:LYS:HE3	7	0.46
(1,1399)	1:583:A:LYS:HG2	1:580:A:LEU:HD21	4	0.46
(1,1399)	1:583:A:LYS:HG2	1:580:A:LEU:HD22	20	0.46
(1,1366)	1:566:A:LEU:HD23	1:631:A:LEU:HD12	4	0.46
(1,1363)	1:562:A:LEU:HD21	1:631:A:LEU:HB2	1	0.46
(1,1325)	1:628:A:LEU:HD11	1:569:A:GLU:HA	18	0.46
(1,1250)	1:626:A:GLU:HG2	1:623:A:GLU:HA	16	0.46
(1,1230)	1:612:A:ALA:HA	1:611:A:MET:HG3	10	0.46
(1,1230)	1:612:A:ALA:HA	1:611:A:MET:HG3	11	0.46
(1,1230)	1:612:A:ALA:HA	1:611:A:MET:HG3	19	0.46
(1,1164)	1:601:A:HIS:HB3	1:605:A:GLN:HG2	1	0.46
(1,1164)	1:601:A:HIS:HB3	1:605:A:GLN:HG2	6	0.46
(1,1164)	1:601:A:HIS:HB3	1:605:A:GLN:HG2	8	0.46
(1,1163)	1:599:A:GLN:HG3	1:600:A:PRO:HD3	12	0.46
(1,1158)	1:600:A:PRO:HD2	1:603:A:GLN:HG2	10	0.46
(1,1147)	1:565:A:LYS:HA	1:565:A:LYS:HD3	4	0.46

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1147)	1:565:A:LYS:HA	1:565:A:LYS:HD3	8	0.46
(1,1147)	1:565:A:LYS:HA	1:565:A:LYS:HD3	12	0.46
(1,1136)	1:600:A:PRO:HD3	1:603:A:GLN:HB3	7	0.46
(1,1120)	1:588:A:GLN:HA	1:611:A:MET:HE1	20	0.46
(1,1062)	1:610:A:ASP:HB2	1:587:A:LEU:HD23	1	0.46
(1,1005)	1:603:A:GLN:HG3	1:604:A:THR:HG23	17	0.46
(1,985)	1:591:A:VAL:HB	1:608:A:LEU:HD22	8	0.46
(1,893)	1:583:A:LYS:HA	1:583:A:LYS:HE3	19	0.46
(1,755)	1:621:A:ALA:HA	1:576:A:LEU:HD22	13	0.46
(1,658)	1:591:A:VAL:HG21	1:596:A:PHE:HB3	4	0.46
(1,658)	1:591:A:VAL:HG21	1:596:A:PHE:HB3	17	0.46
(1,559)	1:596:A:PHE:HE2	1:604:A:THR:HG23	16	0.46
(1,550)	1:596:A:PHE:HD1	1:604:A:THR:HG22	18	0.46
(1,538)	1:635:A:GLY:H	1:631:A:LEU:HD11	14	0.46
(1,339)	1:605:A:GLN:H	1:604:A:THR:HG22	10	0.46
(1,238)	1:575:A:GLN:H	1:575:A:GLN:HB3	5	0.46
(1,172)	1:582:A:ALA:H	1:579:A:ASP:HB2	4	0.46
(1,172)	1:582:A:ALA:H	1:579:A:ASP:HB2	15	0.46
(1,154)	1:585:A:GLU:H	1:584:A:LEU:HB2	17	0.46
(1,92)	1:592:A:ALA:H	1:589:A:THR:HG22	3	0.46
(1,92)	1:592:A:ALA:H	1:589:A:THR:HG23	9	0.46
(1,92)	1:592:A:ALA:H	1:589:A:THR:HG23	10	0.46
(1,26)	1:599:A:GLN:H	1:599:A:GLN:HB3	15	0.46
(1,26)	1:599:A:GLN:H	1:599:A:GLN:HB3	17	0.46
(1,24)	1:599:A:GLN:H	1:599:A:GLN:HG2	15	0.46
(1,2168)	1:626:A:GLU:HA	1:625:A:TRP:HA	7	0.45
(1,2168)	1:626:A:GLU:HA	1:625:A:TRP:HA	11	0.45
(1,2163)	1:567:A:GLN:HA	1:570:A:LEU:HD12	2	0.45
(1,2160)	1:630:A:ALA:HB3	1:627:A:TYR:HB2	9	0.45
(1,2159)	1:627:A:TYR:HB3	1:628:A:LEU:HA	9	0.45
(1,2135)	1:567:A:GLN:HA	1:570:A:LEU:HD12	2	0.45
(1,2124)	1:612:A:ALA:HA	1:611:A:MET:HE2	16	0.45
(1,2124)	1:612:A:ALA:HA	1:611:A:MET:HE2	17	0.45
(1,2059)	1:615:A:GLU:HA	1:619:A:GLU:HG2	8	0.45
(1,2052)	1:603:A:GLN:HG3	1:599:A:GLN:HA	13	0.45
(1,2034)	1:618:A:LEU:HG	1:615:A:GLU:HA	19	0.45
(1,2033)	1:562:A:LEU:HG	1:563:A:SER:HB3	14	0.45
(1,1961)	1:610:A:ASP:HB3	1:587:A:LEU:HB3	15	0.45
(1,1907)	1:591:A:VAL:HA	1:608:A:LEU:HD21	8	0.45
(1,1895)	1:618:A:LEU:HG	1:581:A:GLU:HB2	3	0.45
(1,1894)	1:562:A:LEU:HG	1:567:A:GLN:HG3	4	0.45
(1,1894)	1:576:A:LEU:HG	1:617:A:GLU:HG3	16	0.45

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1865)	1:622:A:PHE:HA	1:623:A:GLU:HA	4	0.45
(1,1854)	1:612:A:ALA:HA	1:611:A:MET:HA	1	0.45
(1,1854)	1:614:A:ALA:HA	1:615:A:GLU:HA	5	0.45
(1,1854)	1:612:A:ALA:HA	1:611:A:MET:HA	7	0.45
(1,1854)	1:612:A:ALA:HA	1:611:A:MET:HA	11	0.45
(1,1854)	1:614:A:ALA:HA	1:615:A:GLU:HA	16	0.45
(1,1812)	1:632:A:LYS:HA	1:631:A:LEU:HD21	15	0.45
(1,1779)	1:614:A:ALA:HA	1:587:A:LEU:HD13	15	0.45
(1,1712)	1:577:A:LEU:HD22	1:625:A:TRP:HA	10	0.45
(1,1705)	1:622:A:PHE:HD1	1:577:A:LEU:HD23	1	0.45
(1,1705)	1:622:A:PHE:HD1	1:577:A:LEU:HD22	3	0.45
(1,1678)	1:627:A:TYR:HE1	1:631:A:LEU:HG	10	0.45
(1,1611)	1:616:A:GLN:H	1:612:A:ALA:HB1	2	0.45
(1,1611)	1:616:A:GLN:H	1:612:A:ALA:HB3	6	0.45
(1,1611)	1:616:A:GLN:H	1:612:A:ALA:HB1	9	0.45
(1,1592)	1:613:A:ALA:H	1:616:A:GLN:HB2	6	0.45
(1,1562)	1:604:A:THR:H	1:599:A:GLN:HB2	16	0.45
(1,1526)	1:576:A:LEU:H	1:576:A:LEU:HD22	5	0.45
(1,1526)	1:576:A:LEU:H	1:576:A:LEU:HD22	16	0.45
(1,1526)	1:576:A:LEU:H	1:576:A:LEU:HD22	17	0.45
(1,1517)	1:578:A:GLU:H	1:577:A:LEU:HG	15	0.45
(1,1510)	1:581:A:GLU:H	1:582:A:ALA:HB3	9	0.45
(1,1480)	1:588:A:GLN:H	1:586:A:ALA:HB3	18	0.45
(1,1468)	1:592:A:ALA:H	1:593:A:ASP:HB3	19	0.45
(1,1399)	1:583:A:LYS:HG2	1:580:A:LEU:HD22	13	0.45
(1,1397)	1:587:A:LEU:HD12	1:583:A:LYS:HA	3	0.45
(1,1387)	1:577:A:LEU:HD22	1:574:A:PRO:HB2	14	0.45
(1,1387)	1:577:A:LEU:HD23	1:574:A:PRO:HB2	20	0.45
(1,1369)	1:591:A:VAL:HG21	1:596:A:PHE:HB2	18	0.45
(1,1367)	1:570:A:LEU:HD22	1:628:A:LEU:HB3	5	0.45
(1,1230)	1:612:A:ALA:HA	1:611:A:MET:HG3	2	0.45
(1,1230)	1:612:A:ALA:HA	1:611:A:MET:HG3	8	0.45
(1,1230)	1:612:A:ALA:HA	1:611:A:MET:HG3	12	0.45
(1,1220)	1:551:A:LYS:HD2	1:551:A:LYS:HA	11	0.45
(1,1165)	1:601:A:HIS:HB2	1:605:A:GLN:HG2	12	0.45
(1,1147)	1:565:A:LYS:HA	1:565:A:LYS:HD2	2	0.45
(1,1120)	1:588:A:GLN:HA	1:611:A:MET:HE2	12	0.45
(1,1062)	1:610:A:ASP:HB2	1:587:A:LEU:HD23	3	0.45
(1,1054)	1:604:A:THR:HG23	1:597:A:PHE:HB2	7	0.45
(1,1054)	1:604:A:THR:HG21	1:597:A:PHE:HB2	13	0.45
(1,1054)	1:604:A:THR:HG23	1:597:A:PHE:HB2	14	0.45
(1,1024)	1:590:A:GLN:HG3	1:589:A:THR:HG21	16	0.45

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,926)	1:583:A:LYS:HG3	1:580:A:LEU:HD22	14	0.45
(1,926)	1:583:A:LYS:HG3	1:580:A:LEU:HD22	18	0.45
(1,926)	1:583:A:LYS:HG3	1:580:A:LEU:HD21	19	0.45
(1,893)	1:583:A:LYS:HA	1:583:A:LYS:HE3	3	0.45
(1,893)	1:583:A:LYS:HA	1:583:A:LYS:HE3	5	0.45
(1,893)	1:583:A:LYS:HA	1:583:A:LYS:HE3	8	0.45
(1,870)	1:556:A:LYS:HA	1:556:A:LYS:HE2	13	0.45
(1,850)	1:604:A:THR:HA	1:607:A:VAL:HG12	15	0.45
(1,755)	1:621:A:ALA:HA	1:576:A:LEU:HD22	9	0.45
(1,725)	1:600:A:PRO:HD3	1:599:A:GLN:HB2	15	0.45
(1,672)	1:607:A:VAL:HG22	1:606:A:LYS:HE2	7	0.45
(1,658)	1:591:A:VAL:HG21	1:596:A:PHE:HB3	16	0.45
(1,658)	1:591:A:VAL:HG21	1:596:A:PHE:HB3	18	0.45
(1,630)	1:577:A:LEU:HD12	1:580:A:LEU:HG	1	0.45
(1,630)	1:577:A:LEU:HD12	1:580:A:LEU:HG	2	0.45
(1,603)	1:622:A:PHE:HD1	1:626:A:GLU:HG2	10	0.45
(1,550)	1:596:A:PHE:HD1	1:604:A:THR:HG23	3	0.45
(1,550)	1:596:A:PHE:HD2	1:604:A:THR:HG21	9	0.45
(1,416)	1:616:A:GLN:H	1:615:A:GLU:HB3	5	0.45
(1,321)	1:604:A:THR:H	1:596:A:PHE:HE1	13	0.45
(1,308)	1:566:A:LEU:H	1:566:A:LEU:HD21	6	0.45
(1,300)	1:567:A:GLN:H	1:566:A:LEU:HD22	16	0.45
(1,172)	1:582:A:ALA:H	1:579:A:ASP:HB2	3	0.45
(1,154)	1:585:A:GLU:H	1:584:A:LEU:HB2	2	0.45
(1,154)	1:585:A:GLU:H	1:584:A:LEU:HB2	4	0.45
(1,154)	1:585:A:GLU:H	1:584:A:LEU:HB2	10	0.45
(1,154)	1:585:A:GLU:H	1:584:A:LEU:HB2	12	0.45
(1,154)	1:585:A:GLU:H	1:584:A:LEU:HB2	16	0.45
(1,110)	1:590:A:GLN:H	1:590:A:GLN:HG3	14	0.45
(1,2168)	1:626:A:GLU:HA	1:625:A:TRP:HA	1	0.44
(1,2168)	1:626:A:GLU:HA	1:625:A:TRP:HA	14	0.44
(1,2159)	1:627:A:TYR:HB3	1:628:A:LEU:HA	3	0.44
(1,2159)	1:627:A:TYR:HB3	1:628:A:LEU:HA	6	0.44
(1,2159)	1:627:A:TYR:HB3	1:628:A:LEU:HA	14	0.44
(1,2120)	1:573:A:LEU:HD22	1:624:A:ARG:HB2	16	0.44
(1,2104)	1:566:A:LEU:HD23	1:631:A:LEU:HB2	13	0.44
(1,2059)	1:615:A:GLU:HA	1:619:A:GLU:HG2	10	0.44
(1,2051)	1:603:A:GLN:HG2	1:600:A:PRO:HA	18	0.44
(1,2047)	1:608:A:LEU:HA	1:611:A:MET:HG2	10	0.44
(1,2034)	1:618:A:LEU:HG	1:615:A:GLU:HA	9	0.44
(1,2014)	1:601:A:HIS:HB3	1:602:A:GLU:HB2	2	0.44
(1,1995)	1:557:A:ARG:HD2	1:555:A:VAL:HG11	9	0.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1992)	1:562:A:LEU:HB2	1:632:A:LYS:HG2	6	0.44
(1,1960)	1:622:A:PHE:HB3	1:619:A:GLU:HB2	19	0.44
(1,1958)	1:622:A:PHE:HB3	1:619:A:GLU:HB2	19	0.44
(1,1901)	1:612:A:ALA:HB3	1:616:A:GLN:HB3	12	0.44
(1,1895)	1:618:A:LEU:HG	1:581:A:GLU:HB2	18	0.44
(1,1868)	1:569:A:GLU:HA	1:566:A:LEU:HA	4	0.44
(1,1868)	1:612:A:ALA:HA	1:611:A:MET:HA	9	0.44
(1,1868)	1:614:A:ALA:HA	1:615:A:GLU:HA	17	0.44
(1,1865)	1:622:A:PHE:HA	1:619:A:GLU:HA	15	0.44
(1,1865)	1:622:A:PHE:HA	1:623:A:GLU:HA	17	0.44
(1,1854)	1:612:A:ALA:HA	1:611:A:MET:HA	9	0.44
(1,1854)	1:612:A:ALA:HA	1:611:A:MET:HA	15	0.44
(1,1854)	1:614:A:ALA:HA	1:615:A:GLU:HA	17	0.44
(1,1854)	1:614:A:ALA:HA	1:615:A:GLU:HA	20	0.44
(1,1852)	1:604:A:THR:HB	1:599:A:GLN:HB2	7	0.44
(1,1836)	1:619:A:GLU:HA	1:618:A:LEU:HD12	2	0.44
(1,1834)	1:583:A:LYS:HA	1:587:A:LEU:HD22	4	0.44
(1,1834)	1:583:A:LYS:HA	1:587:A:LEU:HD21	9	0.44
(1,1723)	1:591:A:VAL:HG13	1:611:A:MET:HG3	9	0.44
(1,1718)	1:604:A:THR:HG23	1:599:A:GLN:HG3	17	0.44
(1,1711)	1:577:A:LEU:HD22	1:626:A:GLU:HG3	9	0.44
(1,1711)	1:577:A:LEU:HD21	1:624:A:ARG:HB3	16	0.44
(1,1701)	1:622:A:PHE:HE2	1:577:A:LEU:HA	5	0.44
(1,1701)	1:622:A:PHE:HE2	1:577:A:LEU:HA	13	0.44
(1,1683)	1:622:A:PHE:HE2	1:618:A:LEU:HD22	6	0.44
(1,1628)	1:621:A:ALA:H	1:620:A:GLN:HB2	6	0.44
(1,1608)	1:616:A:GLN:H	1:612:A:ALA:HA	5	0.44
(1,1608)	1:616:A:GLN:H	1:612:A:ALA:HA	15	0.44
(1,1604)	1:628:A:LEU:H	1:570:A:LEU:HG	15	0.44
(1,1534)	1:572:A:GLN:H	1:571:A:GLU:HB3	6	0.44
(1,1534)	1:572:A:GLN:H	1:571:A:GLU:HB3	10	0.44
(1,1526)	1:576:A:LEU:H	1:576:A:LEU:HD23	15	0.44
(1,1526)	1:576:A:LEU:H	1:576:A:LEU:HD23	20	0.44
(1,1510)	1:581:A:GLU:H	1:582:A:ALA:HB3	20	0.44
(1,1468)	1:592:A:ALA:H	1:593:A:ASP:HB2	5	0.44
(1,1465)	1:606:A:LYS:H	1:606:A:LYS:HG2	16	0.44
(1,1457)	1:597:A:PHE:H	1:598:A:SER:HB2	3	0.44
(1,1457)	1:597:A:PHE:H	1:598:A:SER:HB2	20	0.44
(1,1431)	1:622:A:PHE:HE2	1:618:A:LEU:HD22	6	0.44
(1,1397)	1:587:A:LEU:HD11	1:583:A:LYS:HA	16	0.44
(1,1378)	1:624:A:ARG:HD3	1:573:A:LEU:HD11	6	0.44
(1,1369)	1:591:A:VAL:HG21	1:596:A:PHE:HB2	15	0.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1363)	1:562:A:LEU:HD23	1:631:A:LEU:HB2	13	0.44
(1,1325)	1:628:A:LEU:HD12	1:569:A:GLU:HA	6	0.44
(1,1230)	1:612:A:ALA:HA	1:611:A:MET:HG3	5	0.44
(1,1230)	1:612:A:ALA:HA	1:611:A:MET:HG3	9	0.44
(1,1230)	1:612:A:ALA:HA	1:611:A:MET:HG3	18	0.44
(1,1163)	1:599:A:GLN:HG3	1:600:A:PRO:HD3	2	0.44
(1,1061)	1:610:A:ASP:HB3	1:607:A:VAL:HG11	8	0.44
(1,1020)	1:604:A:THR:HG23	1:599:A:GLN:HG3	17	0.44
(1,1016)	1:588:A:GLN:HG2	1:584:A:LEU:HG	9	0.44
(1,1005)	1:603:A:GLN:HG3	1:604:A:THR:HG22	19	0.44
(1,956)	1:605:A:GLN:HB3	1:608:A:LEU:HD12	19	0.44
(1,929)	1:565:A:LYS:HG2	1:566:A:LEU:HD11	4	0.44
(1,926)	1:583:A:LYS:HG3	1:580:A:LEU:HD21	5	0.44
(1,926)	1:583:A:LYS:HG3	1:580:A:LEU:HD22	6	0.44
(1,922)	1:612:A:ALA:HB3	1:611:A:MET:HE1	14	0.44
(1,893)	1:583:A:LYS:HA	1:583:A:LYS:HE3	13	0.44
(1,893)	1:583:A:LYS:HA	1:583:A:LYS:HE3	17	0.44
(1,850)	1:604:A:THR:HA	1:607:A:VAL:HG13	3	0.44
(1,809)	1:605:A:GLN:HA	1:608:A:LEU:HD23	5	0.44
(1,658)	1:591:A:VAL:HG21	1:596:A:PHE:HB3	8	0.44
(1,658)	1:591:A:VAL:HG23	1:596:A:PHE:HB3	11	0.44
(1,634)	1:577:A:LEU:HD11	1:574:A:PRO:HA	11	0.44
(1,631)	1:577:A:LEU:HD11	1:622:A:PHE:HB3	1	0.44
(1,603)	1:622:A:PHE:HD1	1:626:A:GLU:HG2	9	0.44
(1,559)	1:596:A:PHE:HE1	1:604:A:THR:HG22	11	0.44
(1,550)	1:596:A:PHE:HD1	1:604:A:THR:HG22	11	0.44
(1,550)	1:596:A:PHE:HD1	1:604:A:THR:HG23	19	0.44
(1,416)	1:616:A:GLN:H	1:615:A:GLU:HB3	15	0.44
(1,368)	1:609:A:ALA:H	1:608:A:LEU:HD22	5	0.44
(1,368)	1:609:A:ALA:H	1:608:A:LEU:HD23	6	0.44
(1,368)	1:609:A:ALA:H	1:608:A:LEU:HD23	11	0.44
(1,308)	1:566:A:LEU:H	1:566:A:LEU:HD22	14	0.44
(1,308)	1:566:A:LEU:H	1:566:A:LEU:HD22	19	0.44
(1,172)	1:582:A:ALA:H	1:579:A:ASP:HB2	13	0.44
(1,154)	1:585:A:GLU:H	1:584:A:LEU:HB2	9	0.44
(1,154)	1:585:A:GLU:H	1:584:A:LEU:HB2	18	0.44
(1,154)	1:585:A:GLU:H	1:584:A:LEU:HB2	19	0.44
(1,110)	1:590:A:GLN:H	1:590:A:GLN:HG3	1	0.44
(1,2171)	1:591:A:VAL:HG23	1:597:A:PHE:HZ	6	0.43
(1,2168)	1:626:A:GLU:HA	1:625:A:TRP:HA	2	0.43
(1,2168)	1:626:A:GLU:HA	1:625:A:TRP:HA	6	0.43
(1,2168)	1:626:A:GLU:HA	1:625:A:TRP:HA	18	0.43

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2059)	1:615:A:GLU:HA	1:619:A:GLU:HG2	14	0.43
(1,2056)	1:599:A:GLN:HG2	1:598:A:SER:HB3	13	0.43
(1,2051)	1:603:A:GLN:HG2	1:600:A:PRO:HA	15	0.43
(1,2034)	1:618:A:LEU:HG	1:615:A:GLU:HA	2	0.43
(1,2013)	1:565:A:LYS:HA	1:568:A:ARG:HB3	17	0.43
(1,1965)	1:579:A:ASP:HB2	1:576:A:LEU:HG	12	0.43
(1,1924)	1:614:A:ALA:HB3	1:611:A:MET:HG2	2	0.43
(1,1924)	1:614:A:ALA:HB1	1:611:A:MET:HG2	9	0.43
(1,1917)	1:585:A:GLU:HB2	1:584:A:LEU:HD12	8	0.43
(1,1901)	1:612:A:ALA:HB2	1:616:A:GLN:HB3	8	0.43
(1,1865)	1:622:A:PHE:HA	1:623:A:GLU:HA	20	0.43
(1,1854)	1:614:A:ALA:HA	1:615:A:GLU:HA	2	0.43
(1,1854)	1:614:A:ALA:HA	1:615:A:GLU:HA	13	0.43
(1,1854)	1:612:A:ALA:HA	1:611:A:MET:HA	14	0.43
(1,1854)	1:614:A:ALA:HA	1:615:A:GLU:HA	19	0.43
(1,1852)	1:604:A:THR:HB	1:599:A:GLN:HB2	2	0.43
(1,1852)	1:604:A:THR:HB	1:608:A:LEU:HB2	17	0.43
(1,1836)	1:619:A:GLU:HA	1:618:A:LEU:HD11	16	0.43
(1,1778)	1:612:A:ALA:HA	1:584:A:LEU:HD21	6	0.43
(1,1774)	1:592:A:ALA:HA	1:589:A:THR:HA	2	0.43
(1,1741)	1:628:A:LEU:HD23	1:624:A:ARG:HA	6	0.43
(1,1711)	1:577:A:LEU:HD21	1:626:A:GLU:HG3	7	0.43
(1,1705)	1:622:A:PHE:HD1	1:577:A:LEU:HD23	11	0.43
(1,1701)	1:622:A:PHE:HE2	1:577:A:LEU:HA	1	0.43
(1,1701)	1:622:A:PHE:HE2	1:577:A:LEU:HA	11	0.43
(1,1701)	1:622:A:PHE:HE2	1:577:A:LEU:HA	18	0.43
(1,1700)	1:622:A:PHE:HZ	1:618:A:LEU:HD12	16	0.43
(1,1691)	1:627:A:TYR:HE2	1:624:A:ARG:HA	6	0.43
(1,1621)	1:619:A:GLU:H	1:618:A:LEU:HD23	17	0.43
(1,1621)	1:619:A:GLU:H	1:618:A:LEU:HD21	19	0.43
(1,1617)	1:617:A:GLU:H	1:580:A:LEU:HD21	11	0.43
(1,1588)	1:583:A:LYS:H	1:581:A:GLU:HG2	1	0.43
(1,1468)	1:592:A:ALA:H	1:593:A:ASP:HB3	17	0.43
(1,1449)	1:603:A:GLN:H	1:605:A:GLN:HB2	11	0.43
(1,1412)	1:584:A:LEU:HD22	1:615:A:GLU:HB2	5	0.43
(1,1369)	1:591:A:VAL:HG21	1:596:A:PHE:HB2	14	0.43
(1,1265)	1:593:A:ASP:HB3	1:595:A:SER:HB2	20	0.43
(1,1164)	1:601:A:HIS:HB3	1:605:A:GLN:HG2	5	0.43
(1,1053)	1:577:A:LEU:HD12	1:617:A:GLU:HG3	10	0.43
(1,1019)	1:604:A:THR:HG21	1:599:A:GLN:HG2	4	0.43
(1,1000)	1:565:A:LYS:HB2	1:566:A:LEU:HD11	10	0.43
(1,926)	1:583:A:LYS:HG3	1:580:A:LEU:HD22	15	0.43

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,893)	1:583:A:LYS:HA	1:583:A:LYS:HE3	10	0.43
(1,893)	1:583:A:LYS:HA	1:583:A:LYS:HE3	11	0.43
(1,850)	1:604:A:THR:HA	1:607:A:VAL:HG11	1	0.43
(1,834)	1:619:A:GLU:HA	1:618:A:LEU:HG	14	0.43
(1,658)	1:591:A:VAL:HG22	1:596:A:PHE:HB3	9	0.43
(1,631)	1:577:A:LEU:HD11	1:622:A:PHE:HB3	5	0.43
(1,631)	1:577:A:LEU:HD13	1:622:A:PHE:HB3	9	0.43
(1,569)	1:625:A:TRP:HZ2	1:629:A:GLU:HG2	11	0.43
(1,550)	1:596:A:PHE:HD1	1:604:A:THR:HG22	4	0.43
(1,538)	1:635:A:GLY:H	1:631:A:LEU:HD11	13	0.43
(1,368)	1:609:A:ALA:H	1:608:A:LEU:HD21	3	0.43
(1,368)	1:609:A:ALA:H	1:608:A:LEU:HD21	17	0.43
(1,308)	1:566:A:LEU:H	1:566:A:LEU:HD21	1	0.43
(1,307)	1:566:A:LEU:H	1:566:A:LEU:HD12	7	0.43
(1,172)	1:582:A:ALA:H	1:579:A:ASP:HB2	1	0.43
(1,172)	1:582:A:ALA:H	1:579:A:ASP:HB2	6	0.43
(1,172)	1:582:A:ALA:H	1:579:A:ASP:HB2	10	0.43
(1,172)	1:582:A:ALA:H	1:579:A:ASP:HB2	11	0.43
(1,154)	1:585:A:GLU:H	1:584:A:LEU:HB2	1	0.43
(1,154)	1:585:A:GLU:H	1:584:A:LEU:HB2	8	0.43
(1,154)	1:585:A:GLU:H	1:584:A:LEU:HB2	13	0.43
(1,154)	1:585:A:GLU:H	1:584:A:LEU:HB2	20	0.43
(1,110)	1:590:A:GLN:H	1:590:A:GLN:HG3	4	0.43
(1,2168)	1:626:A:GLU:HA	1:625:A:TRP:HA	8	0.42
(1,2165)	1:606:A:LYS:HA	1:606:A:LYS:HE3	13	0.42
(1,2159)	1:627:A:TYR:HB3	1:628:A:LEU:HA	7	0.42
(1,2159)	1:627:A:TYR:HB3	1:628:A:LEU:HA	10	0.42
(1,2158)	1:591:A:VAL:HG21	1:596:A:PHE:HB2	13	0.42
(1,2105)	1:566:A:LEU:HD23	1:569:A:GLU:HG3	5	0.42
(1,2105)	1:566:A:LEU:HD22	1:628:A:LEU:HG	8	0.42
(1,2052)	1:603:A:GLN:HG3	1:599:A:GLN:HA	7	0.42
(1,2051)	1:603:A:GLN:HG2	1:600:A:PRO:HA	8	0.42
(1,2047)	1:608:A:LEU:HA	1:611:A:MET:HG2	1	0.42
(1,2047)	1:608:A:LEU:HA	1:611:A:MET:HG2	16	0.42
(1,2046)	1:626:A:GLU:HB3	1:627:A:TYR:HA	18	0.42
(1,1965)	1:579:A:ASP:HB2	1:576:A:LEU:HG	4	0.42
(1,1961)	1:610:A:ASP:HB3	1:587:A:LEU:HB3	2	0.42
(1,1937)	1:616:A:GLN:HG3	1:613:A:ALA:HB1	11	0.42
(1,1937)	1:616:A:GLN:HG3	1:613:A:ALA:HB2	17	0.42
(1,1901)	1:613:A:ALA:HB3	1:616:A:GLN:HB2	3	0.42
(1,1901)	1:612:A:ALA:HB1	1:616:A:GLN:HB3	9	0.42
(1,1865)	1:622:A:PHE:HA	1:623:A:GLU:HA	13	0.42

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1854)	1:612:A:ALA:HA	1:611:A:MET:HA	3	0.42
(1,1854)	1:614:A:ALA:HA	1:615:A:GLU:HA	8	0.42
(1,1854)	1:614:A:ALA:HA	1:615:A:GLU:HA	10	0.42
(1,1778)	1:612:A:ALA:HA	1:584:A:LEU:HD21	17	0.42
(1,1729)	1:631:A:LEU:HD23	1:561:A:LYS:HA	14	0.42
(1,1723)	1:591:A:VAL:HG13	1:611:A:MET:HG3	5	0.42
(1,1718)	1:604:A:THR:HG22	1:599:A:GLN:HG3	16	0.42
(1,1708)	1:625:A:TRP:HD1	1:628:A:LEU:HD11	2	0.42
(1,1708)	1:625:A:TRP:HD1	1:628:A:LEU:HD12	20	0.42
(1,1683)	1:622:A:PHE:HE2	1:618:A:LEU:HD22	10	0.42
(1,1678)	1:627:A:TYR:HE1	1:631:A:LEU:HG	2	0.42
(1,1592)	1:613:A:ALA:H	1:616:A:GLN:HB2	2	0.42
(1,1567)	1:607:A:VAL:H	1:606:A:LYS:HB2	9	0.42
(1,1565)	1:607:A:VAL:H	1:610:A:ASP:HB2	20	0.42
(1,1526)	1:576:A:LEU:H	1:576:A:LEU:HD22	11	0.42
(1,1517)	1:578:A:GLU:H	1:577:A:LEU:HG	8	0.42
(1,1510)	1:581:A:GLU:H	1:582:A:ALA:HB1	6	0.42
(1,1506)	1:582:A:ALA:H	1:618:A:LEU:HD23	14	0.42
(1,1468)	1:592:A:ALA:H	1:593:A:ASP:HB2	9	0.42
(1,1420)	1:627:A:TYR:HE2	1:631:A:LEU:HD22	12	0.42
(1,1399)	1:583:A:LYS:HG2	1:580:A:LEU:HD23	11	0.42
(1,1396)	1:632:A:LYS:HG3	1:562:A:LEU:HB2	3	0.42
(1,1335)	1:566:A:LEU:HG	1:562:A:LEU:HD23	17	0.42
(1,1164)	1:601:A:HIS:HB3	1:605:A:GLN:HG2	17	0.42
(1,1062)	1:610:A:ASP:HB2	1:587:A:LEU:HD22	5	0.42
(1,1062)	1:610:A:ASP:HB2	1:587:A:LEU:HD21	11	0.42
(1,1024)	1:590:A:GLN:HG3	1:589:A:THR:HG23	4	0.42
(1,1021)	1:591:A:VAL:HG23	1:590:A:GLN:HG3	18	0.42
(1,1020)	1:604:A:THR:HG22	1:599:A:GLN:HG3	16	0.42
(1,1016)	1:588:A:GLN:HG2	1:584:A:LEU:HG	13	0.42
(1,1005)	1:603:A:GLN:HG3	1:604:A:THR:HG21	4	0.42
(1,1005)	1:603:A:GLN:HG3	1:604:A:THR:HG23	8	0.42
(1,926)	1:583:A:LYS:HG3	1:580:A:LEU:HD22	12	0.42
(1,869)	1:557:A:ARG:HA	1:557:A:ARG:HD2	6	0.42
(1,850)	1:604:A:THR:HA	1:607:A:VAL:HG11	11	0.42
(1,838)	1:623:A:GLU:HA	1:626:A:GLU:HB3	11	0.42
(1,809)	1:605:A:GLN:HA	1:608:A:LEU:HD21	15	0.42
(1,809)	1:605:A:GLN:HA	1:608:A:LEU:HD21	19	0.42
(1,717)	1:621:A:ALA:HB3	1:577:A:LEU:HD21	6	0.42
(1,658)	1:591:A:VAL:HG21	1:596:A:PHE:HB3	14	0.42
(1,634)	1:577:A:LEU:HD11	1:574:A:PRO:HA	10	0.42
(1,634)	1:577:A:LEU:HD13	1:574:A:PRO:HA	12	0.42

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,569)	1:625:A:TRP:HZ2	1:629:A:GLU:HG2	7	0.42
(1,569)	1:625:A:TRP:HZ2	1:629:A:GLU:HG2	13	0.42
(1,569)	1:625:A:TRP:HZ2	1:629:A:GLU:HG2	16	0.42
(1,559)	1:596:A:PHE:HE2	1:604:A:THR:HG21	2	0.42
(1,559)	1:596:A:PHE:HE1	1:604:A:THR:HG23	15	0.42
(1,559)	1:596:A:PHE:HE2	1:604:A:THR:HG21	20	0.42
(1,558)	1:564:A:TYR:HE2	1:568:A:ARG:HB2	5	0.42
(1,550)	1:596:A:PHE:HD2	1:604:A:THR:HG21	2	0.42
(1,550)	1:596:A:PHE:HD1	1:604:A:THR:HG23	6	0.42
(1,550)	1:596:A:PHE:HD1	1:604:A:THR:HG21	8	0.42
(1,429)	1:618:A:LEU:H	1:617:A:GLU:HB2	15	0.42
(1,416)	1:616:A:GLN:H	1:615:A:GLU:HB3	17	0.42
(1,173)	1:612:A:ALA:H	1:611:A:MET:HB2	14	0.42
(1,26)	1:599:A:GLN:H	1:599:A:GLN:HB3	2	0.42
(1,26)	1:599:A:GLN:H	1:599:A:GLN:HB3	3	0.42
(1,26)	1:599:A:GLN:H	1:599:A:GLN:HB3	11	0.42
(1,26)	1:599:A:GLN:H	1:599:A:GLN:HB3	12	0.42
(1,26)	1:599:A:GLN:H	1:599:A:GLN:HB3	13	0.42
(1,26)	1:599:A:GLN:H	1:599:A:GLN:HB3	20	0.42
(1,24)	1:599:A:GLN:H	1:599:A:GLN:HG2	7	0.42
(1,2171)	1:591:A:VAL:HG23	1:597:A:PHE:HZ	1	0.41
(1,2168)	1:626:A:GLU:HA	1:625:A:TRP:HA	5	0.41
(1,2159)	1:627:A:TYR:HB3	1:628:A:LEU:HA	11	0.41
(1,2159)	1:627:A:TYR:HB3	1:628:A:LEU:HA	18	0.41
(1,2105)	1:566:A:LEU:HD23	1:628:A:LEU:HG	6	0.41
(1,2104)	1:566:A:LEU:HD23	1:562:A:LEU:HB2	8	0.41
(1,2046)	1:626:A:GLU:HB3	1:627:A:TYR:HA	11	0.41
(1,2042)	1:573:A:LEU:HG	1:570:A:LEU:HA	17	0.41
(1,2034)	1:618:A:LEU:HG	1:581:A:GLU:HA	4	0.41
(1,1965)	1:579:A:ASP:HB2	1:576:A:LEU:HG	2	0.41
(1,1965)	1:579:A:ASP:HB2	1:576:A:LEU:HG	8	0.41
(1,1958)	1:622:A:PHE:HB3	1:619:A:GLU:HB2	5	0.41
(1,1937)	1:616:A:GLN:HG3	1:613:A:ALA:HB1	8	0.41
(1,1913)	1:585:A:GLU:HB3	1:586:A:ALA:HB1	6	0.41
(1,1874)	1:632:A:LYS:HG2	1:562:A:LEU:HD22	12	0.41
(1,1868)	1:614:A:ALA:HA	1:615:A:GLU:HA	6	0.41
(1,1854)	1:614:A:ALA:HA	1:615:A:GLU:HA	6	0.41
(1,1852)	1:604:A:THR:HB	1:599:A:GLN:HB2	15	0.41
(1,1836)	1:619:A:GLU:HA	1:618:A:LEU:HD12	18	0.41
(1,1828)	1:601:A:HIS:HA	1:602:A:GLU:HG3	19	0.41
(1,1794)	1:566:A:LEU:HA	1:562:A:LEU:HG	19	0.41
(1,1759)	1:609:A:ALA:HB2	1:605:A:GLN:HA	13	0.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1731)	1:607:A:VAL:HG22	1:603:A:GLN:HB3	3	0.41
(1,1711)	1:577:A:LEU:HD22	1:626:A:GLU:HG3	19	0.41
(1,1709)	1:625:A:TRP:HD1	1:573:A:LEU:HB2	20	0.41
(1,1701)	1:622:A:PHE:HE2	1:577:A:LEU:HA	20	0.41
(1,1678)	1:627:A:TYR:HE1	1:631:A:LEU:HG	11	0.41
(1,1569)	1:607:A:VAL:H	1:587:A:LEU:HD23	1	0.41
(1,1567)	1:607:A:VAL:H	1:606:A:LYS:HB2	20	0.41
(1,1565)	1:607:A:VAL:H	1:610:A:ASP:HB2	11	0.41
(1,1562)	1:604:A:THR:H	1:599:A:GLN:HB2	10	0.41
(1,1562)	1:604:A:THR:H	1:599:A:GLN:HB2	18	0.41
(1,1535)	1:572:A:GLN:H	1:573:A:LEU:HD12	19	0.41
(1,1526)	1:576:A:LEU:H	1:576:A:LEU:HD22	18	0.41
(1,1517)	1:578:A:GLU:H	1:577:A:LEU:HG	2	0.41
(1,1510)	1:581:A:GLU:H	1:582:A:ALA:HB1	7	0.41
(1,1510)	1:581:A:GLU:H	1:582:A:ALA:HB2	19	0.41
(1,1506)	1:582:A:ALA:H	1:618:A:LEU:HD11	17	0.41
(1,1484)	1:587:A:LEU:H	1:588:A:GLN:HG2	12	0.41
(1,1469)	1:592:A:ALA:H	1:591:A:VAL:HG13	15	0.41
(1,1449)	1:603:A:GLN:H	1:605:A:GLN:HB2	14	0.41
(1,1431)	1:622:A:PHE:HE2	1:618:A:LEU:HD22	10	0.41
(1,1399)	1:583:A:LYS:HG2	1:580:A:LEU:HD21	19	0.41
(1,1374)	1:577:A:LEU:HD13	1:625:A:TRP:HB3	10	0.41
(1,1369)	1:591:A:VAL:HG23	1:596:A:PHE:HB2	20	0.41
(1,1366)	1:566:A:LEU:HD21	1:631:A:LEU:HD12	3	0.41
(1,1333)	1:573:A:LEU:HD13	1:624:A:ARG:HD2	4	0.41
(1,1333)	1:573:A:LEU:HD12	1:624:A:ARG:HD2	16	0.41
(1,1325)	1:628:A:LEU:HD12	1:569:A:GLU:HA	10	0.41
(1,1291)	1:608:A:LEU:HD13	1:604:A:THR:HG22	20	0.41
(1,1136)	1:600:A:PRO:HD3	1:603:A:GLN:HB3	6	0.41
(1,1057)	1:622:A:PHE:HB3	1:577:A:LEU:HD22	10	0.41
(1,1024)	1:590:A:GLN:HG3	1:589:A:THR:HG23	8	0.41
(1,970)	1:632:A:LYS:HD3	1:570:A:LEU:HD12	10	0.41
(1,956)	1:605:A:GLN:HB3	1:608:A:LEU:HD13	6	0.41
(1,926)	1:583:A:LYS:HG3	1:580:A:LEU:HD23	1	0.41
(1,926)	1:583:A:LYS:HG3	1:580:A:LEU:HD21	9	0.41
(1,926)	1:583:A:LYS:HG3	1:580:A:LEU:HD22	10	0.41
(1,893)	1:583:A:LYS:HA	1:583:A:LYS:HE3	15	0.41
(1,893)	1:583:A:LYS:HA	1:583:A:LYS:HE3	20	0.41
(1,850)	1:604:A:THR:HA	1:607:A:VAL:HG12	5	0.41
(1,755)	1:621:A:ALA:HA	1:576:A:LEU:HD23	3	0.41
(1,668)	1:631:A:LEU:HD12	1:635:A:GLY:HA3	10	0.41
(1,658)	1:591:A:VAL:HG23	1:596:A:PHE:HB3	1	0.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,634)	1:577:A:LEU:HD11	1:574:A:PRO:HA	9	0.41
(1,634)	1:577:A:LEU:HD11	1:574:A:PRO:HA	17	0.41
(1,602)	1:597:A:PHE:HZ	1:608:A:LEU:HD13	20	0.41
(1,599)	1:601:A:HIS:HD2	1:602:A:GLU:HG3	13	0.41
(1,569)	1:625:A:TRP:HZ2	1:629:A:GLU:HG2	6	0.41
(1,559)	1:596:A:PHE:HE1	1:604:A:THR:HG23	19	0.41
(1,550)	1:596:A:PHE:HD1	1:604:A:THR:HG23	15	0.41
(1,416)	1:616:A:GLN:H	1:615:A:GLU:HB3	10	0.41
(1,416)	1:616:A:GLN:H	1:615:A:GLU:HB3	19	0.41
(1,368)	1:609:A:ALA:H	1:608:A:LEU:HD21	1	0.41
(1,368)	1:609:A:ALA:H	1:608:A:LEU:HD23	12	0.41
(1,321)	1:604:A:THR:H	1:596:A:PHE:HE1	2	0.41
(1,283)	1:569:A:GLU:H	1:568:A:ARG:HB3	17	0.41
(1,172)	1:582:A:ALA:H	1:579:A:ASP:HB2	2	0.41
(1,172)	1:582:A:ALA:H	1:579:A:ASP:HB2	5	0.41
(1,172)	1:582:A:ALA:H	1:579:A:ASP:HB2	7	0.41
(1,172)	1:582:A:ALA:H	1:579:A:ASP:HB2	12	0.41
(1,110)	1:590:A:GLN:H	1:590:A:GLN:HG3	16	0.41
(1,26)	1:599:A:GLN:H	1:599:A:GLN:HB3	1	0.41
(1,26)	1:599:A:GLN:H	1:599:A:GLN:HB3	7	0.41
(1,26)	1:599:A:GLN:H	1:599:A:GLN:HB3	19	0.41
(1,2109)	1:608:A:LEU:HD11	1:591:A:VAL:HG12	6	0.4
(1,2109)	1:608:A:LEU:HD11	1:591:A:VAL:HG12	11	0.4
(1,2104)	1:566:A:LEU:HD21	1:631:A:LEU:HB2	18	0.4
(1,2098)	1:581:A:GLU:HG3	1:618:A:LEU:HD22	7	0.4
(1,2059)	1:615:A:GLU:HA	1:619:A:GLU:HG2	7	0.4
(1,2052)	1:603:A:GLN:HG3	1:599:A:GLN:HA	6	0.4
(1,1965)	1:579:A:ASP:HB2	1:576:A:LEU:HG	19	0.4
(1,1961)	1:610:A:ASP:HB3	1:587:A:LEU:HB3	20	0.4
(1,1907)	1:591:A:VAL:HA	1:608:A:LEU:HD21	5	0.4
(1,1868)	1:569:A:GLU:HA	1:566:A:LEU:HA	14	0.4
(1,1852)	1:604:A:THR:HB	1:599:A:GLN:HB2	20	0.4
(1,1836)	1:619:A:GLU:HA	1:618:A:LEU:HD13	15	0.4
(1,1828)	1:601:A:HIS:HA	1:602:A:GLU:HG3	9	0.4
(1,1787)	1:621:A:ALA:HA	1:620:A:GLN:HB2	6	0.4
(1,1779)	1:614:A:ALA:HA	1:580:A:LEU:HD12	17	0.4
(1,1778)	1:612:A:ALA:HA	1:584:A:LEU:HD22	2	0.4
(1,1778)	1:612:A:ALA:HA	1:584:A:LEU:HD21	13	0.4
(1,1774)	1:592:A:ALA:HA	1:589:A:THR:HA	11	0.4
(1,1731)	1:607:A:VAL:HG23	1:603:A:GLN:HB2	6	0.4
(1,1718)	1:604:A:THR:HG21	1:599:A:GLN:HG3	9	0.4
(1,1709)	1:625:A:TRP:HD1	1:573:A:LEU:HB2	17	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1708)	1:625:A:TRP:HD1	1:628:A:LEU:HD13	10	0.4
(1,1708)	1:625:A:TRP:HD1	1:628:A:LEU:HD11	13	0.4
(1,1691)	1:627:A:TYR:HE2	1:624:A:ARG:HA	4	0.4
(1,1690)	1:564:A:TYR:HE1	1:567:A:GLN:HB3	9	0.4
(1,1669)	1:633:A:ASN:H	1:632:A:LYS:HG3	15	0.4
(1,1621)	1:619:A:GLU:H	1:618:A:LEU:HD21	5	0.4
(1,1562)	1:604:A:THR:H	1:599:A:GLN:HB2	7	0.4
(1,1562)	1:604:A:THR:H	1:599:A:GLN:HB2	13	0.4
(1,1517)	1:578:A:GLU:H	1:577:A:LEU:HG	12	0.4
(1,1517)	1:578:A:GLU:H	1:577:A:LEU:HG	18	0.4
(1,1510)	1:581:A:GLU:H	1:582:A:ALA:HB3	16	0.4
(1,1447)	1:568:A:ARG:HD2	1:564:A:TYR:HD2	5	0.4
(1,1426)	1:627:A:TYR:HD2	1:628:A:LEU:HD22	1	0.4
(1,1402)	1:606:A:LYS:HB2	1:606:A:LYS:HE3	6	0.4
(1,1369)	1:591:A:VAL:HG23	1:596:A:PHE:HB2	6	0.4
(1,1367)	1:570:A:LEU:HD21	1:628:A:LEU:HB3	6	0.4
(1,1365)	1:631:A:LEU:HD21	1:566:A:LEU:HD12	6	0.4
(1,1335)	1:566:A:LEU:HG	1:562:A:LEU:HD21	11	0.4
(1,1306)	1:589:A:THR:HG23	1:590:A:GLN:HB2	7	0.4
(1,1220)	1:551:A:LYS:HD2	1:551:A:LYS:HA	6	0.4
(1,1220)	1:551:A:LYS:HD3	1:551:A:LYS:HA	8	0.4
(1,1165)	1:601:A:HIS:HB2	1:605:A:GLN:HG2	1	0.4
(1,1163)	1:599:A:GLN:HG3	1:600:A:PRO:HD3	20	0.4
(1,1155)	1:603:A:GLN:HG3	1:600:A:PRO:HD3	7	0.4
(1,1147)	1:565:A:LYS:HA	1:565:A:LYS:HD3	16	0.4
(1,1062)	1:610:A:ASP:HB2	1:587:A:LEU:HD23	9	0.4
(1,1057)	1:622:A:PHE:HB3	1:577:A:LEU:HD23	1	0.4
(1,1057)	1:622:A:PHE:HB3	1:577:A:LEU:HD21	5	0.4
(1,1057)	1:622:A:PHE:HB3	1:577:A:LEU:HD21	7	0.4
(1,1057)	1:622:A:PHE:HB3	1:577:A:LEU:HD21	12	0.4
(1,1024)	1:590:A:GLN:HG3	1:589:A:THR:HG22	1	0.4
(1,1021)	1:591:A:VAL:HG22	1:590:A:GLN:HG3	1	0.4
(1,1021)	1:591:A:VAL:HG23	1:590:A:GLN:HG3	8	0.4
(1,1021)	1:591:A:VAL:HG23	1:590:A:GLN:HG3	17	0.4
(1,1020)	1:604:A:THR:HG21	1:599:A:GLN:HG3	9	0.4
(1,998)	1:583:A:LYS:HB3	1:587:A:LEU:HD13	12	0.4
(1,998)	1:583:A:LYS:HB3	1:587:A:LEU:HD12	14	0.4
(1,926)	1:583:A:LYS:HG3	1:580:A:LEU:HD23	2	0.4
(1,893)	1:583:A:LYS:HA	1:583:A:LYS:HE3	14	0.4
(1,869)	1:557:A:ARG:HA	1:557:A:ARG:HD2	2	0.4
(1,755)	1:621:A:ALA:HA	1:576:A:LEU:HD21	7	0.4
(1,658)	1:591:A:VAL:HG23	1:596:A:PHE:HB3	10	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,631)	1:577:A:LEU:HD13	1:622:A:PHE:HB3	11	0.4
(1,599)	1:601:A:HIS:HD2	1:602:A:GLU:HG2	2	0.4
(1,564)	1:597:A:PHE:HE2	1:591:A:VAL:HG11	10	0.4
(1,559)	1:596:A:PHE:HE1	1:604:A:THR:HG22	4	0.4
(1,559)	1:596:A:PHE:HE1	1:604:A:THR:HG22	18	0.4
(1,554)	1:627:A:TYR:HE2	1:628:A:LEU:HD21	20	0.4
(1,416)	1:616:A:GLN:H	1:615:A:GLU:HB3	7	0.4
(1,416)	1:616:A:GLN:H	1:615:A:GLU:HB3	12	0.4
(1,368)	1:609:A:ALA:H	1:608:A:LEU:HD21	15	0.4
(1,368)	1:609:A:ALA:H	1:608:A:LEU:HD23	18	0.4
(1,368)	1:609:A:ALA:H	1:608:A:LEU:HD23	20	0.4
(1,300)	1:567:A:GLN:H	1:566:A:LEU:HD23	3	0.4
(1,172)	1:582:A:ALA:H	1:579:A:ASP:HB2	8	0.4
(1,172)	1:582:A:ALA:H	1:579:A:ASP:HB2	14	0.4
(1,172)	1:582:A:ALA:H	1:579:A:ASP:HB2	16	0.4
(1,172)	1:582:A:ALA:H	1:579:A:ASP:HB2	18	0.4
(1,154)	1:585:A:GLU:H	1:584:A:LEU:HB2	6	0.4
(1,125)	1:589:A:THR:H	1:586:A:ALA:HB3	15	0.4
(1,110)	1:590:A:GLN:H	1:590:A:GLN:HG3	6	0.4
(1,110)	1:590:A:GLN:H	1:590:A:GLN:HG3	8	0.4
(1,26)	1:599:A:GLN:H	1:599:A:GLN:HB3	4	0.4
(1,26)	1:599:A:GLN:H	1:599:A:GLN:HB3	5	0.4
(1,26)	1:599:A:GLN:H	1:599:A:GLN:HB3	10	0.4
(1,2171)	1:591:A:VAL:HG22	1:597:A:PHE:HZ	9	0.39
(1,2165)	1:606:A:LYS:HA	1:610:A:ASP:HB2	6	0.39
(1,2159)	1:627:A:TYR:HB3	1:628:A:LEU:HA	17	0.39
(1,2119)	1:569:A:GLU:HB3	1:566:A:LEU:HD13	6	0.39
(1,2114)	1:581:A:GLU:HG3	1:618:A:LEU:HD13	18	0.39
(1,2109)	1:608:A:LEU:HD11	1:591:A:VAL:HG13	10	0.39
(1,2059)	1:615:A:GLU:HA	1:619:A:GLU:HG2	17	0.39
(1,2047)	1:608:A:LEU:HA	1:611:A:MET:HG2	5	0.39
(1,2047)	1:608:A:LEU:HA	1:611:A:MET:HG2	6	0.39
(1,2047)	1:608:A:LEU:HA	1:611:A:MET:HG2	12	0.39
(1,2047)	1:608:A:LEU:HA	1:611:A:MET:HG2	18	0.39
(1,2047)	1:608:A:LEU:HA	1:611:A:MET:HG2	19	0.39
(1,2046)	1:626:A:GLU:HB3	1:627:A:TYR:HA	8	0.39
(1,2046)	1:626:A:GLU:HB3	1:627:A:TYR:HA	14	0.39
(1,2042)	1:573:A:LEU:HG	1:570:A:LEU:HA	13	0.39
(1,1960)	1:622:A:PHE:HB3	1:619:A:GLU:HB2	16	0.39
(1,1958)	1:622:A:PHE:HB3	1:619:A:GLU:HB2	16	0.39
(1,1924)	1:614:A:ALA:HB1	1:611:A:MET:HG2	5	0.39
(1,1871)	1:594:A:ALA:HB2	1:595:A:SER:HB3	13	0.39

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1868)	1:569:A:GLU:HA	1:566:A:LEU:HA	3	0.39
(1,1852)	1:604:A:THR:HB	1:599:A:GLN:HB2	11	0.39
(1,1828)	1:601:A:HIS:HA	1:602:A:GLU:HG3	12	0.39
(1,1790)	1:557:A:ARG:HA	1:555:A:VAL:HG22	11	0.39
(1,1760)	1:594:A:ALA:HB2	1:595:A:SER:HB3	13	0.39
(1,1741)	1:628:A:LEU:HD22	1:624:A:ARG:HA	9	0.39
(1,1741)	1:628:A:LEU:HD23	1:624:A:ARG:HA	19	0.39
(1,1719)	1:604:A:THR:HG21	1:603:A:GLN:HG2	18	0.39
(1,1706)	1:625:A:TRP:HD1	1:628:A:LEU:HB2	19	0.39
(1,1705)	1:622:A:PHE:HD1	1:577:A:LEU:HD21	5	0.39
(1,1701)	1:622:A:PHE:HE2	1:577:A:LEU:HA	10	0.39
(1,1691)	1:627:A:TYR:HE2	1:624:A:ARG:HA	11	0.39
(1,1633)	1:622:A:PHE:H	1:619:A:GLU:HB3	4	0.39
(1,1628)	1:621:A:ALA:H	1:620:A:GLN:HB2	4	0.39
(1,1621)	1:619:A:GLU:H	1:618:A:LEU:HD23	7	0.39
(1,1621)	1:619:A:GLU:H	1:618:A:LEU:HD23	10	0.39
(1,1608)	1:616:A:GLN:H	1:612:A:ALA:HA	14	0.39
(1,1594)	1:614:A:ALA:H	1:615:A:GLU:HG3	1	0.39
(1,1565)	1:607:A:VAL:H	1:610:A:ASP:HB2	15	0.39
(1,1535)	1:572:A:GLN:H	1:573:A:LEU:HD11	15	0.39
(1,1526)	1:576:A:LEU:H	1:576:A:LEU:HD21	7	0.39
(1,1520)	1:577:A:LEU:H	1:574:A:PRO:HB2	3	0.39
(1,1517)	1:578:A:GLU:H	1:577:A:LEU:HG	7	0.39
(1,1517)	1:578:A:GLU:H	1:577:A:LEU:HG	17	0.39
(1,1517)	1:578:A:GLU:H	1:577:A:LEU:HG	20	0.39
(1,1480)	1:588:A:GLN:H	1:586:A:ALA:HB3	7	0.39
(1,1468)	1:592:A:ALA:H	1:593:A:ASP:HB3	10	0.39
(1,1449)	1:603:A:GLN:H	1:605:A:GLN:HB2	12	0.39
(1,1426)	1:627:A:TYR:HD2	1:628:A:LEU:HD22	2	0.39
(1,1420)	1:627:A:TYR:HE1	1:631:A:LEU:HD22	17	0.39
(1,1402)	1:606:A:LYS:HB2	1:606:A:LYS:HE3	8	0.39
(1,1399)	1:583:A:LYS:HG2	1:580:A:LEU:HD23	2	0.39
(1,1399)	1:583:A:LYS:HG2	1:580:A:LEU:HD22	12	0.39
(1,1399)	1:583:A:LYS:HG2	1:580:A:LEU:HD22	16	0.39
(1,1370)	1:604:A:THR:HG23	1:607:A:VAL:HB	19	0.39
(1,1369)	1:591:A:VAL:HG23	1:596:A:PHE:HB2	10	0.39
(1,1369)	1:591:A:VAL:HG22	1:596:A:PHE:HB2	12	0.39
(1,1326)	1:566:A:LEU:HD22	1:563:A:SER:HB3	18	0.39
(1,1309)	1:573:A:LEU:HD21	1:576:A:LEU:HB2	6	0.39
(1,1307)	1:566:A:LEU:HD13	1:565:A:LYS:HA	6	0.39
(1,1303)	1:581:A:GLU:HG3	1:618:A:LEU:HD13	18	0.39
(1,1288)	1:566:A:LEU:HD22	1:562:A:LEU:HD21	2	0.39

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1265)	1:593:A:ASP:HB3	1:595:A:SER:HB2	14	0.39
(1,1250)	1:626:A:GLU:HG2	1:623:A:GLU:HA	4	0.39
(1,1250)	1:626:A:GLU:HG2	1:623:A:GLU:HA	20	0.39
(1,1220)	1:551:A:LYS:HD3	1:551:A:LYS:HA	15	0.39
(1,1165)	1:601:A:HIS:HB2	1:605:A:GLN:HG2	5	0.39
(1,1147)	1:565:A:LYS:HA	1:565:A:LYS:HD3	7	0.39
(1,1147)	1:565:A:LYS:HA	1:565:A:LYS:HD3	10	0.39
(1,1147)	1:565:A:LYS:HA	1:565:A:LYS:HD3	13	0.39
(1,1111)	1:631:A:LEU:HD21	1:562:A:LEU:HB2	14	0.39
(1,1063)	1:610:A:ASP:HB2	1:587:A:LEU:HD12	15	0.39
(1,1057)	1:622:A:PHE:HB3	1:577:A:LEU:HD22	3	0.39
(1,1057)	1:622:A:PHE:HB3	1:577:A:LEU:HD21	4	0.39
(1,1057)	1:622:A:PHE:HB3	1:577:A:LEU:HD22	9	0.39
(1,1053)	1:577:A:LEU:HD13	1:617:A:GLU:HG3	2	0.39
(1,1021)	1:591:A:VAL:HG22	1:590:A:GLN:HG3	6	0.39
(1,1021)	1:591:A:VAL:HG23	1:590:A:GLN:HG3	14	0.39
(1,1016)	1:588:A:GLN:HG2	1:584:A:LEU:HG	2	0.39
(1,1004)	1:604:A:THR:HG21	1:603:A:GLN:HG2	18	0.39
(1,998)	1:583:A:LYS:HB3	1:587:A:LEU:HD12	4	0.39
(1,998)	1:583:A:LYS:HB3	1:587:A:LEU:HD11	17	0.39
(1,926)	1:583:A:LYS:HG3	1:580:A:LEU:HD23	7	0.39
(1,926)	1:583:A:LYS:HG3	1:580:A:LEU:HD22	13	0.39
(1,869)	1:557:A:ARG:HA	1:557:A:ARG:HD3	5	0.39
(1,859)	1:604:A:THR:HB	1:608:A:LEU:HD22	10	0.39
(1,850)	1:604:A:THR:HA	1:607:A:VAL:HG11	6	0.39
(1,809)	1:605:A:GLN:HA	1:608:A:LEU:HD23	20	0.39
(1,755)	1:621:A:ALA:HA	1:576:A:LEU:HD23	10	0.39
(1,670)	1:591:A:VAL:HG21	1:607:A:VAL:HG22	8	0.39
(1,658)	1:591:A:VAL:HG23	1:596:A:PHE:HB3	6	0.39
(1,658)	1:591:A:VAL:HG23	1:596:A:PHE:HB3	7	0.39
(1,658)	1:591:A:VAL:HG22	1:596:A:PHE:HB3	12	0.39
(1,658)	1:591:A:VAL:HG21	1:596:A:PHE:HB3	15	0.39
(1,631)	1:577:A:LEU:HD13	1:622:A:PHE:HB3	17	0.39
(1,602)	1:597:A:PHE:HZ	1:608:A:LEU:HD12	5	0.39
(1,602)	1:597:A:PHE:HZ	1:608:A:LEU:HD13	12	0.39
(1,569)	1:625:A:TRP:HZ2	1:629:A:GLU:HG2	17	0.39
(1,554)	1:627:A:TYR:HE2	1:628:A:LEU:HD21	18	0.39
(1,550)	1:596:A:PHE:HD2	1:604:A:THR:HG21	5	0.39
(1,416)	1:616:A:GLN:H	1:615:A:GLU:HB3	3	0.39
(1,416)	1:616:A:GLN:H	1:615:A:GLU:HB3	14	0.39
(1,368)	1:609:A:ALA:H	1:608:A:LEU:HD23	9	0.39
(1,172)	1:582:A:ALA:H	1:579:A:ASP:HB2	20	0.39

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,110)	1:590:A:GLN:H	1:590:A:GLN:HG3	7	0.39
(1,92)	1:592:A:ALA:H	1:589:A:THR:HG22	7	0.39
(1,26)	1:599:A:GLN:H	1:599:A:GLN:HB3	9	0.39
(1,26)	1:599:A:GLN:H	1:599:A:GLN:HB3	14	0.39
(1,2171)	1:591:A:VAL:HG21	1:597:A:PHE:HZ	8	0.38
(1,2171)	1:591:A:VAL:HG21	1:597:A:PHE:HZ	14	0.38
(1,2169)	1:576:A:LEU:HD11	1:617:A:GLU:HG3	19	0.38
(1,2159)	1:627:A:TYR:HB3	1:628:A:LEU:HA	13	0.38
(1,2139)	1:566:A:LEU:HD21	1:565:A:LYS:HA	2	0.38
(1,2139)	1:566:A:LEU:HD22	1:565:A:LYS:HA	5	0.38
(1,2104)	1:566:A:LEU:HD22	1:631:A:LEU:HB2	20	0.38
(1,2088)	1:576:A:LEU:HD11	1:617:A:GLU:HG3	19	0.38
(1,2059)	1:615:A:GLU:HA	1:619:A:GLU:HG2	2	0.38
(1,2052)	1:603:A:GLN:HG3	1:599:A:GLN:HA	16	0.38
(1,2047)	1:608:A:LEU:HA	1:611:A:MET:HG2	7	0.38
(1,2046)	1:626:A:GLU:HB3	1:627:A:TYR:HA	2	0.38
(1,2036)	1:556:A:LYS:HD3	1:556:A:LYS:HA	2	0.38
(1,2015)	1:565:A:LYS:HB3	1:565:A:LYS:HE2	9	0.38
(1,1965)	1:579:A:ASP:HB2	1:576:A:LEU:HG	17	0.38
(1,1965)	1:579:A:ASP:HB2	1:576:A:LEU:HG	20	0.38
(1,1940)	1:572:A:GLN:HG2	1:568:A:ARG:HG3	12	0.38
(1,1937)	1:616:A:GLN:HG3	1:613:A:ALA:HB2	4	0.38
(1,1907)	1:591:A:VAL:HA	1:608:A:LEU:HD22	20	0.38
(1,1867)	1:564:A:TYR:HA	1:567:A:GLN:HA	18	0.38
(1,1865)	1:622:A:PHE:HA	1:623:A:GLU:HA	9	0.38
(1,1853)	1:554:A:THR:HB	1:555:A:VAL:HG13	6	0.38
(1,1853)	1:554:A:THR:HB	1:555:A:VAL:HG11	12	0.38
(1,1834)	1:583:A:LYS:HA	1:587:A:LEU:HD21	1	0.38
(1,1828)	1:601:A:HIS:HA	1:602:A:GLU:HG3	2	0.38
(1,1813)	1:588:A:GLN:HA	1:584:A:LEU:HD22	13	0.38
(1,1795)	1:579:A:ASP:HA	1:583:A:LYS:HB2	9	0.38
(1,1795)	1:579:A:ASP:HA	1:583:A:LYS:HB2	17	0.38
(1,1795)	1:579:A:ASP:HA	1:583:A:LYS:HB2	19	0.38
(1,1789)	1:556:A:LYS:HA	1:555:A:VAL:HG11	9	0.38
(1,1779)	1:614:A:ALA:HA	1:580:A:LEU:HD11	19	0.38
(1,1778)	1:612:A:ALA:HA	1:584:A:LEU:HD23	18	0.38
(1,1774)	1:592:A:ALA:HA	1:589:A:THR:HA	19	0.38
(1,1736)	1:607:A:VAL:HG12	1:608:A:LEU:HG	9	0.38
(1,1718)	1:604:A:THR:HG23	1:599:A:GLN:HG3	5	0.38
(1,1718)	1:604:A:THR:HG23	1:599:A:GLN:HG3	8	0.38
(1,1694)	1:564:A:TYR:HD2	1:568:A:ARG:HG2	8	0.38
(1,1691)	1:627:A:TYR:HE2	1:624:A:ARG:HA	14	0.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1678)	1:627:A:TYR:HE1	1:631:A:LEU:HG	8	0.38
(1,1669)	1:633:A:ASN:H	1:631:A:LEU:HB3	11	0.38
(1,1633)	1:622:A:PHE:H	1:619:A:GLU:HB3	19	0.38
(1,1628)	1:621:A:ALA:H	1:620:A:GLN:HB2	8	0.38
(1,1625)	1:620:A:GLN:H	1:621:A:ALA:HB3	6	0.38
(1,1617)	1:617:A:GLU:H	1:580:A:LEU:HD23	14	0.38
(1,1608)	1:616:A:GLN:H	1:612:A:ALA:HA	1	0.38
(1,1565)	1:607:A:VAL:H	1:606:A:LYS:HE3	3	0.38
(1,1562)	1:604:A:THR:H	1:599:A:GLN:HB2	8	0.38
(1,1535)	1:572:A:GLN:H	1:573:A:LEU:HD13	9	0.38
(1,1534)	1:572:A:GLN:H	1:571:A:GLU:HB3	16	0.38
(1,1517)	1:578:A:GLU:H	1:577:A:LEU:HG	6	0.38
(1,1515)	1:579:A:ASP:H	1:576:A:LEU:HD13	19	0.38
(1,1468)	1:592:A:ALA:H	1:593:A:ASP:HB2	13	0.38
(1,1456)	1:597:A:PHE:H	1:595:A:SER:HA	13	0.38
(1,1437)	1:564:A:TYR:HD2	1:568:A:ARG:HG2	8	0.38
(1,1399)	1:583:A:LYS:HG2	1:580:A:LEU:HD23	7	0.38
(1,1383)	1:624:A:ARG:HG2	1:621:A:ALA:HA	15	0.38
(1,1369)	1:591:A:VAL:HG21	1:596:A:PHE:HB2	5	0.38
(1,1326)	1:566:A:LEU:HD22	1:563:A:SER:HB3	16	0.38
(1,1325)	1:628:A:LEU:HD11	1:569:A:GLU:HA	20	0.38
(1,1309)	1:573:A:LEU:HD23	1:576:A:LEU:HB2	3	0.38
(1,1265)	1:593:A:ASP:HB3	1:595:A:SER:HB2	11	0.38
(1,1190)	1:562:A:LEU:HB2	1:632:A:LYS:HA	15	0.38
(1,1170)	1:629:A:GLU:HG2	1:626:A:GLU:HA	19	0.38
(1,1147)	1:565:A:LYS:HA	1:565:A:LYS:HD2	11	0.38
(1,1111)	1:631:A:LEU:HD21	1:562:A:LEU:HB2	13	0.38
(1,1021)	1:591:A:VAL:HG23	1:590:A:GLN:HG3	16	0.38
(1,1020)	1:604:A:THR:HG23	1:599:A:GLN:HG3	5	0.38
(1,1020)	1:604:A:THR:HG23	1:599:A:GLN:HG3	8	0.38
(1,1016)	1:588:A:GLN:HG2	1:584:A:LEU:HG	5	0.38
(1,1005)	1:603:A:GLN:HG3	1:604:A:THR:HG22	3	0.38
(1,1005)	1:603:A:GLN:HG3	1:604:A:THR:HG21	18	0.38
(1,1005)	1:603:A:GLN:HG3	1:604:A:THR:HG23	20	0.38
(1,926)	1:583:A:LYS:HG3	1:580:A:LEU:HD23	11	0.38
(1,859)	1:604:A:THR:HB	1:608:A:LEU:HD23	16	0.38
(1,750)	1:604:A:THR:HG21	1:599:A:GLN:HA	14	0.38
(1,717)	1:621:A:ALA:HB3	1:577:A:LEU:HD23	8	0.38
(1,672)	1:607:A:VAL:HG22	1:606:A:LYS:HE2	2	0.38
(1,664)	1:631:A:LEU:HD23	1:566:A:LEU:HB2	1	0.38
(1,664)	1:631:A:LEU:HD21	1:566:A:LEU:HB2	12	0.38
(1,631)	1:577:A:LEU:HD12	1:622:A:PHE:HB3	12	0.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,630)	1:577:A:LEU:HD12	1:580:A:LEU:HG	7	0.38
(1,602)	1:597:A:PHE:HZ	1:608:A:LEU:HD12	7	0.38
(1,569)	1:625:A:TRP:HZ2	1:629:A:GLU:HG2	8	0.38
(1,569)	1:625:A:TRP:HZ2	1:629:A:GLU:HG2	12	0.38
(1,416)	1:616:A:GLN:H	1:615:A:GLU:HB3	9	0.38
(1,416)	1:616:A:GLN:H	1:615:A:GLU:HB3	16	0.38
(1,416)	1:616:A:GLN:H	1:615:A:GLU:HB3	18	0.38
(1,416)	1:616:A:GLN:H	1:615:A:GLU:HB3	20	0.38
(1,368)	1:609:A:ALA:H	1:608:A:LEU:HD23	7	0.38
(1,368)	1:609:A:ALA:H	1:608:A:LEU:HD21	16	0.38
(1,368)	1:609:A:ALA:H	1:608:A:LEU:HD23	19	0.38
(1,327)	1:604:A:THR:H	1:603:A:GLN:HB3	16	0.38
(1,321)	1:604:A:THR:H	1:596:A:PHE:HE1	9	0.38
(1,110)	1:590:A:GLN:H	1:590:A:GLN:HG3	17	0.38
(1,26)	1:599:A:GLN:H	1:599:A:GLN:HB3	16	0.38
(1,2165)	1:606:A:LYS:HA	1:610:A:ASP:HB2	17	0.37
(1,2159)	1:627:A:TYR:HB3	1:628:A:LEU:HA	5	0.37
(1,2159)	1:627:A:TYR:HB3	1:628:A:LEU:HA	8	0.37
(1,2121)	1:581:A:GLU:HG2	1:618:A:LEU:HD21	2	0.37
(1,2109)	1:608:A:LEU:HD13	1:591:A:VAL:HG11	4	0.37
(1,2109)	1:608:A:LEU:HD12	1:591:A:VAL:HG13	18	0.37
(1,2036)	1:561:A:LYS:HD2	1:561:A:LYS:HA	12	0.37
(1,2034)	1:618:A:LEU:HG	1:581:A:GLU:HA	13	0.37
(1,1965)	1:579:A:ASP:HB2	1:576:A:LEU:HG	9	0.37
(1,1965)	1:579:A:ASP:HB2	1:576:A:LEU:HG	10	0.37
(1,1961)	1:610:A:ASP:HB3	1:587:A:LEU:HB3	16	0.37
(1,1961)	1:610:A:ASP:HB3	1:587:A:LEU:HB3	17	0.37
(1,1946)	1:581:A:GLU:HG2	1:618:A:LEU:HD21	2	0.37
(1,1907)	1:591:A:VAL:HA	1:608:A:LEU:HD23	3	0.37
(1,1868)	1:569:A:GLU:HA	1:566:A:LEU:HA	8	0.37
(1,1867)	1:564:A:TYR:HA	1:567:A:GLN:HA	13	0.37
(1,1865)	1:622:A:PHE:HA	1:623:A:GLU:HA	1	0.37
(1,1852)	1:604:A:THR:HB	1:599:A:GLN:HB2	3	0.37
(1,1806)	1:577:A:LEU:HA	1:581:A:GLU:HB2	7	0.37
(1,1797)	1:576:A:LEU:HA	1:576:A:LEU:HD21	10	0.37
(1,1797)	1:576:A:LEU:HA	1:576:A:LEU:HD23	19	0.37
(1,1736)	1:607:A:VAL:HG12	1:608:A:LEU:HG	13	0.37
(1,1731)	1:607:A:VAL:HG22	1:603:A:GLN:HB2	14	0.37
(1,1723)	1:591:A:VAL:HG13	1:611:A:MET:HG3	3	0.37
(1,1723)	1:591:A:VAL:HG11	1:611:A:MET:HG3	15	0.37
(1,1711)	1:577:A:LEU:HD22	1:624:A:ARG:HB3	10	0.37
(1,1711)	1:577:A:LEU:HD21	1:626:A:GLU:HG3	20	0.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1691)	1:627:A:TYR:HE2	1:624:A:ARG:HA	3	0.37
(1,1689)	1:596:A:PHE:HD1	1:607:A:VAL:HB	20	0.37
(1,1678)	1:627:A:TYR:HE1	1:631:A:LEU:HG	13	0.37
(1,1678)	1:627:A:TYR:HE1	1:631:A:LEU:HG	14	0.37
(1,1628)	1:621:A:ALA:H	1:620:A:GLN:HB2	14	0.37
(1,1628)	1:621:A:ALA:H	1:620:A:GLN:HB2	19	0.37
(1,1628)	1:621:A:ALA:H	1:620:A:GLN:HB2	20	0.37
(1,1567)	1:607:A:VAL:H	1:606:A:LYS:HB2	15	0.37
(1,1563)	1:605:A:GLN:H	1:605:A:GLN:HE22	17	0.37
(1,1562)	1:604:A:THR:H	1:599:A:GLN:HB2	19	0.37
(1,1538)	1:571:A:GLU:H	1:628:A:LEU:HD13	16	0.37
(1,1535)	1:572:A:GLN:H	1:573:A:LEU:HD13	11	0.37
(1,1535)	1:572:A:GLN:H	1:573:A:LEU:HD11	12	0.37
(1,1526)	1:576:A:LEU:H	1:576:A:LEU:HD23	1	0.37
(1,1517)	1:578:A:GLU:H	1:577:A:LEU:HG	4	0.37
(1,1510)	1:581:A:GLU:H	1:582:A:ALA:HB3	17	0.37
(1,1457)	1:597:A:PHE:H	1:598:A:SER:HB2	18	0.37
(1,1399)	1:583:A:LYS:HG2	1:580:A:LEU:HD22	3	0.37
(1,1399)	1:583:A:LYS:HG2	1:580:A:LEU:HD21	5	0.37
(1,1399)	1:583:A:LYS:HG2	1:580:A:LEU:HD22	14	0.37
(1,1369)	1:591:A:VAL:HG23	1:596:A:PHE:HB2	1	0.37
(1,1367)	1:570:A:LEU:HD22	1:628:A:LEU:HB3	12	0.37
(1,1325)	1:628:A:LEU:HD12	1:569:A:GLU:HA	7	0.37
(1,1323)	1:576:A:LEU:HA	1:576:A:LEU:HD21	10	0.37
(1,1323)	1:576:A:LEU:HA	1:576:A:LEU:HD23	19	0.37
(1,1307)	1:566:A:LEU:HD11	1:565:A:LYS:HA	18	0.37
(1,1307)	1:566:A:LEU:HD13	1:565:A:LYS:HA	20	0.37
(1,1265)	1:593:A:ASP:HB3	1:595:A:SER:HB2	10	0.37
(1,1165)	1:601:A:HIS:HB2	1:605:A:GLN:HG2	3	0.37
(1,1165)	1:601:A:HIS:HB2	1:605:A:GLN:HG2	15	0.37
(1,1147)	1:565:A:LYS:HA	1:565:A:LYS:HD3	5	0.37
(1,1136)	1:600:A:PRO:HD3	1:603:A:GLN:HB2	18	0.37
(1,1057)	1:622:A:PHE:HB3	1:577:A:LEU:HD22	2	0.37
(1,1057)	1:622:A:PHE:HB3	1:577:A:LEU:HD23	8	0.37
(1,1057)	1:622:A:PHE:HB3	1:577:A:LEU:HD23	13	0.37
(1,1057)	1:622:A:PHE:HB3	1:577:A:LEU:HD23	14	0.37
(1,1057)	1:622:A:PHE:HB3	1:577:A:LEU:HD21	20	0.37
(1,1021)	1:591:A:VAL:HG22	1:590:A:GLN:HG3	7	0.37
(1,1021)	1:591:A:VAL:HG22	1:590:A:GLN:HG3	11	0.37
(1,1016)	1:588:A:GLN:HG2	1:584:A:LEU:HG	15	0.37
(1,926)	1:583:A:LYS:HG3	1:580:A:LEU:HD21	4	0.37
(1,893)	1:583:A:LYS:HA	1:583:A:LYS:HE3	16	0.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,851)	1:604:A:THR:HA	1:608:A:LEU:HD12	13	0.37
(1,755)	1:621:A:ALA:HA	1:576:A:LEU:HD21	19	0.37
(1,717)	1:621:A:ALA:HB2	1:577:A:LEU:HD21	5	0.37
(1,652)	1:591:A:VAL:HG13	1:608:A:LEU:HA	3	0.37
(1,634)	1:577:A:LEU:HD12	1:574:A:PRO:HA	4	0.37
(1,634)	1:577:A:LEU:HD11	1:574:A:PRO:HA	13	0.37
(1,602)	1:597:A:PHE:HZ	1:608:A:LEU:HD12	8	0.37
(1,554)	1:627:A:TYR:HE2	1:628:A:LEU:HD22	13	0.37
(1,507)	1:629:A:GLU:H	1:570:A:LEU:HD23	8	0.37
(1,473)	1:623:A:GLU:H	1:623:A:GLU:HB2	1	0.37
(1,416)	1:616:A:GLN:H	1:615:A:GLU:HB3	6	0.37
(1,416)	1:616:A:GLN:H	1:615:A:GLU:HB3	11	0.37
(1,368)	1:609:A:ALA:H	1:608:A:LEU:HD22	2	0.37
(1,368)	1:609:A:ALA:H	1:608:A:LEU:HD22	13	0.37
(1,368)	1:609:A:ALA:H	1:608:A:LEU:HD21	14	0.37
(1,308)	1:566:A:LEU:H	1:566:A:LEU:HD23	3	0.37
(1,299)	1:567:A:GLN:H	1:566:A:LEU:HD13	10	0.37
(1,283)	1:569:A:GLU:H	1:568:A:ARG:HB3	2	0.37
(1,283)	1:569:A:GLU:H	1:568:A:ARG:HB3	9	0.37
(1,283)	1:569:A:GLU:H	1:568:A:ARG:HB3	14	0.37
(1,172)	1:582:A:ALA:H	1:579:A:ASP:HB2	19	0.37
(1,2171)	1:591:A:VAL:HG23	1:597:A:PHE:HZ	3	0.36
(1,2163)	1:567:A:GLN:HA	1:570:A:LEU:HD13	13	0.36
(1,2160)	1:630:A:ALA:HB1	1:627:A:TYR:HB2	3	0.36
(1,2159)	1:627:A:TYR:HB3	1:628:A:LEU:HA	20	0.36
(1,2135)	1:567:A:GLN:HA	1:570:A:LEU:HD13	13	0.36
(1,2105)	1:566:A:LEU:HD22	1:628:A:LEU:HG	2	0.36
(1,2104)	1:566:A:LEU:HD23	1:631:A:LEU:HB2	17	0.36
(1,2059)	1:615:A:GLU:HA	1:619:A:GLU:HG2	19	0.36
(1,2051)	1:603:A:GLN:HG2	1:600:A:PRO:HA	17	0.36
(1,2047)	1:608:A:LEU:HA	1:611:A:MET:HG2	11	0.36
(1,2034)	1:618:A:LEU:HG	1:615:A:GLU:HA	18	0.36
(1,2019)	1:551:A:LYS:HB3	1:551:A:LYS:HE2	5	0.36
(1,1992)	1:562:A:LEU:HB3	1:631:A:LEU:HG	10	0.36
(1,1965)	1:579:A:ASP:HB2	1:576:A:LEU:HG	3	0.36
(1,1965)	1:579:A:ASP:HB2	1:576:A:LEU:HG	5	0.36
(1,1963)	1:596:A:PHE:HB3	1:591:A:VAL:HG11	4	0.36
(1,1946)	1:581:A:GLU:HG2	1:618:A:LEU:HD21	18	0.36
(1,1894)	1:562:A:LEU:HG	1:567:A:GLN:HG3	9	0.36
(1,1894)	1:576:A:LEU:HG	1:617:A:GLU:HG3	12	0.36
(1,1889)	1:568:A:ARG:HG2	1:569:A:GLU:HB2	19	0.36
(1,1868)	1:569:A:GLU:HA	1:566:A:LEU:HA	7	0.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1855)	1:572:A:GLN:HA	1:571:A:GLU:HA	5	0.36
(1,1855)	1:572:A:GLN:HA	1:571:A:GLU:HA	20	0.36
(1,1836)	1:619:A:GLU:HA	1:618:A:LEU:HD11	6	0.36
(1,1806)	1:577:A:LEU:HA	1:581:A:GLU:HB2	1	0.36
(1,1778)	1:612:A:ALA:HA	1:584:A:LEU:HD23	12	0.36
(1,1774)	1:592:A:ALA:HA	1:589:A:THR:HA	1	0.36
(1,1741)	1:628:A:LEU:HD23	1:624:A:ARG:HA	4	0.36
(1,1741)	1:628:A:LEU:HD23	1:624:A:ARG:HA	18	0.36
(1,1719)	1:604:A:THR:HG22	1:603:A:GLN:HG2	1	0.36
(1,1719)	1:604:A:THR:HG21	1:603:A:GLN:HG2	4	0.36
(1,1719)	1:604:A:THR:HG21	1:603:A:GLN:HG2	11	0.36
(1,1708)	1:625:A:TRP:HD1	1:628:A:LEU:HD12	11	0.36
(1,1708)	1:625:A:TRP:HD1	1:628:A:LEU:HD11	15	0.36
(1,1700)	1:622:A:PHE:HZ	1:618:A:LEU:HD22	14	0.36
(1,1691)	1:627:A:TYR:HE2	1:624:A:ARG:HA	10	0.36
(1,1691)	1:627:A:TYR:HE2	1:624:A:ARG:HA	18	0.36
(1,1683)	1:622:A:PHE:HE2	1:618:A:LEU:HD22	7	0.36
(1,1625)	1:620:A:GLN:H	1:621:A:ALA:HB1	9	0.36
(1,1625)	1:620:A:GLN:H	1:621:A:ALA:HB3	18	0.36
(1,1588)	1:613:A:ALA:H	1:616:A:GLN:HG3	2	0.36
(1,1588)	1:583:A:LYS:H	1:581:A:GLU:HG2	3	0.36
(1,1567)	1:607:A:VAL:H	1:606:A:LYS:HB2	2	0.36
(1,1563)	1:605:A:GLN:H	1:605:A:GLN:HE22	20	0.36
(1,1562)	1:604:A:THR:H	1:599:A:GLN:HB2	6	0.36
(1,1520)	1:577:A:LEU:H	1:574:A:PRO:HB2	12	0.36
(1,1517)	1:578:A:GLU:H	1:577:A:LEU:HG	5	0.36
(1,1517)	1:578:A:GLU:H	1:577:A:LEU:HG	11	0.36
(1,1517)	1:578:A:GLU:H	1:577:A:LEU:HG	13	0.36
(1,1517)	1:578:A:GLU:H	1:577:A:LEU:HG	19	0.36
(1,1468)	1:592:A:ALA:H	1:593:A:ASP:HB2	4	0.36
(1,1468)	1:592:A:ALA:H	1:593:A:ASP:HB2	16	0.36
(1,1431)	1:622:A:PHE:HE2	1:618:A:LEU:HD22	7	0.36
(1,1412)	1:584:A:LEU:HD22	1:615:A:GLU:HB2	16	0.36
(1,1412)	1:584:A:LEU:HD23	1:615:A:GLU:HB2	20	0.36
(1,1402)	1:606:A:LYS:HB2	1:606:A:LYS:HE3	15	0.36
(1,1384)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	19	0.36
(1,1378)	1:624:A:ARG:HD3	1:573:A:LEU:HD13	5	0.36
(1,1378)	1:624:A:ARG:HD3	1:573:A:LEU:HD13	18	0.36
(1,1370)	1:604:A:THR:HG21	1:607:A:VAL:HB	8	0.36
(1,1370)	1:604:A:THR:HG21	1:607:A:VAL:HB	9	0.36
(1,1363)	1:562:A:LEU:HD23	1:631:A:LEU:HB2	18	0.36
(1,1309)	1:573:A:LEU:HD21	1:576:A:LEU:HB2	20	0.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1307)	1:566:A:LEU:HD11	1:565:A:LYS:HA	1	0.36
(1,1288)	1:566:A:LEU:HD22	1:562:A:LEU:HD23	19	0.36
(1,1165)	1:601:A:HIS:HB2	1:605:A:GLN:HG2	2	0.36
(1,1147)	1:565:A:LYS:HA	1:565:A:LYS:HD2	20	0.36
(1,1062)	1:610:A:ASP:HB2	1:587:A:LEU:HD23	8	0.36
(1,1057)	1:622:A:PHE:HB3	1:577:A:LEU:HD21	16	0.36
(1,1057)	1:622:A:PHE:HB3	1:577:A:LEU:HD21	17	0.36
(1,1057)	1:622:A:PHE:HB3	1:577:A:LEU:HD21	18	0.36
(1,1021)	1:591:A:VAL:HG23	1:590:A:GLN:HG3	4	0.36
(1,1005)	1:603:A:GLN:HG3	1:604:A:THR:HG22	1	0.36
(1,1004)	1:604:A:THR:HG22	1:603:A:GLN:HG2	1	0.36
(1,1004)	1:604:A:THR:HG21	1:603:A:GLN:HG2	4	0.36
(1,1004)	1:604:A:THR:HG21	1:603:A:GLN:HG2	11	0.36
(1,990)	1:591:A:VAL:HG21	1:611:A:MET:HG2	10	0.36
(1,985)	1:591:A:VAL:HB	1:608:A:LEU:HD21	17	0.36
(1,938)	1:631:A:LEU:HG	1:562:A:LEU:HD23	2	0.36
(1,929)	1:565:A:LYS:HG2	1:566:A:LEU:HD12	14	0.36
(1,925)	1:565:A:LYS:HG3	1:566:A:LEU:HD12	16	0.36
(1,893)	1:583:A:LYS:HA	1:583:A:LYS:HE3	6	0.36
(1,809)	1:605:A:GLN:HA	1:608:A:LEU:HD21	6	0.36
(1,750)	1:604:A:THR:HG23	1:599:A:GLN:HA	8	0.36
(1,725)	1:600:A:PRO:HD3	1:599:A:GLN:HB2	11	0.36
(1,664)	1:631:A:LEU:HD22	1:566:A:LEU:HB2	5	0.36
(1,631)	1:577:A:LEU:HD13	1:622:A:PHE:HB3	13	0.36
(1,569)	1:625:A:TRP:HZ2	1:629:A:GLU:HG2	14	0.36
(1,554)	1:627:A:TYR:HE2	1:628:A:LEU:HD23	10	0.36
(1,542)	1:625:A:TRP:HE1	1:629:A:GLU:HG3	1	0.36
(1,473)	1:623:A:GLU:H	1:623:A:GLU:HB2	9	0.36
(1,429)	1:618:A:LEU:H	1:617:A:GLU:HB2	7	0.36
(1,416)	1:616:A:GLN:H	1:615:A:GLU:HB3	4	0.36
(1,368)	1:609:A:ALA:H	1:608:A:LEU:HD23	4	0.36
(1,368)	1:609:A:ALA:H	1:608:A:LEU:HD22	8	0.36
(1,339)	1:605:A:GLN:H	1:604:A:THR:HG21	7	0.36
(1,321)	1:604:A:THR:H	1:596:A:PHE:HE1	1	0.36
(1,321)	1:604:A:THR:H	1:596:A:PHE:HE1	3	0.36
(1,321)	1:604:A:THR:H	1:596:A:PHE:HE1	11	0.36
(1,307)	1:566:A:LEU:H	1:566:A:LEU:HD11	15	0.36
(1,26)	1:599:A:GLN:H	1:599:A:GLN:HB3	6	0.36
(1,26)	1:599:A:GLN:H	1:599:A:GLN:HB3	18	0.36
(1,2171)	1:591:A:VAL:HG21	1:597:A:PHE:HZ	18	0.35
(1,2120)	1:573:A:LEU:HD22	1:624:A:ARG:HB2	13	0.35
(1,2114)	1:581:A:GLU:HG3	1:618:A:LEU:HD13	12	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2109)	1:608:A:LEU:HD12	1:591:A:VAL:HG11	1	0.35
(1,2059)	1:615:A:GLU:HA	1:619:A:GLU:HG2	13	0.35
(1,2047)	1:608:A:LEU:HA	1:611:A:MET:HG2	17	0.35
(1,2046)	1:626:A:GLU:HB3	1:627:A:TYR:HA	3	0.35
(1,2027)	1:564:A:TYR:HB3	1:567:A:GLN:HB2	5	0.35
(1,1961)	1:610:A:ASP:HB3	1:587:A:LEU:HB3	3	0.35
(1,1937)	1:616:A:GLN:HG3	1:613:A:ALA:HB3	16	0.35
(1,1924)	1:614:A:ALA:HB3	1:611:A:MET:HG2	20	0.35
(1,1867)	1:564:A:TYR:HA	1:567:A:GLN:HA	8	0.35
(1,1852)	1:604:A:THR:HB	1:599:A:GLN:HB2	1	0.35
(1,1789)	1:556:A:LYS:HA	1:555:A:VAL:HG12	20	0.35
(1,1774)	1:592:A:ALA:HA	1:589:A:THR:HA	6	0.35
(1,1774)	1:592:A:ALA:HA	1:589:A:THR:HA	14	0.35
(1,1741)	1:628:A:LEU:HD22	1:624:A:ARG:HA	7	0.35
(1,1719)	1:604:A:THR:HG22	1:603:A:GLN:HG2	19	0.35
(1,1711)	1:577:A:LEU:HD21	1:626:A:GLU:HG3	4	0.35
(1,1706)	1:625:A:TRP:HD1	1:628:A:LEU:HB2	18	0.35
(1,1700)	1:622:A:PHE:HZ	1:618:A:LEU:HD13	2	0.35
(1,1694)	1:564:A:TYR:HD2	1:568:A:ARG:HG2	1	0.35
(1,1694)	1:564:A:TYR:HD2	1:568:A:ARG:HG2	6	0.35
(1,1691)	1:627:A:TYR:HE2	1:624:A:ARG:HA	16	0.35
(1,1678)	1:627:A:TYR:HE1	1:631:A:LEU:HG	16	0.35
(1,1625)	1:620:A:GLN:H	1:621:A:ALA:HB3	2	0.35
(1,1625)	1:620:A:GLN:H	1:621:A:ALA:HB2	3	0.35
(1,1625)	1:620:A:GLN:H	1:621:A:ALA:HB3	5	0.35
(1,1625)	1:620:A:GLN:H	1:618:A:LEU:HB3	12	0.35
(1,1625)	1:620:A:GLN:H	1:621:A:ALA:HB3	19	0.35
(1,1611)	1:616:A:GLN:H	1:612:A:ALA:HB2	3	0.35
(1,1608)	1:616:A:GLN:H	1:612:A:ALA:HA	4	0.35
(1,1608)	1:616:A:GLN:H	1:612:A:ALA:HA	10	0.35
(1,1588)	1:583:A:LYS:H	1:581:A:GLU:HG2	10	0.35
(1,1569)	1:607:A:VAL:H	1:608:A:LEU:HD23	11	0.35
(1,1535)	1:572:A:GLN:H	1:573:A:LEU:HD13	14	0.35
(1,1437)	1:564:A:TYR:HD2	1:568:A:ARG:HG2	1	0.35
(1,1437)	1:564:A:TYR:HD2	1:568:A:ARG:HG2	6	0.35
(1,1420)	1:627:A:TYR:HE1	1:631:A:LEU:HD21	18	0.35
(1,1402)	1:606:A:LYS:HB2	1:606:A:LYS:HE3	17	0.35
(1,1399)	1:583:A:LYS:HG2	1:580:A:LEU:HD23	1	0.35
(1,1378)	1:624:A:ARG:HD3	1:573:A:LEU:HD12	2	0.35
(1,1378)	1:624:A:ARG:HD3	1:573:A:LEU:HD11	14	0.35
(1,1369)	1:591:A:VAL:HG21	1:596:A:PHE:HB2	8	0.35
(1,1363)	1:562:A:LEU:HD22	1:631:A:LEU:HB2	16	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1326)	1:566:A:LEU:HD22	1:563:A:SER:HB3	14	0.35
(1,1325)	1:628:A:LEU:HD11	1:569:A:GLU:HA	5	0.35
(1,1320)	1:562:A:LEU:HA	1:562:A:LEU:HD13	7	0.35
(1,1320)	1:562:A:LEU:HA	1:562:A:LEU:HD13	15	0.35
(1,1309)	1:573:A:LEU:HD21	1:576:A:LEU:HB2	7	0.35
(1,1309)	1:573:A:LEU:HD23	1:576:A:LEU:HB2	12	0.35
(1,1307)	1:566:A:LEU:HD12	1:565:A:LYS:HA	12	0.35
(1,1307)	1:566:A:LEU:HD13	1:565:A:LYS:HA	13	0.35
(1,1307)	1:566:A:LEU:HD13	1:565:A:LYS:HA	17	0.35
(1,1303)	1:581:A:GLU:HG3	1:618:A:LEU:HD13	12	0.35
(1,1147)	1:565:A:LYS:HA	1:565:A:LYS:HD2	1	0.35
(1,1120)	1:588:A:GLN:HA	1:611:A:MET:HE3	15	0.35
(1,1111)	1:631:A:LEU:HD21	1:562:A:LEU:HB2	20	0.35
(1,1057)	1:622:A:PHE:HB3	1:577:A:LEU:HD23	11	0.35
(1,1057)	1:622:A:PHE:HB3	1:577:A:LEU:HD22	19	0.35
(1,1016)	1:588:A:GLN:HG2	1:584:A:LEU:HG	19	0.35
(1,1005)	1:603:A:GLN:HG3	1:604:A:THR:HG23	9	0.35
(1,1005)	1:603:A:GLN:HG3	1:604:A:THR:HG21	11	0.35
(1,1005)	1:603:A:GLN:HG3	1:604:A:THR:HG22	15	0.35
(1,1004)	1:604:A:THR:HG22	1:603:A:GLN:HG2	19	0.35
(1,985)	1:591:A:VAL:HB	1:608:A:LEU:HD23	4	0.35
(1,985)	1:591:A:VAL:HB	1:608:A:LEU:HD23	12	0.35
(1,969)	1:573:A:LEU:HG	1:576:A:LEU:HD23	10	0.35
(1,929)	1:565:A:LYS:HG2	1:566:A:LEU:HD12	19	0.35
(1,906)	1:596:A:PHE:HA	1:599:A:GLN:HG2	7	0.35
(1,850)	1:604:A:THR:HA	1:607:A:VAL:HG12	20	0.35
(1,843)	1:625:A:TRP:HA	1:573:A:LEU:HD12	1	0.35
(1,809)	1:605:A:GLN:HA	1:608:A:LEU:HD21	7	0.35
(1,805)	1:629:A:GLU:HA	1:570:A:LEU:HD21	15	0.35
(1,750)	1:604:A:THR:HG23	1:599:A:GLN:HA	5	0.35
(1,664)	1:631:A:LEU:HD22	1:566:A:LEU:HB2	8	0.35
(1,664)	1:631:A:LEU:HD21	1:566:A:LEU:HB2	13	0.35
(1,634)	1:577:A:LEU:HD12	1:574:A:PRO:HA	15	0.35
(1,603)	1:622:A:PHE:HD1	1:626:A:GLU:HG2	1	0.35
(1,603)	1:622:A:PHE:HD1	1:626:A:GLU:HG2	6	0.35
(1,602)	1:597:A:PHE:HZ	1:608:A:LEU:HD11	2	0.35
(1,602)	1:597:A:PHE:HZ	1:608:A:LEU:HD11	10	0.35
(1,602)	1:597:A:PHE:HZ	1:608:A:LEU:HD12	15	0.35
(1,599)	1:601:A:HIS:HD2	1:602:A:GLU:HG3	16	0.35
(1,569)	1:625:A:TRP:HZ2	1:629:A:GLU:HG2	5	0.35
(1,569)	1:625:A:TRP:HZ2	1:629:A:GLU:HG2	19	0.35
(1,559)	1:596:A:PHE:HE1	1:604:A:THR:HG23	3	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,554)	1:627:A:TYR:HE2	1:628:A:LEU:HD22	11	0.35
(1,554)	1:627:A:TYR:HE2	1:628:A:LEU:HD23	17	0.35
(1,507)	1:629:A:GLU:H	1:570:A:LEU:HD22	18	0.35
(1,473)	1:623:A:GLU:H	1:623:A:GLU:HB2	4	0.35
(1,473)	1:623:A:GLU:H	1:623:A:GLU:HB2	13	0.35
(1,473)	1:623:A:GLU:H	1:623:A:GLU:HB2	20	0.35
(1,339)	1:605:A:GLN:H	1:604:A:THR:HG22	6	0.35
(1,339)	1:605:A:GLN:H	1:604:A:THR:HG22	13	0.35
(1,283)	1:569:A:GLU:H	1:568:A:ARG:HB3	3	0.35
(1,283)	1:569:A:GLU:H	1:568:A:ARG:HB3	15	0.35
(1,172)	1:582:A:ALA:H	1:579:A:ASP:HB2	17	0.35
(1,92)	1:592:A:ALA:H	1:589:A:THR:HG22	5	0.35
(1,2171)	1:591:A:VAL:HG21	1:597:A:PHE:HZ	15	0.34
(1,2166)	1:562:A:LEU:HD12	1:561:A:LYS:HG3	19	0.34
(1,2160)	1:630:A:ALA:HB3	1:627:A:TYR:HB2	14	0.34
(1,2159)	1:627:A:TYR:HB3	1:628:A:LEU:HA	12	0.34
(1,2109)	1:608:A:LEU:HD12	1:591:A:VAL:HG11	16	0.34
(1,2105)	1:566:A:LEU:HD21	1:628:A:LEU:HG	12	0.34
(1,2059)	1:615:A:GLU:HA	1:619:A:GLU:HG2	20	0.34
(1,2052)	1:603:A:GLN:HG3	1:599:A:GLN:HA	19	0.34
(1,2051)	1:603:A:GLN:HG2	1:600:A:PRO:HA	1	0.34
(1,2051)	1:603:A:GLN:HG2	1:600:A:PRO:HA	19	0.34
(1,2042)	1:573:A:LEU:HG	1:570:A:LEU:HA	5	0.34
(1,2036)	1:556:A:LYS:HD2	1:556:A:LYS:HA	6	0.34
(1,1992)	1:562:A:LEU:HB2	1:631:A:LEU:HG	20	0.34
(1,1965)	1:579:A:ASP:HB2	1:576:A:LEU:HG	13	0.34
(1,1944)	1:585:A:GLU:HG3	1:586:A:ALA:HB2	17	0.34
(1,1943)	1:590:A:GLN:HG2	1:589:A:THR:HG22	5	0.34
(1,1937)	1:616:A:GLN:HG3	1:613:A:ALA:HB3	13	0.34
(1,1852)	1:604:A:THR:HB	1:599:A:GLN:HB2	12	0.34
(1,1828)	1:601:A:HIS:HA	1:602:A:GLU:HG3	18	0.34
(1,1795)	1:579:A:ASP:HA	1:583:A:LYS:HB2	12	0.34
(1,1795)	1:579:A:ASP:HA	1:583:A:LYS:HB2	14	0.34
(1,1795)	1:579:A:ASP:HA	1:583:A:LYS:HB2	18	0.34
(1,1795)	1:579:A:ASP:HA	1:583:A:LYS:HB2	20	0.34
(1,1779)	1:614:A:ALA:HA	1:580:A:LEU:HD11	1	0.34
(1,1774)	1:592:A:ALA:HA	1:589:A:THR:HA	3	0.34
(1,1774)	1:592:A:ALA:HA	1:589:A:THR:HA	15	0.34
(1,1729)	1:631:A:LEU:HD21	1:561:A:LYS:HA	5	0.34
(1,1719)	1:604:A:THR:HG23	1:603:A:GLN:HG2	8	0.34
(1,1718)	1:604:A:THR:HG21	1:599:A:GLN:HG3	14	0.34
(1,1717)	1:604:A:THR:HG23	1:608:A:LEU:HG	6	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1708)	1:625:A:TRP:HD1	1:628:A:LEU:HD11	16	0.34
(1,1691)	1:627:A:TYR:HE2	1:624:A:ARG:HA	19	0.34
(1,1678)	1:627:A:TYR:HE1	1:631:A:LEU:HG	20	0.34
(1,1588)	1:583:A:LYS:H	1:581:A:GLU:HG2	8	0.34
(1,1588)	1:583:A:LYS:H	1:581:A:GLU:HG2	16	0.34
(1,1565)	1:607:A:VAL:H	1:606:A:LYS:HE2	8	0.34
(1,1535)	1:572:A:GLN:H	1:573:A:LEU:HD12	4	0.34
(1,1517)	1:578:A:GLU:H	1:577:A:LEU:HG	1	0.34
(1,1517)	1:578:A:GLU:H	1:577:A:LEU:HG	3	0.34
(1,1517)	1:578:A:GLU:H	1:577:A:LEU:HG	10	0.34
(1,1517)	1:578:A:GLU:H	1:577:A:LEU:HG	14	0.34
(1,1474)	1:589:A:THR:H	1:586:A:ALA:HA	1	0.34
(1,1474)	1:589:A:THR:H	1:586:A:ALA:HA	20	0.34
(1,1420)	1:627:A:TYR:HE1	1:631:A:LEU:HD22	13	0.34
(1,1384)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	18	0.34
(1,1382)	1:573:A:LEU:HD13	1:624:A:ARG:HG2	8	0.34
(1,1370)	1:604:A:THR:HG23	1:607:A:VAL:HB	1	0.34
(1,1370)	1:604:A:THR:HG22	1:607:A:VAL:HB	11	0.34
(1,1147)	1:565:A:LYS:HA	1:565:A:LYS:HD2	17	0.34
(1,1062)	1:610:A:ASP:HB2	1:587:A:LEU:HD22	13	0.34
(1,1057)	1:622:A:PHE:HB3	1:577:A:LEU:HD21	6	0.34
(1,1057)	1:622:A:PHE:HB3	1:577:A:LEU:HD22	15	0.34
(1,1056)	1:622:A:PHE:HB2	1:577:A:LEU:HD22	9	0.34
(1,1020)	1:604:A:THR:HG21	1:599:A:GLN:HG3	14	0.34
(1,1016)	1:588:A:GLN:HG2	1:584:A:LEU:HG	18	0.34
(1,1004)	1:604:A:THR:HG23	1:603:A:GLN:HG2	8	0.34
(1,985)	1:591:A:VAL:HB	1:608:A:LEU:HD23	9	0.34
(1,970)	1:632:A:LYS:HD2	1:570:A:LEU:HD11	16	0.34
(1,956)	1:605:A:GLN:HB3	1:608:A:LEU:HD11	7	0.34
(1,925)	1:565:A:LYS:HG3	1:566:A:LEU:HD11	3	0.34
(1,850)	1:604:A:THR:HA	1:607:A:VAL:HG13	14	0.34
(1,730)	1:600:A:PRO:HD3	1:603:A:GLN:HG2	1	0.34
(1,717)	1:621:A:ALA:HB1	1:577:A:LEU:HD21	3	0.34
(1,652)	1:591:A:VAL:HG11	1:608:A:LEU:HA	15	0.34
(1,602)	1:597:A:PHE:HZ	1:608:A:LEU:HD12	3	0.34
(1,585)	1:596:A:PHE:HZ	1:607:A:VAL:HG13	1	0.34
(1,581)	1:601:A:HIS:HD2	1:605:A:GLN:HG2	16	0.34
(1,569)	1:625:A:TRP:HZ2	1:629:A:GLU:HG2	1	0.34
(1,569)	1:625:A:TRP:HZ2	1:629:A:GLU:HG2	3	0.34
(1,569)	1:625:A:TRP:HZ2	1:629:A:GLU:HG2	9	0.34
(1,569)	1:625:A:TRP:HZ2	1:629:A:GLU:HG2	15	0.34
(1,507)	1:629:A:GLU:H	1:570:A:LEU:HD22	5	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,473)	1:623:A:GLU:H	1:623:A:GLU:HB2	19	0.34
(1,416)	1:616:A:GLN:H	1:615:A:GLU:HB3	1	0.34
(1,416)	1:616:A:GLN:H	1:615:A:GLU:HB3	2	0.34
(1,339)	1:605:A:GLN:H	1:604:A:THR:HG22	16	0.34
(1,321)	1:604:A:THR:H	1:596:A:PHE:HE1	5	0.34
(1,307)	1:566:A:LEU:H	1:566:A:LEU:HD13	5	0.34
(1,283)	1:569:A:GLU:H	1:568:A:ARG:HB3	4	0.34
(1,274)	1:570:A:LEU:H	1:569:A:GLU:HG2	5	0.34
(1,173)	1:612:A:ALA:H	1:611:A:MET:HB2	13	0.34
(1,172)	1:582:A:ALA:H	1:579:A:ASP:HB2	9	0.34
(1,2171)	1:591:A:VAL:HG21	1:597:A:PHE:HZ	17	0.33
(1,2171)	1:591:A:VAL:HG23	1:597:A:PHE:HZ	20	0.33
(1,2139)	1:566:A:LEU:HD21	1:565:A:LYS:HA	11	0.33
(1,2047)	1:608:A:LEU:HA	1:611:A:MET:HG2	9	0.33
(1,2047)	1:608:A:LEU:HA	1:611:A:MET:HG2	15	0.33
(1,2033)	1:562:A:LEU:HG	1:563:A:SER:HB3	19	0.33
(1,2027)	1:564:A:TYR:HB3	1:567:A:GLN:HB2	18	0.33
(1,1987)	1:614:A:ALA:HB3	1:587:A:LEU:HB2	10	0.33
(1,1961)	1:610:A:ASP:HB3	1:587:A:LEU:HB3	1	0.33
(1,1958)	1:622:A:PHE:HB3	1:619:A:GLU:HB2	15	0.33
(1,1944)	1:585:A:GLU:HG3	1:586:A:ALA:HB1	11	0.33
(1,1939)	1:572:A:GLN:HG3	1:568:A:ARG:HG2	15	0.33
(1,1901)	1:613:A:ALA:HB2	1:616:A:GLN:HB2	2	0.33
(1,1868)	1:569:A:GLU:HA	1:566:A:LEU:HA	12	0.33
(1,1834)	1:583:A:LYS:HA	1:587:A:LEU:HD23	13	0.33
(1,1813)	1:588:A:GLN:HA	1:584:A:LEU:HD22	9	0.33
(1,1796)	1:580:A:LEU:HA	1:580:A:LEU:HD23	1	0.33
(1,1774)	1:592:A:ALA:HA	1:589:A:THR:HA	9	0.33
(1,1774)	1:592:A:ALA:HA	1:589:A:THR:HA	13	0.33
(1,1774)	1:592:A:ALA:HA	1:589:A:THR:HA	16	0.33
(1,1774)	1:592:A:ALA:HA	1:589:A:THR:HA	20	0.33
(1,1763)	1:621:A:ALA:HB1	1:617:A:GLU:HG2	10	0.33
(1,1756)	1:614:A:ALA:HB3	1:587:A:LEU:HB2	10	0.33
(1,1719)	1:604:A:THR:HG23	1:603:A:GLN:HG2	2	0.33
(1,1719)	1:604:A:THR:HG23	1:603:A:GLN:HG2	20	0.33
(1,1717)	1:604:A:THR:HG21	1:608:A:LEU:HG	5	0.33
(1,1712)	1:577:A:LEU:HD23	1:625:A:TRP:HA	14	0.33
(1,1711)	1:577:A:LEU:HD21	1:626:A:GLU:HG3	17	0.33
(1,1709)	1:625:A:TRP:HD1	1:573:A:LEU:HB2	16	0.33
(1,1706)	1:625:A:TRP:HD1	1:628:A:LEU:HB2	9	0.33
(1,1706)	1:625:A:TRP:HD1	1:628:A:LEU:HB2	20	0.33
(1,1694)	1:564:A:TYR:HD2	1:568:A:ARG:HG3	2	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1682)	1:622:A:PHE:HD2	1:577:A:LEU:HD11	14	0.33
(1,1678)	1:627:A:TYR:HE1	1:631:A:LEU:HG	3	0.33
(1,1678)	1:627:A:TYR:HE1	1:631:A:LEU:HG	6	0.33
(1,1678)	1:627:A:TYR:HE1	1:631:A:LEU:HG	9	0.33
(1,1678)	1:627:A:TYR:HE1	1:631:A:LEU:HG	15	0.33
(1,1628)	1:621:A:ALA:H	1:620:A:GLN:HB2	3	0.33
(1,1625)	1:620:A:GLN:H	1:621:A:ALA:HB2	4	0.33
(1,1608)	1:616:A:GLN:H	1:612:A:ALA:HA	11	0.33
(1,1535)	1:572:A:GLN:H	1:573:A:LEU:HD13	6	0.33
(1,1526)	1:576:A:LEU:H	1:576:A:LEU:HD23	10	0.33
(1,1517)	1:578:A:GLU:H	1:577:A:LEU:HG	9	0.33
(1,1510)	1:581:A:GLU:H	1:582:A:ALA:HB1	1	0.33
(1,1468)	1:592:A:ALA:H	1:593:A:ASP:HB3	14	0.33
(1,1449)	1:603:A:GLN:H	1:599:A:GLN:HB2	15	0.33
(1,1443)	1:564:A:TYR:HE2	1:564:A:TYR:HA	3	0.33
(1,1437)	1:564:A:TYR:HD2	1:568:A:ARG:HG3	2	0.33
(1,1402)	1:606:A:LYS:HB2	1:606:A:LYS:HE2	16	0.33
(1,1399)	1:583:A:LYS:HG2	1:580:A:LEU:HD22	10	0.33
(1,1370)	1:604:A:THR:HG21	1:607:A:VAL:HB	2	0.33
(1,1369)	1:591:A:VAL:HG21	1:596:A:PHE:HB2	16	0.33
(1,1325)	1:628:A:LEU:HD12	1:569:A:GLU:HA	19	0.33
(1,1309)	1:573:A:LEU:HD21	1:576:A:LEU:HB2	2	0.33
(1,1307)	1:566:A:LEU:HD13	1:565:A:LYS:HA	8	0.33
(1,1292)	1:577:A:LEU:HD21	1:573:A:LEU:HD12	6	0.33
(1,1291)	1:608:A:LEU:HD11	1:604:A:THR:HG21	6	0.33
(1,1265)	1:593:A:ASP:HB3	1:595:A:SER:HB2	18	0.33
(1,1164)	1:601:A:HIS:HB3	1:605:A:GLN:HG2	4	0.33
(1,1163)	1:599:A:GLN:HG3	1:600:A:PRO:HD3	9	0.33
(1,1063)	1:610:A:ASP:HB2	1:587:A:LEU:HD13	17	0.33
(1,1063)	1:610:A:ASP:HB2	1:587:A:LEU:HD13	19	0.33
(1,1005)	1:603:A:GLN:HG3	1:604:A:THR:HG23	12	0.33
(1,1004)	1:604:A:THR:HG23	1:603:A:GLN:HG2	2	0.33
(1,1004)	1:604:A:THR:HG23	1:603:A:GLN:HG2	20	0.33
(1,998)	1:583:A:LYS:HB3	1:587:A:LEU:HD13	9	0.33
(1,998)	1:583:A:LYS:HB3	1:587:A:LEU:HD11	19	0.33
(1,985)	1:591:A:VAL:HB	1:608:A:LEU:HD23	20	0.33
(1,929)	1:565:A:LYS:HG2	1:566:A:LEU:HD13	2	0.33
(1,859)	1:604:A:THR:HB	1:608:A:LEU:HD22	18	0.33
(1,805)	1:629:A:GLU:HA	1:570:A:LEU:HD21	14	0.33
(1,755)	1:621:A:ALA:HA	1:576:A:LEU:HD23	15	0.33
(1,717)	1:621:A:ALA:HB3	1:577:A:LEU:HD23	14	0.33
(1,717)	1:621:A:ALA:HB2	1:577:A:LEU:HD22	19	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,664)	1:631:A:LEU:HD23	1:566:A:LEU:HB2	16	0.33
(1,634)	1:577:A:LEU:HD12	1:574:A:PRO:HA	3	0.33
(1,634)	1:577:A:LEU:HD12	1:574:A:PRO:HA	7	0.33
(1,625)	1:577:A:LEU:HD11	1:573:A:LEU:HD21	1	0.33
(1,601)	1:601:A:HIS:HD2	1:605:A:GLN:HB3	13	0.33
(1,585)	1:596:A:PHE:HZ	1:607:A:VAL:HG11	11	0.33
(1,569)	1:625:A:TRP:HZ2	1:629:A:GLU:HG2	2	0.33
(1,569)	1:625:A:TRP:HZ2	1:629:A:GLU:HG2	4	0.33
(1,569)	1:625:A:TRP:HZ2	1:629:A:GLU:HG2	18	0.33
(1,554)	1:627:A:TYR:HE2	1:628:A:LEU:HD21	5	0.33
(1,368)	1:609:A:ALA:H	1:608:A:LEU:HD23	10	0.33
(1,327)	1:604:A:THR:H	1:603:A:GLN:HB3	5	0.33
(1,321)	1:604:A:THR:H	1:596:A:PHE:HE1	6	0.33
(1,321)	1:604:A:THR:H	1:596:A:PHE:HE1	20	0.33
(1,173)	1:612:A:ALA:H	1:611:A:MET:HB2	4	0.33
(1,110)	1:590:A:GLN:H	1:590:A:GLN:HG3	11	0.33
(1,2160)	1:630:A:ALA:HB2	1:627:A:TYR:HB2	17	0.32
(1,2124)	1:612:A:ALA:HA	1:611:A:MET:HE1	19	0.32
(1,2105)	1:566:A:LEU:HD23	1:628:A:LEU:HG	13	0.32
(1,2047)	1:608:A:LEU:HA	1:611:A:MET:HG2	4	0.32
(1,2047)	1:608:A:LEU:HA	1:611:A:MET:HG2	8	0.32
(1,2046)	1:626:A:GLU:HB3	1:627:A:TYR:HA	7	0.32
(1,2042)	1:573:A:LEU:HG	1:570:A:LEU:HA	8	0.32
(1,1992)	1:562:A:LEU:HB2	1:632:A:LYS:HG2	13	0.32
(1,1965)	1:579:A:ASP:HB2	1:576:A:LEU:HG	14	0.32
(1,1939)	1:572:A:GLN:HG3	1:573:A:LEU:HB3	20	0.32
(1,1901)	1:613:A:ALA:HB1	1:616:A:GLN:HB2	6	0.32
(1,1901)	1:613:A:ALA:HB2	1:616:A:GLN:HB2	18	0.32
(1,1868)	1:569:A:GLU:HA	1:566:A:LEU:HA	19	0.32
(1,1868)	1:569:A:GLU:HA	1:566:A:LEU:HA	20	0.32
(1,1867)	1:564:A:TYR:HA	1:567:A:GLN:HA	1	0.32
(1,1855)	1:572:A:GLN:HA	1:571:A:GLU:HA	9	0.32
(1,1853)	1:554:A:THR:HB	1:555:A:VAL:HG23	19	0.32
(1,1852)	1:604:A:THR:HB	1:608:A:LEU:HB2	6	0.32
(1,1834)	1:583:A:LYS:HA	1:587:A:LEU:HD23	5	0.32
(1,1806)	1:577:A:LEU:HA	1:581:A:GLU:HB2	2	0.32
(1,1806)	1:577:A:LEU:HA	1:581:A:GLU:HB2	12	0.32
(1,1806)	1:577:A:LEU:HA	1:581:A:GLU:HB2	14	0.32
(1,1806)	1:577:A:LEU:HA	1:581:A:GLU:HB2	15	0.32
(1,1797)	1:576:A:LEU:HA	1:576:A:LEU:HD21	1	0.32
(1,1797)	1:576:A:LEU:HA	1:576:A:LEU:HD23	11	0.32
(1,1796)	1:580:A:LEU:HA	1:580:A:LEU:HD21	4	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1796)	1:580:A:LEU:HA	1:580:A:LEU:HD23	7	0.32
(1,1787)	1:621:A:ALA:HA	1:620:A:GLN:HB2	8	0.32
(1,1779)	1:614:A:ALA:HA	1:580:A:LEU:HD11	12	0.32
(1,1779)	1:614:A:ALA:HA	1:580:A:LEU:HD13	13	0.32
(1,1774)	1:592:A:ALA:HA	1:589:A:THR:HA	8	0.32
(1,1736)	1:607:A:VAL:HG13	1:611:A:MET:HE2	1	0.32
(1,1719)	1:604:A:THR:HG23	1:603:A:GLN:HG2	12	0.32
(1,1706)	1:625:A:TRP:HD1	1:628:A:LEU:HB2	8	0.32
(1,1706)	1:625:A:TRP:HD1	1:628:A:LEU:HB2	12	0.32
(1,1700)	1:622:A:PHE:HZ	1:618:A:LEU:HD11	15	0.32
(1,1691)	1:627:A:TYR:HE2	1:624:A:ARG:HA	1	0.32
(1,1628)	1:621:A:ALA:H	1:620:A:GLN:HB2	9	0.32
(1,1628)	1:621:A:ALA:H	1:620:A:GLN:HB2	17	0.32
(1,1617)	1:617:A:GLU:H	1:580:A:LEU:HD23	8	0.32
(1,1617)	1:617:A:GLU:H	1:580:A:LEU:HD23	17	0.32
(1,1608)	1:616:A:GLN:H	1:612:A:ALA:HA	7	0.32
(1,1588)	1:583:A:LYS:H	1:581:A:GLU:HG2	13	0.32
(1,1569)	1:607:A:VAL:H	1:608:A:LEU:HD23	10	0.32
(1,1567)	1:607:A:VAL:H	1:606:A:LYS:HB2	3	0.32
(1,1567)	1:607:A:VAL:H	1:606:A:LYS:HB2	13	0.32
(1,1546)	1:568:A:ARG:H	1:567:A:GLN:HG3	1	0.32
(1,1520)	1:577:A:LEU:H	1:574:A:PRO:HB2	1	0.32
(1,1451)	1:599:A:GLN:H	1:600:A:PRO:HD3	12	0.32
(1,1443)	1:564:A:TYR:HE1	1:564:A:TYR:HA	5	0.32
(1,1402)	1:606:A:LYS:HB2	1:606:A:LYS:HE3	20	0.32
(1,1399)	1:583:A:LYS:HG2	1:580:A:LEU:HD22	15	0.32
(1,1376)	1:566:A:LEU:HD22	1:563:A:SER:HB2	16	0.32
(1,1369)	1:591:A:VAL:HG22	1:596:A:PHE:HB2	9	0.32
(1,1335)	1:566:A:LEU:HG	1:562:A:LEU:HD22	10	0.32
(1,1323)	1:576:A:LEU:HA	1:576:A:LEU:HD21	1	0.32
(1,1323)	1:576:A:LEU:HA	1:576:A:LEU:HD23	11	0.32
(1,1319)	1:567:A:GLN:HA	1:562:A:LEU:HD13	14	0.32
(1,1309)	1:573:A:LEU:HD23	1:576:A:LEU:HB2	17	0.32
(1,1291)	1:608:A:LEU:HD12	1:604:A:THR:HG22	5	0.32
(1,1250)	1:626:A:GLU:HG2	1:623:A:GLU:HA	11	0.32
(1,1250)	1:626:A:GLU:HG2	1:623:A:GLU:HA	13	0.32
(1,1165)	1:601:A:HIS:HB2	1:605:A:GLN:HG2	6	0.32
(1,1136)	1:600:A:PRO:HD3	1:603:A:GLN:HB3	10	0.32
(1,1063)	1:610:A:ASP:HB2	1:587:A:LEU:HD12	1	0.32
(1,1056)	1:622:A:PHE:HB2	1:577:A:LEU:HD21	12	0.32
(1,1034)	1:569:A:GLU:HG2	1:573:A:LEU:HD12	5	0.32
(1,1023)	1:590:A:GLN:HG3	1:587:A:LEU:HD23	2	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1016)	1:588:A:GLN:HG2	1:584:A:LEU:HG	12	0.32
(1,1004)	1:604:A:THR:HG23	1:603:A:GLN:HG2	12	0.32
(1,906)	1:596:A:PHE:HA	1:599:A:GLN:HG2	10	0.32
(1,906)	1:596:A:PHE:HA	1:599:A:GLN:HG2	12	0.32
(1,850)	1:604:A:THR:HA	1:607:A:VAL:HG13	9	0.32
(1,805)	1:629:A:GLU:HA	1:570:A:LEU:HD22	5	0.32
(1,725)	1:600:A:PRO:HD3	1:599:A:GLN:HB2	20	0.32
(1,664)	1:631:A:LEU:HD21	1:566:A:LEU:HB2	14	0.32
(1,634)	1:577:A:LEU:HD12	1:574:A:PRO:HA	5	0.32
(1,630)	1:577:A:LEU:HD13	1:580:A:LEU:HG	16	0.32
(1,585)	1:596:A:PHE:HZ	1:607:A:VAL:HG12	5	0.32
(1,585)	1:596:A:PHE:HZ	1:607:A:VAL:HG13	13	0.32
(1,581)	1:601:A:HIS:HD2	1:605:A:GLN:HG2	10	0.32
(1,569)	1:625:A:TRP:HZ2	1:629:A:GLU:HG2	10	0.32
(1,559)	1:596:A:PHE:HE1	1:604:A:THR:HG23	6	0.32
(1,339)	1:605:A:GLN:H	1:604:A:THR:HG22	3	0.32
(1,339)	1:605:A:GLN:H	1:604:A:THR:HG23	5	0.32
(1,321)	1:604:A:THR:H	1:596:A:PHE:HE1	14	0.32
(1,283)	1:569:A:GLU:H	1:568:A:ARG:HB3	7	0.32
(1,283)	1:569:A:GLU:H	1:568:A:ARG:HB3	11	0.32
(1,18)	1:599:A:GLN:H	1:596:A:PHE:HD1	13	0.32
(1,2169)	1:576:A:LEU:HD12	1:617:A:GLU:HG3	11	0.31
(1,2160)	1:630:A:ALA:HB3	1:627:A:TYR:HB2	4	0.31
(1,2088)	1:576:A:LEU:HD12	1:617:A:GLU:HG3	11	0.31
(1,2059)	1:615:A:GLU:HA	1:619:A:GLU:HG2	15	0.31
(1,2051)	1:603:A:GLN:HG2	1:600:A:PRO:HA	9	0.31
(1,1868)	1:569:A:GLU:HA	1:566:A:LEU:HA	13	0.31
(1,1868)	1:569:A:GLU:HA	1:566:A:LEU:HA	18	0.31
(1,1867)	1:564:A:TYR:HA	1:567:A:GLN:HA	12	0.31
(1,1867)	1:564:A:TYR:HA	1:567:A:GLN:HA	20	0.31
(1,1855)	1:572:A:GLN:HA	1:571:A:GLU:HA	3	0.31
(1,1855)	1:572:A:GLN:HA	1:571:A:GLU:HA	16	0.31
(1,1813)	1:588:A:GLN:HA	1:584:A:LEU:HD23	15	0.31
(1,1806)	1:577:A:LEU:HA	1:581:A:GLU:HB2	11	0.31
(1,1797)	1:576:A:LEU:HA	1:576:A:LEU:HD21	4	0.31
(1,1797)	1:576:A:LEU:HA	1:576:A:LEU:HD22	7	0.31
(1,1797)	1:576:A:LEU:HA	1:576:A:LEU:HD21	15	0.31
(1,1797)	1:576:A:LEU:HA	1:576:A:LEU:HD23	17	0.31
(1,1796)	1:580:A:LEU:HA	1:580:A:LEU:HD22	20	0.31
(1,1778)	1:612:A:ALA:HA	1:584:A:LEU:HD21	9	0.31
(1,1743)	1:628:A:LEU:HD23	1:625:A:TRP:HA	4	0.31
(1,1718)	1:604:A:THR:HG22	1:599:A:GLN:HG3	19	0.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1694)	1:564:A:TYR:HD2	1:568:A:ARG:HG2	13	0.31
(1,1693)	1:627:A:TYR:HD1	1:631:A:LEU:HD11	12	0.31
(1,1689)	1:596:A:PHE:HD1	1:607:A:VAL:HB	2	0.31
(1,1683)	1:622:A:PHE:HE2	1:618:A:LEU:HD21	18	0.31
(1,1678)	1:627:A:TYR:HE1	1:631:A:LEU:HG	4	0.31
(1,1633)	1:622:A:PHE:H	1:619:A:GLU:HB3	5	0.31
(1,1628)	1:621:A:ALA:H	1:620:A:GLN:HB2	5	0.31
(1,1628)	1:621:A:ALA:H	1:620:A:GLN:HB2	13	0.31
(1,1625)	1:620:A:GLN:H	1:618:A:LEU:HB3	14	0.31
(1,1608)	1:616:A:GLN:H	1:612:A:ALA:HA	16	0.31
(1,1608)	1:616:A:GLN:H	1:612:A:ALA:HA	19	0.31
(1,1594)	1:614:A:ALA:H	1:615:A:GLU:HG3	3	0.31
(1,1588)	1:583:A:LYS:H	1:581:A:GLU:HG2	4	0.31
(1,1569)	1:607:A:VAL:H	1:608:A:LEU:HD22	13	0.31
(1,1567)	1:607:A:VAL:H	1:606:A:LYS:HB2	8	0.31
(1,1567)	1:607:A:VAL:H	1:606:A:LYS:HB2	12	0.31
(1,1567)	1:607:A:VAL:H	1:606:A:LYS:HB2	14	0.31
(1,1546)	1:568:A:ARG:H	1:567:A:GLN:HG3	17	0.31
(1,1535)	1:572:A:GLN:H	1:573:A:LEU:HD12	17	0.31
(1,1491)	1:585:A:GLU:H	1:584:A:LEU:HG	5	0.31
(1,1474)	1:589:A:THR:H	1:586:A:ALA:HA	8	0.31
(1,1474)	1:589:A:THR:H	1:586:A:ALA:HA	9	0.31
(1,1474)	1:589:A:THR:H	1:586:A:ALA:HA	16	0.31
(1,1468)	1:592:A:ALA:H	1:593:A:ASP:HB3	3	0.31
(1,1457)	1:597:A:PHE:H	1:598:A:SER:HB2	16	0.31
(1,1443)	1:564:A:TYR:HE2	1:564:A:TYR:HA	14	0.31
(1,1443)	1:564:A:TYR:HE1	1:564:A:TYR:HA	18	0.31
(1,1437)	1:564:A:TYR:HD2	1:568:A:ARG:HG2	13	0.31
(1,1397)	1:587:A:LEU:HD11	1:583:A:LYS:HA	1	0.31
(1,1335)	1:566:A:LEU:HG	1:562:A:LEU:HD21	13	0.31
(1,1323)	1:576:A:LEU:HA	1:576:A:LEU:HD21	4	0.31
(1,1323)	1:576:A:LEU:HA	1:576:A:LEU:HD22	7	0.31
(1,1323)	1:576:A:LEU:HA	1:576:A:LEU:HD23	14	0.31
(1,1323)	1:576:A:LEU:HA	1:576:A:LEU:HD21	15	0.31
(1,1323)	1:576:A:LEU:HA	1:576:A:LEU:HD23	17	0.31
(1,1309)	1:573:A:LEU:HD22	1:576:A:LEU:HB2	8	0.31
(1,1309)	1:573:A:LEU:HD23	1:576:A:LEU:HB2	9	0.31
(1,1292)	1:577:A:LEU:HD22	1:573:A:LEU:HD13	15	0.31
(1,1210)	1:606:A:LYS:HA	1:605:A:GLN:HB2	13	0.31
(1,1152)	1:565:A:LYS:HB2	1:565:A:LYS:HE3	19	0.31
(1,1063)	1:610:A:ASP:HB2	1:587:A:LEU:HD13	6	0.31
(1,1062)	1:610:A:ASP:HB2	1:587:A:LEU:HD22	7	0.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1056)	1:622:A:PHE:HB2	1:577:A:LEU:HD22	3	0.31
(1,1056)	1:622:A:PHE:HB2	1:577:A:LEU:HD21	5	0.31
(1,1025)	1:590:A:GLN:HG2	1:591:A:VAL:HG23	8	0.31
(1,1025)	1:590:A:GLN:HG2	1:591:A:VAL:HG23	14	0.31
(1,1020)	1:604:A:THR:HG22	1:599:A:GLN:HG3	19	0.31
(1,1016)	1:588:A:GLN:HG2	1:584:A:LEU:HG	1	0.31
(1,1016)	1:588:A:GLN:HG2	1:584:A:LEU:HG	3	0.31
(1,1016)	1:588:A:GLN:HG2	1:584:A:LEU:HG	14	0.31
(1,1005)	1:603:A:GLN:HG3	1:604:A:THR:HG23	2	0.31
(1,928)	1:583:A:LYS:HG3	1:587:A:LEU:HD22	15	0.31
(1,870)	1:556:A:LYS:HA	1:556:A:LYS:HE2	16	0.31
(1,850)	1:604:A:THR:HA	1:607:A:VAL:HG13	8	0.31
(1,850)	1:604:A:THR:HA	1:607:A:VAL:HG13	13	0.31
(1,819)	1:604:A:THR:HG22	1:601:A:HIS:HA	10	0.31
(1,725)	1:600:A:PRO:HD3	1:599:A:GLN:HB2	1	0.31
(1,672)	1:607:A:VAL:HG21	1:606:A:LYS:HE3	16	0.31
(1,652)	1:591:A:VAL:HG11	1:608:A:LEU:HA	8	0.31
(1,652)	1:591:A:VAL:HG12	1:608:A:LEU:HA	17	0.31
(1,650)	1:591:A:VAL:HG13	1:588:A:GLN:HA	16	0.31
(1,603)	1:622:A:PHE:HD1	1:626:A:GLU:HG2	14	0.31
(1,602)	1:597:A:PHE:HZ	1:608:A:LEU:HD13	19	0.31
(1,586)	1:625:A:TRP:HD1	1:577:A:LEU:HD22	1	0.31
(1,569)	1:625:A:TRP:HZ2	1:629:A:GLU:HG2	20	0.31
(1,559)	1:596:A:PHE:HE1	1:604:A:THR:HG23	13	0.31
(1,544)	1:625:A:TRP:HE1	1:570:A:LEU:HD13	1	0.31
(1,507)	1:629:A:GLU:H	1:570:A:LEU:HD21	4	0.31
(1,507)	1:629:A:GLU:H	1:570:A:LEU:HD22	7	0.31
(1,429)	1:618:A:LEU:H	1:617:A:GLU:HB2	2	0.31
(1,369)	1:609:A:ALA:H	1:608:A:LEU:HD11	3	0.31
(1,327)	1:604:A:THR:H	1:603:A:GLN:HB3	10	0.31
(1,264)	1:571:A:GLU:H	1:571:A:GLU:HG3	19	0.31
(1,58)	1:596:A:PHE:H	1:594:A:ALA:HB2	13	0.31
(1,55)	1:596:A:PHE:H	1:595:A:SER:HB2	13	0.31
(1,2169)	1:576:A:LEU:HD12	1:617:A:GLU:HG3	15	0.3
(1,2163)	1:567:A:GLN:HA	1:570:A:LEU:HD13	18	0.3
(1,2135)	1:567:A:GLN:HA	1:570:A:LEU:HD13	18	0.3
(1,2124)	1:612:A:ALA:HA	1:611:A:MET:HE3	12	0.3
(1,2088)	1:576:A:LEU:HD12	1:617:A:GLU:HG3	15	0.3
(1,2059)	1:615:A:GLU:HA	1:619:A:GLU:HG2	4	0.3
(1,2047)	1:608:A:LEU:HA	1:611:A:MET:HG2	3	0.3
(1,2046)	1:626:A:GLU:HB3	1:627:A:TYR:HA	10	0.3
(1,2046)	1:623:A:GLU:HA	1:626:A:GLU:HB3	12	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2027)	1:564:A:TYR:HB3	1:567:A:GLN:HB2	8	0.3
(1,1965)	1:579:A:ASP:HB2	1:576:A:LEU:HG	11	0.3
(1,1963)	1:596:A:PHE:HB3	1:591:A:VAL:HG11	1	0.3
(1,1963)	1:596:A:PHE:HB3	1:591:A:VAL:HG12	15	0.3
(1,1963)	1:596:A:PHE:HB3	1:591:A:VAL:HG13	19	0.3
(1,1939)	1:572:A:GLN:HG3	1:568:A:ARG:HG2	16	0.3
(1,1907)	1:591:A:VAL:HA	1:608:A:LEU:HD23	15	0.3
(1,1894)	1:576:A:LEU:HG	1:617:A:GLU:HG3	1	0.3
(1,1868)	1:569:A:GLU:HA	1:566:A:LEU:HA	11	0.3
(1,1855)	1:572:A:GLN:HA	1:571:A:GLU:HA	6	0.3
(1,1855)	1:572:A:GLN:HA	1:571:A:GLU:HA	10	0.3
(1,1855)	1:572:A:GLN:HA	1:571:A:GLU:HA	12	0.3
(1,1855)	1:572:A:GLN:HA	1:571:A:GLU:HA	19	0.3
(1,1806)	1:577:A:LEU:HA	1:581:A:GLU:HB2	6	0.3
(1,1806)	1:577:A:LEU:HA	1:581:A:GLU:HB2	9	0.3
(1,1797)	1:576:A:LEU:HA	1:576:A:LEU:HD22	6	0.3
(1,1797)	1:628:A:LEU:HD23	1:624:A:ARG:HA	14	0.3
(1,1797)	1:576:A:LEU:HA	1:576:A:LEU:HD21	20	0.3
(1,1796)	1:580:A:LEU:HA	1:580:A:LEU:HD22	8	0.3
(1,1796)	1:580:A:LEU:HA	1:580:A:LEU:HD22	12	0.3
(1,1796)	1:580:A:LEU:HA	1:580:A:LEU:HD22	15	0.3
(1,1795)	1:579:A:ASP:HA	1:583:A:LYS:HB2	8	0.3
(1,1787)	1:621:A:ALA:HA	1:620:A:GLN:HB2	4	0.3
(1,1774)	1:592:A:ALA:HA	1:589:A:THR:HA	4	0.3
(1,1774)	1:592:A:ALA:HA	1:589:A:THR:HA	10	0.3
(1,1741)	1:628:A:LEU:HD23	1:624:A:ARG:HA	14	0.3
(1,1719)	1:604:A:THR:HG22	1:603:A:GLN:HG2	3	0.3
(1,1718)	1:604:A:THR:HG23	1:599:A:GLN:HG3	1	0.3
(1,1711)	1:577:A:LEU:HD21	1:626:A:GLU:HG3	5	0.3
(1,1709)	1:625:A:TRP:HD1	1:573:A:LEU:HB2	13	0.3
(1,1708)	1:625:A:TRP:HD1	1:628:A:LEU:HD13	6	0.3
(1,1706)	1:625:A:TRP:HD1	1:628:A:LEU:HB2	2	0.3
(1,1706)	1:625:A:TRP:HD1	1:628:A:LEU:HB2	3	0.3
(1,1701)	1:622:A:PHE:HE2	1:577:A:LEU:HA	6	0.3
(1,1683)	1:622:A:PHE:HE2	1:618:A:LEU:HD23	11	0.3
(1,1668)	1:633:A:ASN:H	1:629:A:GLU:HA	12	0.3
(1,1628)	1:621:A:ALA:H	1:620:A:GLN:HB2	18	0.3
(1,1625)	1:620:A:GLN:H	1:618:A:LEU:HB3	11	0.3
(1,1621)	1:619:A:GLU:H	1:618:A:LEU:HD22	1	0.3
(1,1588)	1:583:A:LYS:H	1:581:A:GLU:HG2	5	0.3
(1,1569)	1:607:A:VAL:H	1:587:A:LEU:HD21	4	0.3
(1,1569)	1:607:A:VAL:H	1:587:A:LEU:HD22	5	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1567)	1:607:A:VAL:H	1:606:A:LYS:HB2	4	0.3
(1,1526)	1:576:A:LEU:H	1:576:A:LEU:HD22	19	0.3
(1,1520)	1:577:A:LEU:H	1:574:A:PRO:HB2	2	0.3
(1,1474)	1:589:A:THR:H	1:586:A:ALA:HA	6	0.3
(1,1474)	1:589:A:THR:H	1:586:A:ALA:HA	19	0.3
(1,1457)	1:597:A:PHE:H	1:598:A:SER:HB2	19	0.3
(1,1451)	1:599:A:GLN:H	1:600:A:PRO:HD3	20	0.3
(1,1443)	1:564:A:TYR:HE1	1:564:A:TYR:HA	7	0.3
(1,1443)	1:564:A:TYR:HE1	1:564:A:TYR:HA	17	0.3
(1,1443)	1:564:A:TYR:HE1	1:564:A:TYR:HA	19	0.3
(1,1431)	1:622:A:PHE:HE2	1:618:A:LEU:HD21	18	0.3
(1,1402)	1:606:A:LYS:HB2	1:606:A:LYS:HE2	10	0.3
(1,1367)	1:570:A:LEU:HD21	1:628:A:LEU:HB3	10	0.3
(1,1336)	1:570:A:LEU:HD21	1:570:A:LEU:HA	19	0.3
(1,1328)	1:573:A:LEU:HD11	1:574:A:PRO:HD3	1	0.3
(1,1328)	1:573:A:LEU:HD11	1:574:A:PRO:HD3	8	0.3
(1,1323)	1:576:A:LEU:HA	1:576:A:LEU:HD22	6	0.3
(1,1323)	1:576:A:LEU:HA	1:576:A:LEU:HD21	20	0.3
(1,1309)	1:573:A:LEU:HD23	1:576:A:LEU:HB2	15	0.3
(1,1163)	1:599:A:GLN:HG3	1:600:A:PRO:HD3	1	0.3
(1,1147)	1:565:A:LYS:HA	1:565:A:LYS:HD3	19	0.3
(1,1136)	1:600:A:PRO:HD3	1:603:A:GLN:HB3	14	0.3
(1,1063)	1:610:A:ASP:HB2	1:587:A:LEU:HD13	11	0.3
(1,1056)	1:622:A:PHE:HB2	1:577:A:LEU:HD23	1	0.3
(1,1056)	1:622:A:PHE:HB2	1:577:A:LEU:HD23	13	0.3
(1,1056)	1:622:A:PHE:HB2	1:577:A:LEU:HD21	20	0.3
(1,1020)	1:604:A:THR:HG23	1:599:A:GLN:HG3	1	0.3
(1,1004)	1:604:A:THR:HG22	1:603:A:GLN:HG2	3	0.3
(1,1004)	1:604:A:THR:HG23	1:603:A:GLN:HG2	17	0.3
(1,985)	1:591:A:VAL:HB	1:608:A:LEU:HD21	3	0.3
(1,969)	1:573:A:LEU:HG	1:576:A:LEU:HD23	1	0.3
(1,938)	1:631:A:LEU:HG	1:562:A:LEU:HD23	11	0.3
(1,928)	1:583:A:LYS:HG3	1:587:A:LEU:HD21	20	0.3
(1,893)	1:583:A:LYS:HA	1:583:A:LYS:HE2	1	0.3
(1,838)	1:623:A:GLU:HA	1:626:A:GLU:HB3	12	0.3
(1,805)	1:629:A:GLU:HA	1:570:A:LEU:HD21	4	0.3
(1,750)	1:604:A:THR:HG22	1:599:A:GLN:HA	16	0.3
(1,717)	1:621:A:ALA:HB1	1:577:A:LEU:HD21	4	0.3
(1,658)	1:591:A:VAL:HG21	1:596:A:PHE:HB3	5	0.3
(1,658)	1:591:A:VAL:HG23	1:596:A:PHE:HB3	20	0.3
(1,603)	1:622:A:PHE:HD1	1:626:A:GLU:HG2	2	0.3
(1,603)	1:622:A:PHE:HD1	1:626:A:GLU:HG2	13	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,581)	1:601:A:HIS:HD2	1:605:A:GLN:HG3	4	0.3
(1,564)	1:597:A:PHE:HE2	1:591:A:VAL:HG12	16	0.3
(1,558)	1:564:A:TYR:HE2	1:568:A:ARG:HB2	1	0.3
(1,558)	1:564:A:TYR:HE2	1:568:A:ARG:HB2	6	0.3
(1,558)	1:564:A:TYR:HE2	1:568:A:ARG:HB2	18	0.3
(1,554)	1:627:A:TYR:HE2	1:628:A:LEU:HD23	6	0.3
(1,550)	1:596:A:PHE:HD1	1:604:A:THR:HG22	14	0.3
(1,327)	1:604:A:THR:H	1:603:A:GLN:HB3	13	0.3
(1,321)	1:604:A:THR:H	1:596:A:PHE:HE1	7	0.3
(1,321)	1:604:A:THR:H	1:596:A:PHE:HE1	10	0.3
(1,299)	1:567:A:GLN:H	1:566:A:LEU:HD12	2	0.3
(1,283)	1:569:A:GLU:H	1:568:A:ARG:HB3	16	0.3
(1,124)	1:589:A:THR:H	1:589:A:THR:HG22	15	0.3
(1,64)	1:595:A:SER:H	1:596:A:PHE:HB2	4	0.3
(1,58)	1:596:A:PHE:H	1:594:A:ALA:HB1	11	0.3
(1,2171)	1:591:A:VAL:HG22	1:597:A:PHE:HZ	2	0.29
(1,2124)	1:612:A:ALA:HA	1:611:A:MET:HE3	10	0.29
(1,2120)	1:573:A:LEU:HD22	1:624:A:ARG:HB2	15	0.29
(1,2046)	1:626:A:GLU:HB3	1:627:A:TYR:HA	6	0.29
(1,2034)	1:618:A:LEU:HG	1:615:A:GLU:HA	6	0.29
(1,2027)	1:564:A:TYR:HB3	1:567:A:GLN:HB2	10	0.29
(1,2027)	1:564:A:TYR:HB3	1:567:A:GLN:HB2	13	0.29
(1,1992)	1:562:A:LEU:HB2	1:632:A:LYS:HG2	3	0.29
(1,1961)	1:610:A:ASP:HB3	1:587:A:LEU:HB3	8	0.29
(1,1927)	1:632:A:LYS:HB2	1:562:A:LEU:HD23	18	0.29
(1,1920)	1:613:A:ALA:HB1	1:617:A:GLU:HB2	10	0.29
(1,1894)	1:576:A:LEU:HG	1:617:A:GLU:HG3	18	0.29
(1,1888)	1:568:A:ARG:HG2	1:571:A:GLU:HB3	19	0.29
(1,1867)	1:564:A:TYR:HA	1:567:A:GLN:HA	10	0.29
(1,1855)	1:572:A:GLN:HA	1:571:A:GLU:HA	1	0.29
(1,1855)	1:572:A:GLN:HA	1:571:A:GLU:HA	18	0.29
(1,1806)	1:577:A:LEU:HA	1:581:A:GLU:HB2	3	0.29
(1,1806)	1:577:A:LEU:HA	1:581:A:GLU:HB2	18	0.29
(1,1797)	1:576:A:LEU:HA	1:576:A:LEU:HD23	18	0.29
(1,1796)	1:580:A:LEU:HA	1:580:A:LEU:HD23	2	0.29
(1,1796)	1:580:A:LEU:HA	1:580:A:LEU:HD22	10	0.29
(1,1795)	1:579:A:ASP:HA	1:583:A:LYS:HB2	11	0.29
(1,1787)	1:621:A:ALA:HA	1:620:A:GLN:HB2	19	0.29
(1,1776)	1:600:A:PRO:HG2	1:599:A:GLN:HA	7	0.29
(1,1774)	1:592:A:ALA:HA	1:589:A:THR:HA	12	0.29
(1,1774)	1:592:A:ALA:HA	1:589:A:THR:HA	17	0.29
(1,1749)	1:613:A:ALA:HB1	1:617:A:GLU:HB2	10	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1719)	1:604:A:THR:HG23	1:603:A:GLN:HG2	9	0.29
(1,1718)	1:604:A:THR:HG22	1:599:A:GLN:HG3	13	0.29
(1,1708)	1:625:A:TRP:HD1	1:628:A:LEU:HD13	12	0.29
(1,1683)	1:622:A:PHE:HE2	1:618:A:LEU:HD21	4	0.29
(1,1678)	1:627:A:TYR:HE1	1:631:A:LEU:HG	18	0.29
(1,1625)	1:620:A:GLN:H	1:621:A:ALA:HB1	7	0.29
(1,1625)	1:620:A:GLN:H	1:618:A:LEU:HB3	16	0.29
(1,1617)	1:617:A:GLU:H	1:580:A:LEU:HD23	15	0.29
(1,1591)	1:583:A:LYS:H	1:583:A:LYS:HG3	14	0.29
(1,1588)	1:583:A:LYS:H	1:581:A:GLU:HG2	9	0.29
(1,1588)	1:583:A:LYS:H	1:581:A:GLU:HG2	15	0.29
(1,1577)	1:609:A:ALA:H	1:608:A:LEU:HG	6	0.29
(1,1569)	1:607:A:VAL:H	1:608:A:LEU:HD21	3	0.29
(1,1567)	1:607:A:VAL:H	1:606:A:LYS:HB2	18	0.29
(1,1565)	1:607:A:VAL:H	1:610:A:ASP:HB2	9	0.29
(1,1535)	1:572:A:GLN:H	1:573:A:LEU:HD12	7	0.29
(1,1520)	1:577:A:LEU:H	1:574:A:PRO:HB2	16	0.29
(1,1518)	1:578:A:GLU:H	1:618:A:LEU:HD22	14	0.29
(1,1491)	1:585:A:GLU:H	1:584:A:LEU:HG	18	0.29
(1,1474)	1:589:A:THR:H	1:586:A:ALA:HA	2	0.29
(1,1443)	1:564:A:TYR:HE1	1:564:A:TYR:HA	2	0.29
(1,1443)	1:564:A:TYR:HE2	1:564:A:TYR:HA	4	0.29
(1,1443)	1:564:A:TYR:HE1	1:564:A:TYR:HA	6	0.29
(1,1443)	1:564:A:TYR:HE1	1:564:A:TYR:HA	15	0.29
(1,1431)	1:622:A:PHE:HE2	1:618:A:LEU:HD21	4	0.29
(1,1431)	1:622:A:PHE:HE2	1:618:A:LEU:HD23	11	0.29
(1,1422)	1:627:A:TYR:HD1	1:631:A:LEU:HD11	12	0.29
(1,1420)	1:627:A:TYR:HE1	1:631:A:LEU:HD22	20	0.29
(1,1370)	1:604:A:THR:HG23	1:607:A:VAL:HB	15	0.29
(1,1367)	1:570:A:LEU:HD21	1:628:A:LEU:HB3	15	0.29
(1,1335)	1:566:A:LEU:HG	1:562:A:LEU:HD21	2	0.29
(1,1326)	1:566:A:LEU:HD22	1:563:A:SER:HB3	19	0.29
(1,1326)	1:566:A:LEU:HD23	1:563:A:SER:HB3	20	0.29
(1,1325)	1:628:A:LEU:HD12	1:569:A:GLU:HA	16	0.29
(1,1323)	1:576:A:LEU:HA	1:576:A:LEU:HD23	18	0.29
(1,1295)	1:573:A:LEU:HD13	1:624:A:ARG:HG3	1	0.29
(1,1220)	1:551:A:LYS:HD2	1:551:A:LYS:HA	18	0.29
(1,1147)	1:565:A:LYS:HA	1:565:A:LYS:HD2	15	0.29
(1,1079)	1:573:A:LEU:HB3	1:577:A:LEU:HD21	10	0.29
(1,1063)	1:610:A:ASP:HB2	1:587:A:LEU:HD13	3	0.29
(1,1063)	1:610:A:ASP:HB2	1:587:A:LEU:HD12	9	0.29
(1,1063)	1:610:A:ASP:HB2	1:587:A:LEU:HD13	16	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1056)	1:622:A:PHE:HB2	1:577:A:LEU:HD21	17	0.29
(1,1025)	1:590:A:GLN:HG2	1:591:A:VAL:HG23	16	0.29
(1,1025)	1:590:A:GLN:HG2	1:591:A:VAL:HG23	18	0.29
(1,1020)	1:604:A:THR:HG22	1:599:A:GLN:HG3	13	0.29
(1,1016)	1:588:A:GLN:HG2	1:584:A:LEU:HG	4	0.29
(1,1016)	1:588:A:GLN:HG2	1:584:A:LEU:HG	16	0.29
(1,1014)	1:605:A:GLN:HG2	1:608:A:LEU:HD11	18	0.29
(1,1004)	1:604:A:THR:HG23	1:603:A:GLN:HG2	9	0.29
(1,929)	1:565:A:LYS:HG2	1:566:A:LEU:HD13	9	0.29
(1,870)	1:556:A:LYS:HA	1:556:A:LYS:HE3	12	0.29
(1,851)	1:604:A:THR:HA	1:608:A:LEU:HD11	1	0.29
(1,851)	1:604:A:THR:HA	1:608:A:LEU:HD11	7	0.29
(1,850)	1:604:A:THR:HA	1:607:A:VAL:HG11	7	0.29
(1,725)	1:600:A:PRO:HD3	1:599:A:GLN:HB2	2	0.29
(1,725)	1:600:A:PRO:HD3	1:599:A:GLN:HB2	3	0.29
(1,717)	1:621:A:ALA:HB2	1:577:A:LEU:HD21	18	0.29
(1,630)	1:577:A:LEU:HD11	1:580:A:LEU:HG	11	0.29
(1,601)	1:601:A:HIS:HD2	1:605:A:GLN:HB3	9	0.29
(1,599)	1:601:A:HIS:HD2	1:602:A:GLU:HG3	17	0.29
(1,559)	1:596:A:PHE:HE1	1:604:A:THR:HG22	14	0.29
(1,558)	1:564:A:TYR:HE2	1:568:A:ARG:HB2	8	0.29
(1,554)	1:627:A:TYR:HE2	1:628:A:LEU:HD22	8	0.29
(1,538)	1:635:A:GLY:H	1:631:A:LEU:HD11	1	0.29
(1,538)	1:635:A:GLY:H	1:631:A:LEU:HD11	6	0.29
(1,327)	1:604:A:THR:H	1:603:A:GLN:HB3	14	0.29
(1,321)	1:604:A:THR:H	1:596:A:PHE:HE1	16	0.29
(1,299)	1:567:A:GLN:H	1:566:A:LEU:HD11	11	0.29
(1,173)	1:612:A:ALA:H	1:611:A:MET:HB2	16	0.29
(1,58)	1:596:A:PHE:H	1:594:A:ALA:HB1	5	0.29
(1,58)	1:596:A:PHE:H	1:594:A:ALA:HB1	12	0.29
(1,58)	1:596:A:PHE:H	1:594:A:ALA:HB1	19	0.29
(1,58)	1:596:A:PHE:H	1:594:A:ALA:HB3	20	0.29
(1,2171)	1:591:A:VAL:HG23	1:597:A:PHE:HZ	19	0.28
(1,2165)	1:606:A:LYS:HA	1:610:A:ASP:HB2	1	0.28
(1,2121)	1:581:A:GLU:HG2	1:618:A:LEU:HD23	15	0.28
(1,2114)	1:581:A:GLU:HG3	1:618:A:LEU:HD12	14	0.28
(1,2105)	1:566:A:LEU:HD23	1:628:A:LEU:HG	15	0.28
(1,2059)	1:615:A:GLU:HA	1:619:A:GLU:HG2	5	0.28
(1,2052)	1:603:A:GLN:HG3	1:599:A:GLN:HA	17	0.28
(1,2047)	1:608:A:LEU:HA	1:611:A:MET:HG2	2	0.28
(1,2046)	1:623:A:GLU:HA	1:626:A:GLU:HB3	19	0.28
(1,2027)	1:564:A:TYR:HB3	1:567:A:GLN:HB2	1	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1963)	1:596:A:PHE:HB3	1:591:A:VAL:HG13	18	0.28
(1,1961)	1:610:A:ASP:HB3	1:587:A:LEU:HB3	11	0.28
(1,1946)	1:581:A:GLU:HG2	1:618:A:LEU:HD23	15	0.28
(1,1943)	1:590:A:GLN:HG2	1:589:A:THR:HG22	15	0.28
(1,1940)	1:620:A:GLN:HG2	1:621:A:ALA:HB1	5	0.28
(1,1933)	1:611:A:MET:HB2	1:584:A:LEU:HD23	1	0.28
(1,1933)	1:611:A:MET:HB2	1:608:A:LEU:HD23	6	0.28
(1,1868)	1:569:A:GLU:HA	1:566:A:LEU:HA	15	0.28
(1,1855)	1:572:A:GLN:HA	1:571:A:GLU:HA	4	0.28
(1,1855)	1:572:A:GLN:HA	1:571:A:GLU:HA	8	0.28
(1,1852)	1:604:A:THR:HB	1:608:A:LEU:HB2	5	0.28
(1,1849)	1:604:A:THR:HA	1:599:A:GLN:HB2	14	0.28
(1,1797)	1:576:A:LEU:HA	1:576:A:LEU:HD23	5	0.28
(1,1796)	1:580:A:LEU:HA	1:580:A:LEU:HD21	9	0.28
(1,1796)	1:580:A:LEU:HA	1:580:A:LEU:HD23	11	0.28
(1,1787)	1:621:A:ALA:HA	1:620:A:GLN:HB2	14	0.28
(1,1787)	1:621:A:ALA:HA	1:620:A:GLN:HB2	20	0.28
(1,1778)	1:612:A:ALA:HA	1:584:A:LEU:HD22	11	0.28
(1,1778)	1:612:A:ALA:HA	1:584:A:LEU:HD22	15	0.28
(1,1778)	1:612:A:ALA:HA	1:584:A:LEU:HD23	20	0.28
(1,1736)	1:607:A:VAL:HG11	1:608:A:LEU:HG	5	0.28
(1,1731)	1:607:A:VAL:HG23	1:603:A:GLN:HB3	1	0.28
(1,1731)	1:607:A:VAL:HG23	1:603:A:GLN:HB2	10	0.28
(1,1731)	1:607:A:VAL:HG23	1:603:A:GLN:HB2	13	0.28
(1,1706)	1:625:A:TRP:HD1	1:628:A:LEU:HB2	13	0.28
(1,1693)	1:627:A:TYR:HD1	1:631:A:LEU:HD11	10	0.28
(1,1678)	1:627:A:TYR:HE1	1:631:A:LEU:HG	1	0.28
(1,1678)	1:627:A:TYR:HE1	1:631:A:LEU:HG	17	0.28
(1,1633)	1:622:A:PHE:H	1:619:A:GLU:HB3	9	0.28
(1,1625)	1:620:A:GLN:H	1:618:A:LEU:HB3	1	0.28
(1,1617)	1:617:A:GLU:H	1:580:A:LEU:HD22	4	0.28
(1,1577)	1:609:A:ALA:H	1:608:A:LEU:HG	5	0.28
(1,1569)	1:607:A:VAL:H	1:587:A:LEU:HD22	7	0.28
(1,1567)	1:607:A:VAL:H	1:606:A:LYS:HB2	1	0.28
(1,1567)	1:607:A:VAL:H	1:606:A:LYS:HB2	10	0.28
(1,1530)	1:573:A:LEU:H	1:572:A:GLN:HB3	13	0.28
(1,1520)	1:577:A:LEU:H	1:574:A:PRO:HB2	4	0.28
(1,1515)	1:579:A:ASP:H	1:576:A:LEU:HD11	14	0.28
(1,1491)	1:585:A:GLU:H	1:584:A:LEU:HG	6	0.28
(1,1459)	1:593:A:ASP:H	1:594:A:ALA:H	9	0.28
(1,1457)	1:597:A:PHE:H	1:598:A:SER:HB2	9	0.28
(1,1451)	1:599:A:GLN:H	1:600:A:PRO:HD3	2	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1451)	1:599:A:GLN:H	1:600:A:PRO:HD3	11	0.28
(1,1420)	1:627:A:TYR:HE1	1:631:A:LEU:HD23	8	0.28
(1,1402)	1:606:A:LYS:HB2	1:606:A:LYS:HE2	1	0.28
(1,1402)	1:606:A:LYS:HB2	1:606:A:LYS:HE2	12	0.28
(1,1396)	1:632:A:LYS:HG3	1:562:A:LEU:HB2	7	0.28
(1,1384)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	12	0.28
(1,1377)	1:565:A:LYS:HD3	1:563:A:SER:HB2	11	0.28
(1,1325)	1:628:A:LEU:HD12	1:569:A:GLU:HA	8	0.28
(1,1323)	1:576:A:LEU:HA	1:576:A:LEU:HD21	3	0.28
(1,1323)	1:576:A:LEU:HA	1:576:A:LEU:HD23	5	0.28
(1,1323)	1:576:A:LEU:HA	1:576:A:LEU:HD22	8	0.28
(1,1309)	1:573:A:LEU:HD22	1:576:A:LEU:HB2	19	0.28
(1,1303)	1:581:A:GLU:HG3	1:618:A:LEU:HD12	14	0.28
(1,1292)	1:577:A:LEU:HD22	1:573:A:LEU:HD13	2	0.28
(1,1265)	1:593:A:ASP:HB3	1:595:A:SER:HB3	12	0.28
(1,1250)	1:626:A:GLU:HG2	1:623:A:GLU:HA	1	0.28
(1,1210)	1:606:A:LYS:HA	1:605:A:GLN:HB3	6	0.28
(1,1063)	1:610:A:ASP:HB2	1:587:A:LEU:HD12	13	0.28
(1,1056)	1:622:A:PHE:HB2	1:577:A:LEU:HD23	8	0.28
(1,1025)	1:590:A:GLN:HG2	1:591:A:VAL:HG23	4	0.28
(1,1025)	1:590:A:GLN:HG2	1:591:A:VAL:HG22	7	0.28
(1,1023)	1:590:A:GLN:HG3	1:587:A:LEU:HD23	12	0.28
(1,1016)	1:588:A:GLN:HG2	1:584:A:LEU:HG	10	0.28
(1,972)	1:629:A:GLU:HB2	1:570:A:LEU:HD11	12	0.28
(1,972)	1:629:A:GLU:HB2	1:570:A:LEU:HD13	15	0.28
(1,859)	1:604:A:THR:HB	1:608:A:LEU:HD22	4	0.28
(1,850)	1:604:A:THR:HA	1:607:A:VAL:HG12	2	0.28
(1,838)	1:623:A:GLU:HA	1:626:A:GLU:HB3	19	0.28
(1,805)	1:629:A:GLU:HA	1:570:A:LEU:HD22	7	0.28
(1,725)	1:600:A:PRO:HD3	1:599:A:GLN:HB2	9	0.28
(1,717)	1:621:A:ALA:HB2	1:577:A:LEU:HD21	20	0.28
(1,665)	1:631:A:LEU:HD23	1:631:A:LEU:HA	1	0.28
(1,665)	1:631:A:LEU:HD21	1:631:A:LEU:HA	13	0.28
(1,652)	1:591:A:VAL:HG13	1:608:A:LEU:HA	4	0.28
(1,634)	1:577:A:LEU:HD12	1:574:A:PRO:HA	19	0.28
(1,603)	1:622:A:PHE:HD1	1:626:A:GLU:HG2	3	0.28
(1,603)	1:622:A:PHE:HD1	1:626:A:GLU:HG2	19	0.28
(1,603)	1:622:A:PHE:HD1	1:626:A:GLU:HG2	20	0.28
(1,599)	1:601:A:HIS:HD2	1:602:A:GLU:HG3	4	0.28
(1,559)	1:596:A:PHE:HE2	1:604:A:THR:HG21	5	0.28
(1,339)	1:605:A:GLN:H	1:604:A:THR:HG21	14	0.28
(1,339)	1:605:A:GLN:H	1:604:A:THR:HG23	20	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,327)	1:604:A:THR:H	1:603:A:GLN:HB3	6	0.28
(1,264)	1:571:A:GLU:H	1:571:A:GLU:HG3	9	0.28
(1,262)	1:571:A:GLU:H	1:571:A:GLU:HG2	1	0.28
(1,173)	1:612:A:ALA:H	1:611:A:MET:HB2	12	0.28
(1,26)	1:599:A:GLN:H	1:599:A:GLN:HB3	8	0.28
(1,2169)	1:576:A:LEU:HD12	1:617:A:GLU:HG3	7	0.27
(1,2163)	1:567:A:GLN:HA	1:570:A:LEU:HD13	11	0.27
(1,2135)	1:567:A:GLN:HA	1:570:A:LEU:HD13	11	0.27
(1,2105)	1:566:A:LEU:HD23	1:628:A:LEU:HG	7	0.27
(1,2088)	1:576:A:LEU:HD12	1:617:A:GLU:HG3	7	0.27
(1,2052)	1:603:A:GLN:HG3	1:599:A:GLN:HA	4	0.27
(1,2047)	1:608:A:LEU:HA	1:611:A:MET:HG2	20	0.27
(1,2027)	1:564:A:TYR:HB3	1:567:A:GLN:HB2	20	0.27
(1,1963)	1:596:A:PHE:HB3	1:591:A:VAL:HG13	10	0.27
(1,1950)	1:576:A:LEU:HG	1:617:A:GLU:HG3	5	0.27
(1,1939)	1:572:A:GLN:HG3	1:568:A:ARG:HG3	13	0.27
(1,1937)	1:616:A:GLN:HG3	1:613:A:ALA:HB1	12	0.27
(1,1933)	1:611:A:MET:HB2	1:608:A:LEU:HD23	9	0.27
(1,1867)	1:564:A:TYR:HA	1:567:A:GLN:HA	5	0.27
(1,1867)	1:564:A:TYR:HA	1:567:A:GLN:HA	16	0.27
(1,1855)	1:572:A:GLN:HA	1:571:A:GLU:HA	11	0.27
(1,1855)	1:572:A:GLN:HA	1:571:A:GLU:HA	13	0.27
(1,1855)	1:572:A:GLN:HA	1:571:A:GLU:HA	15	0.27
(1,1828)	1:601:A:HIS:HA	1:602:A:GLU:HG2	8	0.27
(1,1797)	1:576:A:LEU:HA	1:576:A:LEU:HD22	2	0.27
(1,1797)	1:576:A:LEU:HA	1:576:A:LEU:HD23	13	0.27
(1,1797)	1:576:A:LEU:HA	1:576:A:LEU:HD23	16	0.27
(1,1795)	1:579:A:ASP:HA	1:583:A:LYS:HB2	3	0.27
(1,1795)	1:579:A:ASP:HA	1:583:A:LYS:HB2	7	0.27
(1,1778)	1:612:A:ALA:HA	1:584:A:LEU:HD22	16	0.27
(1,1774)	1:592:A:ALA:HA	1:589:A:THR:HA	18	0.27
(1,1730)	1:607:A:VAL:HG23	1:587:A:LEU:HD23	3	0.27
(1,1718)	1:604:A:THR:HG23	1:599:A:GLN:HG3	20	0.27
(1,1691)	1:627:A:TYR:HE2	1:624:A:ARG:HA	8	0.27
(1,1669)	1:633:A:ASN:H	1:631:A:LEU:HB3	4	0.27
(1,1608)	1:616:A:GLN:H	1:612:A:ALA:HA	13	0.27
(1,1591)	1:583:A:LYS:H	1:583:A:LYS:HG3	2	0.27
(1,1577)	1:609:A:ALA:H	1:608:A:LEU:HG	3	0.27
(1,1577)	1:609:A:ALA:H	1:608:A:LEU:HG	7	0.27
(1,1568)	1:607:A:VAL:H	1:606:A:LYS:HG2	20	0.27
(1,1567)	1:607:A:VAL:H	1:606:A:LYS:HB2	17	0.27
(1,1562)	1:604:A:THR:H	1:599:A:GLN:HB2	4	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1530)	1:573:A:LEU:H	1:572:A:GLN:HB3	6	0.27
(1,1520)	1:577:A:LEU:H	1:574:A:PRO:HB2	5	0.27
(1,1520)	1:577:A:LEU:H	1:578:A:GLU:HG3	7	0.27
(1,1520)	1:577:A:LEU:H	1:574:A:PRO:HB2	8	0.27
(1,1520)	1:577:A:LEU:H	1:578:A:GLU:HG3	10	0.27
(1,1520)	1:577:A:LEU:H	1:574:A:PRO:HB2	19	0.27
(1,1509)	1:581:A:GLU:H	1:580:A:LEU:HG	17	0.27
(1,1491)	1:585:A:GLU:H	1:584:A:LEU:HG	8	0.27
(1,1459)	1:593:A:ASP:H	1:594:A:ALA:H	13	0.27
(1,1457)	1:597:A:PHE:H	1:598:A:SER:HB2	13	0.27
(1,1443)	1:564:A:TYR:HE1	1:564:A:TYR:HA	1	0.27
(1,1443)	1:564:A:TYR:HE1	1:564:A:TYR:HA	9	0.27
(1,1443)	1:564:A:TYR:HE1	1:564:A:TYR:HA	16	0.27
(1,1443)	1:564:A:TYR:HE1	1:564:A:TYR:HA	20	0.27
(1,1426)	1:627:A:TYR:HD2	1:628:A:LEU:HD22	8	0.27
(1,1426)	1:627:A:TYR:HD2	1:628:A:LEU:HD21	10	0.27
(1,1420)	1:627:A:TYR:HE1	1:631:A:LEU:HD21	11	0.27
(1,1402)	1:606:A:LYS:HB2	1:606:A:LYS:HE2	18	0.27
(1,1384)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	5	0.27
(1,1378)	1:624:A:ARG:HD3	1:573:A:LEU:HD13	4	0.27
(1,1370)	1:604:A:THR:HG22	1:607:A:VAL:HB	4	0.27
(1,1367)	1:570:A:LEU:HD21	1:628:A:LEU:HB3	17	0.27
(1,1333)	1:573:A:LEU:HD11	1:624:A:ARG:HD2	12	0.27
(1,1325)	1:628:A:LEU:HD13	1:569:A:GLU:HA	13	0.27
(1,1323)	1:576:A:LEU:HA	1:576:A:LEU:HD22	2	0.27
(1,1323)	1:576:A:LEU:HA	1:576:A:LEU:HD23	13	0.27
(1,1323)	1:576:A:LEU:HA	1:576:A:LEU:HD23	16	0.27
(1,1309)	1:573:A:LEU:HD23	1:576:A:LEU:HB2	14	0.27
(1,1165)	1:601:A:HIS:HB2	1:605:A:GLN:HG2	7	0.27
(1,1136)	1:600:A:PRO:HD3	1:603:A:GLN:HB3	5	0.27
(1,1025)	1:590:A:GLN:HG2	1:591:A:VAL:HG22	1	0.27
(1,1025)	1:590:A:GLN:HG2	1:591:A:VAL:HG22	6	0.27
(1,1024)	1:590:A:GLN:HG3	1:589:A:THR:HG21	6	0.27
(1,1023)	1:590:A:GLN:HG3	1:587:A:LEU:HD22	9	0.27
(1,1020)	1:604:A:THR:HG23	1:599:A:GLN:HG3	20	0.27
(1,1016)	1:588:A:GLN:HG2	1:584:A:LEU:HG	20	0.27
(1,1014)	1:605:A:GLN:HG2	1:608:A:LEU:HD11	16	0.27
(1,972)	1:629:A:GLU:HB2	1:570:A:LEU:HD12	4	0.27
(1,972)	1:629:A:GLU:HB2	1:570:A:LEU:HD13	7	0.27
(1,928)	1:583:A:LYS:HG3	1:587:A:LEU:HD23	7	0.27
(1,928)	1:583:A:LYS:HG3	1:587:A:LEU:HD21	18	0.27
(1,750)	1:604:A:THR:HG22	1:599:A:GLN:HA	6	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,750)	1:604:A:THR:HG23	1:599:A:GLN:HA	17	0.27
(1,730)	1:600:A:PRO:HD3	1:603:A:GLN:HG2	12	0.27
(1,725)	1:600:A:PRO:HD3	1:599:A:GLN:HB2	12	0.27
(1,717)	1:621:A:ALA:HB3	1:577:A:LEU:HD21	17	0.27
(1,712)	1:594:A:ALA:HB2	1:593:A:ASP:HA	3	0.27
(1,691)	1:628:A:LEU:HD13	1:569:A:GLU:HB2	11	0.27
(1,665)	1:631:A:LEU:HD23	1:631:A:LEU:HA	9	0.27
(1,634)	1:577:A:LEU:HD12	1:574:A:PRO:HA	2	0.27
(1,634)	1:577:A:LEU:HD13	1:574:A:PRO:HA	16	0.27
(1,603)	1:622:A:PHE:HD1	1:626:A:GLU:HG2	17	0.27
(1,602)	1:597:A:PHE:HZ	1:608:A:LEU:HD12	17	0.27
(1,599)	1:601:A:HIS:HD2	1:602:A:GLU:HG2	9	0.27
(1,585)	1:596:A:PHE:HZ	1:607:A:VAL:HG13	3	0.27
(1,585)	1:596:A:PHE:HZ	1:607:A:VAL:HG13	6	0.27
(1,585)	1:596:A:PHE:HZ	1:607:A:VAL:HG13	14	0.27
(1,558)	1:564:A:TYR:HE2	1:568:A:ARG:HB2	10	0.27
(1,552)	1:596:A:PHE:HD1	1:607:A:VAL:HG23	7	0.27
(1,550)	1:596:A:PHE:HD1	1:604:A:THR:HG23	13	0.27
(1,542)	1:625:A:TRP:HE1	1:629:A:GLU:HG3	19	0.27
(1,507)	1:629:A:GLU:H	1:570:A:LEU:HD21	3	0.27
(1,429)	1:618:A:LEU:H	1:617:A:GLU:HB2	5	0.27
(1,429)	1:618:A:LEU:H	1:617:A:GLU:HB2	19	0.27
(1,327)	1:604:A:THR:H	1:603:A:GLN:HB3	7	0.27
(1,283)	1:569:A:GLU:H	1:568:A:ARG:HB3	19	0.27
(1,274)	1:570:A:LEU:H	1:569:A:GLU:HG2	17	0.27
(1,262)	1:571:A:GLU:H	1:571:A:GLU:HG2	2	0.27
(1,149)	1:586:A:ALA:H	1:589:A:THR:HG22	17	0.27
(1,58)	1:596:A:PHE:H	1:594:A:ALA:HB3	6	0.27
(1,58)	1:596:A:PHE:H	1:594:A:ALA:HB1	7	0.27
(1,58)	1:596:A:PHE:H	1:594:A:ALA:HB3	10	0.27
(1,2171)	1:591:A:VAL:HG23	1:597:A:PHE:HZ	11	0.26
(1,2146)	1:615:A:GLU:HG2	1:584:A:LEU:HG	17	0.26
(1,2139)	1:566:A:LEU:HD22	1:565:A:LYS:HA	15	0.26
(1,2121)	1:581:A:GLU:HG2	1:618:A:LEU:HD22	7	0.26
(1,2119)	1:569:A:GLU:HB3	1:566:A:LEU:HD11	1	0.26
(1,2109)	1:608:A:LEU:HD12	1:591:A:VAL:HG11	7	0.26
(1,2052)	1:603:A:GLN:HG3	1:599:A:GLN:HA	18	0.26
(1,2027)	1:564:A:TYR:HB3	1:567:A:GLN:HB2	6	0.26
(1,1961)	1:610:A:ASP:HB3	1:587:A:LEU:HB3	5	0.26
(1,1951)	1:615:A:GLU:HG2	1:584:A:LEU:HG	11	0.26
(1,1951)	1:615:A:GLU:HG2	1:584:A:LEU:HG	17	0.26
(1,1946)	1:581:A:GLU:HG2	1:618:A:LEU:HD22	7	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1944)	1:585:A:GLU:HG3	1:586:A:ALA:HB1	1	0.26
(1,1939)	1:572:A:GLN:HG3	1:568:A:ARG:HG3	1	0.26
(1,1868)	1:569:A:GLU:HA	1:566:A:LEU:HA	2	0.26
(1,1867)	1:564:A:TYR:HA	1:567:A:GLN:HA	6	0.26
(1,1867)	1:564:A:TYR:HA	1:567:A:GLN:HA	17	0.26
(1,1849)	1:604:A:THR:HA	1:599:A:GLN:HB2	8	0.26
(1,1813)	1:588:A:GLN:HA	1:584:A:LEU:HD21	18	0.26
(1,1806)	1:577:A:LEU:HA	1:581:A:GLU:HB2	10	0.26
(1,1797)	1:576:A:LEU:HA	1:576:A:LEU:HD23	9	0.26
(1,1796)	1:580:A:LEU:HA	1:580:A:LEU:HD22	6	0.26
(1,1796)	1:580:A:LEU:HA	1:580:A:LEU:HD21	19	0.26
(1,1795)	1:579:A:ASP:HA	1:583:A:LYS:HB2	2	0.26
(1,1789)	1:556:A:LYS:HA	1:555:A:VAL:HG13	2	0.26
(1,1787)	1:621:A:ALA:HA	1:620:A:GLN:HB2	3	0.26
(1,1787)	1:621:A:ALA:HA	1:620:A:GLN:HB2	17	0.26
(1,1779)	1:614:A:ALA:HA	1:580:A:LEU:HD12	2	0.26
(1,1767)	1:600:A:PRO:HD2	1:603:A:GLN:HG2	5	0.26
(1,1745)	1:614:A:ALA:HB2	1:580:A:LEU:HD22	4	0.26
(1,1745)	1:614:A:ALA:HB2	1:580:A:LEU:HD23	14	0.26
(1,1718)	1:604:A:THR:HG23	1:599:A:GLN:HG3	2	0.26
(1,1710)	1:577:A:LEU:HD22	1:574:A:PRO:HG3	11	0.26
(1,1700)	1:622:A:PHE:HZ	1:618:A:LEU:HD12	4	0.26
(1,1693)	1:627:A:TYR:HD1	1:631:A:LEU:HD13	2	0.26
(1,1693)	1:627:A:TYR:HD1	1:631:A:LEU:HD11	5	0.26
(1,1693)	1:627:A:TYR:HD1	1:631:A:LEU:HD12	9	0.26
(1,1693)	1:627:A:TYR:HD1	1:631:A:LEU:HD13	17	0.26
(1,1693)	1:627:A:TYR:HD1	1:631:A:LEU:HD11	20	0.26
(1,1678)	1:627:A:TYR:HE1	1:631:A:LEU:HG	7	0.26
(1,1670)	1:633:A:ASN:H	1:631:A:LEU:HB2	13	0.26
(1,1625)	1:620:A:GLN:H	1:621:A:ALA:HB1	13	0.26
(1,1625)	1:620:A:GLN:H	1:621:A:ALA:HB3	20	0.26
(1,1608)	1:616:A:GLN:H	1:612:A:ALA:HA	8	0.26
(1,1608)	1:616:A:GLN:H	1:612:A:ALA:HA	18	0.26
(1,1608)	1:616:A:GLN:H	1:612:A:ALA:HA	20	0.26
(1,1577)	1:609:A:ALA:H	1:608:A:LEU:HG	11	0.26
(1,1569)	1:607:A:VAL:H	1:587:A:LEU:HD23	18	0.26
(1,1565)	1:607:A:VAL:H	1:610:A:ASP:HB2	13	0.26
(1,1546)	1:568:A:ARG:H	1:567:A:GLN:HG3	13	0.26
(1,1520)	1:577:A:LEU:H	1:574:A:PRO:HB2	13	0.26
(1,1520)	1:577:A:LEU:H	1:574:A:PRO:HB2	18	0.26
(1,1515)	1:579:A:ASP:H	1:576:A:LEU:HD11	6	0.26
(1,1503)	1:582:A:ALA:H	1:581:A:GLU:HB2	5	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1503)	1:582:A:ALA:H	1:581:A:GLU:HB2	7	0.26
(1,1491)	1:585:A:GLU:H	1:584:A:LEU:HG	2	0.26
(1,1459)	1:593:A:ASP:H	1:594:A:ALA:H	1	0.26
(1,1459)	1:593:A:ASP:H	1:594:A:ALA:H	15	0.26
(1,1459)	1:593:A:ASP:H	1:594:A:ALA:H	18	0.26
(1,1459)	1:593:A:ASP:H	1:594:A:ALA:H	20	0.26
(1,1451)	1:599:A:GLN:H	1:600:A:PRO:HD3	3	0.26
(1,1451)	1:599:A:GLN:H	1:600:A:PRO:HD3	6	0.26
(1,1451)	1:599:A:GLN:H	1:600:A:PRO:HD3	9	0.26
(1,1422)	1:627:A:TYR:HD1	1:631:A:LEU:HD11	10	0.26
(1,1420)	1:627:A:TYR:HE1	1:631:A:LEU:HD22	3	0.26
(1,1420)	1:627:A:TYR:HE1	1:631:A:LEU:HD22	4	0.26
(1,1420)	1:627:A:TYR:HE1	1:631:A:LEU:HD22	14	0.26
(1,1418)	1:596:A:PHE:HE2	1:591:A:VAL:HG21	16	0.26
(1,1384)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	6	0.26
(1,1384)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	9	0.26
(1,1384)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	14	0.26
(1,1377)	1:565:A:LYS:HD3	1:563:A:SER:HB2	16	0.26
(1,1370)	1:604:A:THR:HG21	1:607:A:VAL:HB	17	0.26
(1,1369)	1:591:A:VAL:HG23	1:596:A:PHE:HB2	19	0.26
(1,1335)	1:566:A:LEU:HG	1:562:A:LEU:HD21	20	0.26
(1,1323)	1:576:A:LEU:HA	1:576:A:LEU:HD23	9	0.26
(1,1265)	1:593:A:ASP:HB3	1:595:A:SER:HB2	15	0.26
(1,1210)	1:606:A:LYS:HA	1:605:A:GLN:HB3	7	0.26
(1,1170)	1:629:A:GLU:HG2	1:626:A:GLU:HA	20	0.26
(1,1158)	1:600:A:PRO:HD2	1:603:A:GLN:HG2	5	0.26
(1,1136)	1:600:A:PRO:HD3	1:603:A:GLN:HB3	13	0.26
(1,1094)	1:632:A:LYS:HE3	1:570:A:LEU:HD11	19	0.26
(1,1063)	1:610:A:ASP:HB2	1:587:A:LEU:HD11	2	0.26
(1,1063)	1:610:A:ASP:HB2	1:587:A:LEU:HD11	20	0.26
(1,1056)	1:622:A:PHE:HB2	1:577:A:LEU:HD23	14	0.26
(1,1025)	1:590:A:GLN:HG2	1:591:A:VAL:HG23	17	0.26
(1,1024)	1:590:A:GLN:HG3	1:589:A:THR:HG23	7	0.26
(1,1020)	1:604:A:THR:HG23	1:599:A:GLN:HG3	2	0.26
(1,1016)	1:588:A:GLN:HG2	1:584:A:LEU:HG	6	0.26
(1,1016)	1:588:A:GLN:HG2	1:584:A:LEU:HG	7	0.26
(1,1016)	1:588:A:GLN:HG2	1:584:A:LEU:HG	17	0.26
(1,972)	1:629:A:GLU:HB2	1:570:A:LEU:HD11	3	0.26
(1,972)	1:629:A:GLU:HB2	1:570:A:LEU:HD11	5	0.26
(1,972)	1:629:A:GLU:HB2	1:570:A:LEU:HD11	10	0.26
(1,928)	1:583:A:LYS:HG3	1:587:A:LEU:HD21	8	0.26
(1,928)	1:583:A:LYS:HG3	1:587:A:LEU:HD21	17	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,928)	1:583:A:LYS:HG3	1:587:A:LEU:HD22	19	0.26
(1,859)	1:604:A:THR:HB	1:608:A:LEU:HD22	12	0.26
(1,809)	1:605:A:GLN:HA	1:608:A:LEU:HD22	1	0.26
(1,755)	1:621:A:ALA:HA	1:576:A:LEU:HD21	12	0.26
(1,665)	1:631:A:LEU:HD23	1:631:A:LEU:HA	2	0.26
(1,665)	1:631:A:LEU:HD23	1:631:A:LEU:HA	7	0.26
(1,665)	1:631:A:LEU:HD23	1:631:A:LEU:HA	8	0.26
(1,665)	1:631:A:LEU:HD21	1:631:A:LEU:HA	16	0.26
(1,665)	1:631:A:LEU:HD21	1:631:A:LEU:HA	19	0.26
(1,664)	1:631:A:LEU:HD21	1:566:A:LEU:HB2	20	0.26
(1,604)	1:622:A:PHE:HD2	1:618:A:LEU:HG	14	0.26
(1,599)	1:601:A:HIS:HD2	1:602:A:GLU:HG3	20	0.26
(1,558)	1:564:A:TYR:HE2	1:568:A:ARG:HB2	12	0.26
(1,429)	1:618:A:LEU:H	1:617:A:GLU:HB2	12	0.26
(1,369)	1:609:A:ALA:H	1:608:A:LEU:HD13	11	0.26
(1,369)	1:609:A:ALA:H	1:608:A:LEU:HD11	15	0.26
(1,339)	1:605:A:GLN:H	1:604:A:THR:HG22	15	0.26
(1,182)	1:581:A:GLU:H	1:580:A:LEU:HD12	6	0.26
(1,182)	1:581:A:GLU:H	1:580:A:LEU:HD13	17	0.26
(1,173)	1:612:A:ALA:H	1:611:A:MET:HB2	17	0.26
(1,58)	1:596:A:PHE:H	1:594:A:ALA:HB3	9	0.26
(1,58)	1:596:A:PHE:H	1:594:A:ALA:HB3	15	0.26
(1,58)	1:596:A:PHE:H	1:594:A:ALA:HB3	18	0.26
(1,2105)	1:566:A:LEU:HD22	1:628:A:LEU:HG	3	0.25
(1,2098)	1:581:A:GLU:HG3	1:618:A:LEU:HD21	2	0.25
(1,2051)	1:603:A:GLN:HG2	1:600:A:PRO:HA	3	0.25
(1,2036)	1:561:A:LYS:HD3	1:561:A:LYS:HA	17	0.25
(1,2027)	1:564:A:TYR:HB3	1:567:A:GLN:HB2	12	0.25
(1,2027)	1:564:A:TYR:HB3	1:567:A:GLN:HB2	16	0.25
(1,2027)	1:564:A:TYR:HB3	1:567:A:GLN:HB2	19	0.25
(1,1963)	1:596:A:PHE:HB3	1:591:A:VAL:HG11	14	0.25
(1,1963)	1:596:A:PHE:HB3	1:591:A:VAL:HG13	17	0.25
(1,1945)	1:585:A:GLU:HG2	1:586:A:ALA:HB2	8	0.25
(1,1940)	1:620:A:GLN:HG2	1:621:A:ALA:HB1	18	0.25
(1,1907)	1:591:A:VAL:HA	1:608:A:LEU:HD22	19	0.25
(1,1901)	1:612:A:ALA:HB2	1:616:A:GLN:HB3	16	0.25
(1,1895)	1:618:A:LEU:HG	1:581:A:GLU:HB2	1	0.25
(1,1849)	1:604:A:THR:HA	1:599:A:GLN:HB2	5	0.25
(1,1828)	1:601:A:HIS:HA	1:602:A:GLU:HG3	20	0.25
(1,1813)	1:588:A:GLN:HA	1:584:A:LEU:HD23	4	0.25
(1,1796)	1:580:A:LEU:HA	1:580:A:LEU:HD21	5	0.25
(1,1796)	1:580:A:LEU:HA	1:580:A:LEU:HD22	16	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1796)	1:580:A:LEU:HA	1:580:A:LEU:HD22	18	0.25
(1,1795)	1:579:A:ASP:HA	1:583:A:LYS:HB2	13	0.25
(1,1787)	1:621:A:ALA:HA	1:620:A:GLN:HB2	18	0.25
(1,1774)	1:592:A:ALA:HA	1:589:A:THR:HA	7	0.25
(1,1742)	1:628:A:LEU:HD21	1:566:A:LEU:HB2	1	0.25
(1,1719)	1:604:A:THR:HG22	1:603:A:GLN:HG2	15	0.25
(1,1711)	1:577:A:LEU:HD21	1:626:A:GLU:HG3	12	0.25
(1,1708)	1:625:A:TRP:HD1	1:628:A:LEU:HD13	1	0.25
(1,1693)	1:627:A:TYR:HD1	1:631:A:LEU:HD13	1	0.25
(1,1693)	1:627:A:TYR:HD1	1:631:A:LEU:HD13	11	0.25
(1,1693)	1:627:A:TYR:HD1	1:631:A:LEU:HD13	13	0.25
(1,1693)	1:627:A:TYR:HD1	1:631:A:LEU:HD13	18	0.25
(1,1693)	1:627:A:TYR:HD1	1:631:A:LEU:HD13	19	0.25
(1,1689)	1:596:A:PHE:HD1	1:607:A:VAL:HB	10	0.25
(1,1683)	1:622:A:PHE:HE2	1:618:A:LEU:HD23	13	0.25
(1,1669)	1:633:A:ASN:H	1:631:A:LEU:HB3	2	0.25
(1,1669)	1:633:A:ASN:H	1:631:A:LEU:HB3	9	0.25
(1,1669)	1:633:A:ASN:H	1:631:A:LEU:HB3	16	0.25
(1,1625)	1:620:A:GLN:H	1:621:A:ALA:HB3	10	0.25
(1,1625)	1:620:A:GLN:H	1:618:A:LEU:HB3	15	0.25
(1,1625)	1:620:A:GLN:H	1:621:A:ALA:HB1	17	0.25
(1,1594)	1:614:A:ALA:H	1:615:A:GLU:HG3	19	0.25
(1,1591)	1:583:A:LYS:H	1:583:A:LYS:HG3	5	0.25
(1,1591)	1:583:A:LYS:H	1:583:A:LYS:HG3	6	0.25
(1,1591)	1:583:A:LYS:H	1:583:A:LYS:HG3	8	0.25
(1,1591)	1:583:A:LYS:H	1:583:A:LYS:HG3	11	0.25
(1,1591)	1:583:A:LYS:H	1:583:A:LYS:HG3	16	0.25
(1,1591)	1:583:A:LYS:H	1:583:A:LYS:HG3	19	0.25
(1,1588)	1:583:A:LYS:H	1:581:A:GLU:HG2	11	0.25
(1,1577)	1:609:A:ALA:H	1:608:A:LEU:HG	18	0.25
(1,1568)	1:607:A:VAL:H	1:606:A:LYS:HG2	9	0.25
(1,1567)	1:607:A:VAL:H	1:606:A:LYS:HB2	6	0.25
(1,1546)	1:568:A:ARG:H	1:567:A:GLN:HG3	6	0.25
(1,1535)	1:572:A:GLN:H	1:573:A:LEU:HD11	2	0.25
(1,1451)	1:599:A:GLN:H	1:600:A:PRO:HD3	1	0.25
(1,1443)	1:564:A:TYR:HE1	1:564:A:TYR:HA	10	0.25
(1,1443)	1:564:A:TYR:HE1	1:564:A:TYR:HA	13	0.25
(1,1437)	1:564:A:TYR:HD2	1:568:A:ARG:HG2	10	0.25
(1,1426)	1:627:A:TYR:HD2	1:628:A:LEU:HD23	11	0.25
(1,1426)	1:627:A:TYR:HD2	1:628:A:LEU:HD21	16	0.25
(1,1402)	1:606:A:LYS:HB2	1:606:A:LYS:HE2	3	0.25
(1,1370)	1:604:A:THR:HG21	1:607:A:VAL:HB	20	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1369)	1:591:A:VAL:HG23	1:596:A:PHE:HB2	3	0.25
(1,1335)	1:566:A:LEU:HG	1:562:A:LEU:HD21	4	0.25
(1,1333)	1:573:A:LEU:HD13	1:624:A:ARG:HD2	7	0.25
(1,1309)	1:573:A:LEU:HD22	1:576:A:LEU:HB2	4	0.25
(1,1309)	1:573:A:LEU:HD22	1:576:A:LEU:HB2	11	0.25
(1,1309)	1:573:A:LEU:HD23	1:576:A:LEU:HB2	13	0.25
(1,1295)	1:573:A:LEU:HD13	1:624:A:ARG:HG3	10	0.25
(1,1271)	1:576:A:LEU:HD11	1:621:A:ALA:HB1	19	0.25
(1,1266)	1:596:A:PHE:HA	1:593:A:ASP:HB2	4	0.25
(1,1210)	1:606:A:LYS:HA	1:605:A:GLN:HB3	5	0.25
(1,1210)	1:606:A:LYS:HA	1:605:A:GLN:HB2	9	0.25
(1,1164)	1:601:A:HIS:HB3	1:605:A:GLN:HG2	10	0.25
(1,1155)	1:603:A:GLN:HG3	1:600:A:PRO:HD3	6	0.25
(1,1062)	1:610:A:ASP:HB2	1:587:A:LEU:HD21	4	0.25
(1,1004)	1:604:A:THR:HG22	1:603:A:GLN:HG2	15	0.25
(1,998)	1:583:A:LYS:HB3	1:587:A:LEU:HD13	15	0.25
(1,991)	1:611:A:MET:HG3	1:587:A:LEU:HD12	14	0.25
(1,851)	1:604:A:THR:HA	1:608:A:LEU:HD11	2	0.25
(1,850)	1:604:A:THR:HA	1:607:A:VAL:HG13	17	0.25
(1,820)	1:601:A:HIS:HA	1:605:A:GLN:HB2	14	0.25
(1,820)	1:601:A:HIS:HA	1:605:A:GLN:HB2	19	0.25
(1,809)	1:605:A:GLN:HA	1:608:A:LEU:HD22	2	0.25
(1,730)	1:600:A:PRO:HD3	1:603:A:GLN:HG2	11	0.25
(1,691)	1:628:A:LEU:HD13	1:569:A:GLU:HB2	2	0.25
(1,665)	1:631:A:LEU:HD23	1:631:A:LEU:HA	5	0.25
(1,665)	1:631:A:LEU:HD21	1:631:A:LEU:HA	6	0.25
(1,664)	1:631:A:LEU:HD21	1:566:A:LEU:HB2	4	0.25
(1,658)	1:591:A:VAL:HG21	1:596:A:PHE:HB3	13	0.25
(1,652)	1:591:A:VAL:HG11	1:608:A:LEU:HA	11	0.25
(1,630)	1:577:A:LEU:HD12	1:580:A:LEU:HG	15	0.25
(1,602)	1:597:A:PHE:HZ	1:608:A:LEU:HD11	6	0.25
(1,599)	1:601:A:HIS:HD2	1:602:A:GLU:HG2	14	0.25
(1,581)	1:601:A:HIS:HD2	1:605:A:GLN:HG2	18	0.25
(1,554)	1:627:A:TYR:HE2	1:628:A:LEU:HD22	9	0.25
(1,552)	1:596:A:PHE:HD1	1:607:A:VAL:HG21	20	0.25
(1,545)	1:577:A:LEU:HD22	1:577:A:LEU:HD23	7	0.25
(1,339)	1:605:A:GLN:H	1:604:A:THR:HG23	2	0.25
(1,264)	1:571:A:GLU:H	1:571:A:GLU:HG3	4	0.25
(1,173)	1:612:A:ALA:H	1:611:A:MET:HB2	8	0.25
(1,173)	1:612:A:ALA:H	1:611:A:MET:HB2	10	0.25
(1,173)	1:612:A:ALA:H	1:611:A:MET:HB2	18	0.25
(1,162)	1:584:A:LEU:H	1:583:A:LYS:HG3	10	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,92)	1:592:A:ALA:H	1:589:A:THR:HG22	15	0.25
(1,58)	1:596:A:PHE:H	1:594:A:ALA:HB2	8	0.25
(1,58)	1:596:A:PHE:H	1:594:A:ALA:HB3	16	0.25
(1,58)	1:596:A:PHE:H	1:594:A:ALA:HB3	17	0.25
(1,2167)	1:606:A:LYS:HB3	1:606:A:LYS:HE3	4	0.24
(1,2163)	1:567:A:GLN:HA	1:570:A:LEU:HD13	9	0.24
(1,2146)	1:588:A:GLN:HG2	1:584:A:LEU:HG	11	0.24
(1,2139)	1:566:A:LEU:HD22	1:565:A:LYS:HA	7	0.24
(1,2135)	1:567:A:GLN:HA	1:570:A:LEU:HD13	9	0.24
(1,2105)	1:566:A:LEU:HD21	1:628:A:LEU:HG	19	0.24
(1,2105)	1:566:A:LEU:HD22	1:628:A:LEU:HG	20	0.24
(1,2056)	1:572:A:GLN:HG3	1:569:A:GLU:HA	11	0.24
(1,2048)	1:611:A:MET:HG3	1:584:A:LEU:HA	14	0.24
(1,1963)	1:596:A:PHE:HB3	1:591:A:VAL:HG11	7	0.24
(1,1963)	1:596:A:PHE:HB3	1:591:A:VAL:HG12	11	0.24
(1,1963)	1:596:A:PHE:HB3	1:591:A:VAL:HG11	16	0.24
(1,1947)	1:581:A:GLU:HG2	1:584:A:LEU:HD13	17	0.24
(1,1946)	1:581:A:GLU:HG2	1:618:A:LEU:HD23	9	0.24
(1,1933)	1:611:A:MET:HB2	1:584:A:LEU:HD23	5	0.24
(1,1933)	1:611:A:MET:HB2	1:608:A:LEU:HD23	20	0.24
(1,1920)	1:613:A:ALA:HB3	1:617:A:GLU:HB2	13	0.24
(1,1901)	1:612:A:ALA:HB1	1:616:A:GLN:HB3	17	0.24
(1,1867)	1:564:A:TYR:HA	1:567:A:GLN:HA	11	0.24
(1,1867)	1:564:A:TYR:HA	1:567:A:GLN:HA	14	0.24
(1,1855)	1:572:A:GLN:HA	1:571:A:GLU:HA	7	0.24
(1,1855)	1:572:A:GLN:HA	1:571:A:GLU:HA	14	0.24
(1,1855)	1:572:A:GLN:HA	1:571:A:GLU:HA	17	0.24
(1,1813)	1:588:A:GLN:HA	1:584:A:LEU:HD22	10	0.24
(1,1813)	1:588:A:GLN:HA	1:584:A:LEU:HD23	19	0.24
(1,1806)	1:577:A:LEU:HA	1:581:A:GLU:HB2	16	0.24
(1,1797)	1:628:A:LEU:HD22	1:624:A:ARG:HA	8	0.24
(1,1797)	1:576:A:LEU:HA	1:576:A:LEU:HD22	12	0.24
(1,1796)	1:580:A:LEU:HA	1:580:A:LEU:HD22	3	0.24
(1,1796)	1:580:A:LEU:HA	1:580:A:LEU:HD22	17	0.24
(1,1795)	1:579:A:ASP:HA	1:583:A:LYS:HB2	15	0.24
(1,1789)	1:556:A:LYS:HA	1:555:A:VAL:HG11	14	0.24
(1,1787)	1:621:A:ALA:HA	1:620:A:GLN:HB2	5	0.24
(1,1787)	1:621:A:ALA:HA	1:620:A:GLN:HB2	9	0.24
(1,1787)	1:621:A:ALA:HA	1:620:A:GLN:HB2	13	0.24
(1,1749)	1:613:A:ALA:HB3	1:617:A:GLU:HB2	13	0.24
(1,1741)	1:628:A:LEU:HD22	1:624:A:ARG:HA	8	0.24
(1,1731)	1:607:A:VAL:HG21	1:603:A:GLN:HB2	7	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1731)	1:607:A:VAL:HG21	1:603:A:GLN:HB3	11	0.24
(1,1711)	1:577:A:LEU:HD23	1:626:A:GLU:HG3	14	0.24
(1,1711)	1:577:A:LEU:HD21	1:626:A:GLU:HG3	18	0.24
(1,1709)	1:625:A:TRP:HD1	1:573:A:LEU:HB2	14	0.24
(1,1693)	1:627:A:TYR:HD1	1:631:A:LEU:HD11	7	0.24
(1,1693)	1:627:A:TYR:HD1	1:631:A:LEU:HD13	14	0.24
(1,1689)	1:596:A:PHE:HD1	1:607:A:VAL:HB	11	0.24
(1,1683)	1:622:A:PHE:HE2	1:618:A:LEU:HD23	12	0.24
(1,1682)	1:622:A:PHE:HD2	1:577:A:LEU:HD13	18	0.24
(1,1678)	1:627:A:TYR:HE1	1:631:A:LEU:HG	19	0.24
(1,1670)	1:633:A:ASN:H	1:631:A:LEU:HB2	15	0.24
(1,1669)	1:633:A:ASN:H	1:631:A:LEU:HB3	12	0.24
(1,1633)	1:622:A:PHE:H	1:619:A:GLU:HB3	3	0.24
(1,1594)	1:614:A:ALA:H	1:615:A:GLU:HG3	16	0.24
(1,1591)	1:583:A:LYS:H	1:583:A:LYS:HG3	3	0.24
(1,1591)	1:583:A:LYS:H	1:583:A:LYS:HG3	10	0.24
(1,1591)	1:583:A:LYS:H	1:583:A:LYS:HG3	17	0.24
(1,1591)	1:583:A:LYS:H	1:583:A:LYS:HG3	20	0.24
(1,1577)	1:609:A:ALA:H	1:608:A:LEU:HG	16	0.24
(1,1568)	1:607:A:VAL:H	1:606:A:LYS:HG2	2	0.24
(1,1567)	1:607:A:VAL:H	1:606:A:LYS:HB2	7	0.24
(1,1563)	1:605:A:GLN:H	1:605:A:GLN:HE22	19	0.24
(1,1538)	1:571:A:GLU:H	1:628:A:LEU:HD12	12	0.24
(1,1535)	1:572:A:GLN:H	1:573:A:LEU:HD12	5	0.24
(1,1520)	1:577:A:LEU:H	1:574:A:PRO:HB2	6	0.24
(1,1503)	1:582:A:ALA:H	1:581:A:GLU:HB2	1	0.24
(1,1503)	1:582:A:ALA:H	1:581:A:GLU:HB2	2	0.24
(1,1503)	1:582:A:ALA:H	1:581:A:GLU:HB2	8	0.24
(1,1503)	1:582:A:ALA:H	1:581:A:GLU:HB2	10	0.24
(1,1503)	1:582:A:ALA:H	1:581:A:GLU:HB2	14	0.24
(1,1491)	1:585:A:GLU:H	1:584:A:LEU:HG	3	0.24
(1,1491)	1:585:A:GLU:H	1:584:A:LEU:HG	4	0.24
(1,1491)	1:585:A:GLU:H	1:584:A:LEU:HG	9	0.24
(1,1474)	1:589:A:THR:H	1:586:A:ALA:HA	14	0.24
(1,1459)	1:593:A:ASP:H	1:594:A:ALA:H	10	0.24
(1,1459)	1:593:A:ASP:H	1:594:A:ALA:H	17	0.24
(1,1457)	1:597:A:PHE:H	1:598:A:SER:HB2	2	0.24
(1,1456)	1:597:A:PHE:H	1:595:A:SER:HA	8	0.24
(1,1443)	1:564:A:TYR:HE1	1:564:A:TYR:HA	11	0.24
(1,1431)	1:622:A:PHE:HE2	1:618:A:LEU:HD23	12	0.24
(1,1431)	1:622:A:PHE:HE2	1:618:A:LEU:HD23	13	0.24
(1,1422)	1:627:A:TYR:HD1	1:631:A:LEU:HD13	2	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1422)	1:627:A:TYR:HD1	1:631:A:LEU:HD12	9	0.24
(1,1422)	1:627:A:TYR:HD1	1:631:A:LEU:HD13	17	0.24
(1,1422)	1:627:A:TYR:HD1	1:631:A:LEU:HD11	20	0.24
(1,1420)	1:627:A:TYR:HE1	1:631:A:LEU:HD21	19	0.24
(1,1418)	1:596:A:PHE:HE2	1:591:A:VAL:HG21	8	0.24
(1,1405)	1:606:A:LYS:HD2	1:607:A:VAL:HG21	11	0.24
(1,1401)	1:606:A:LYS:HB3	1:606:A:LYS:HE3	4	0.24
(1,1384)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	10	0.24
(1,1378)	1:624:A:ARG:HD3	1:573:A:LEU:HD12	13	0.24
(1,1369)	1:591:A:VAL:HG22	1:596:A:PHE:HB2	2	0.24
(1,1325)	1:628:A:LEU:HD12	1:569:A:GLU:HA	3	0.24
(1,1323)	1:576:A:LEU:HA	1:576:A:LEU:HD22	12	0.24
(1,1250)	1:626:A:GLU:HG2	1:623:A:GLU:HA	9	0.24
(1,1210)	1:606:A:LYS:HA	1:605:A:GLN:HB3	1	0.24
(1,1165)	1:601:A:HIS:HB2	1:605:A:GLN:HG2	10	0.24
(1,1164)	1:601:A:HIS:HB3	1:605:A:GLN:HG2	16	0.24
(1,1162)	1:600:A:PRO:HD3	1:599:A:GLN:HG2	17	0.24
(1,1062)	1:610:A:ASP:HB2	1:587:A:LEU:HD21	14	0.24
(1,1062)	1:610:A:ASP:HB2	1:587:A:LEU:HD23	18	0.24
(1,1016)	1:588:A:GLN:HG2	1:584:A:LEU:HG	11	0.24
(1,1009)	1:603:A:GLN:HG2	1:599:A:GLN:HB3	6	0.24
(1,991)	1:611:A:MET:HG3	1:587:A:LEU:HD12	13	0.24
(1,985)	1:591:A:VAL:HB	1:608:A:LEU:HD23	6	0.24
(1,972)	1:629:A:GLU:HB2	1:570:A:LEU:HD13	1	0.24
(1,972)	1:629:A:GLU:HB2	1:570:A:LEU:HD12	13	0.24
(1,851)	1:604:A:THR:HA	1:608:A:LEU:HD12	4	0.24
(1,850)	1:604:A:THR:HA	1:607:A:VAL:HG12	10	0.24
(1,820)	1:601:A:HIS:HA	1:605:A:GLN:HB2	6	0.24
(1,774)	1:610:A:ASP:HA	1:587:A:LEU:HD13	17	0.24
(1,774)	1:610:A:ASP:HA	1:587:A:LEU:HD13	19	0.24
(1,750)	1:604:A:THR:HG22	1:599:A:GLN:HA	19	0.24
(1,717)	1:621:A:ALA:HB3	1:577:A:LEU:HD22	1	0.24
(1,712)	1:594:A:ALA:HB1	1:593:A:ASP:HA	4	0.24
(1,665)	1:631:A:LEU:HD21	1:631:A:LEU:HA	4	0.24
(1,665)	1:631:A:LEU:HD21	1:631:A:LEU:HA	15	0.24
(1,665)	1:631:A:LEU:HD22	1:631:A:LEU:HA	20	0.24
(1,642)	1:604:A:THR:HG23	1:596:A:PHE:HA	19	0.24
(1,585)	1:596:A:PHE:HZ	1:607:A:VAL:HG11	15	0.24
(1,558)	1:564:A:TYR:HE2	1:568:A:ARG:HB2	20	0.24
(1,554)	1:627:A:TYR:HE2	1:628:A:LEU:HD21	3	0.24
(1,554)	1:627:A:TYR:HE2	1:628:A:LEU:HD23	12	0.24
(1,552)	1:596:A:PHE:HD1	1:607:A:VAL:HG23	2	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,552)	1:596:A:PHE:HD1	1:607:A:VAL:HG23	11	0.24
(1,552)	1:596:A:PHE:HD1	1:607:A:VAL:HG21	14	0.24
(1,545)	1:577:A:LEU:HD22	1:577:A:LEU:HD21	1	0.24
(1,545)	1:577:A:LEU:HD21	1:577:A:LEU:HD23	2	0.24
(1,545)	1:577:A:LEU:HD21	1:577:A:LEU:HD23	3	0.24
(1,545)	1:577:A:LEU:HD22	1:577:A:LEU:HD23	4	0.24
(1,545)	1:577:A:LEU:HD22	1:577:A:LEU:HD21	5	0.24
(1,545)	1:577:A:LEU:HD22	1:577:A:LEU:HD23	6	0.24
(1,545)	1:577:A:LEU:HD21	1:577:A:LEU:HD23	8	0.24
(1,545)	1:577:A:LEU:HD21	1:577:A:LEU:HD23	9	0.24
(1,545)	1:577:A:LEU:HD22	1:577:A:LEU:HD23	10	0.24
(1,545)	1:577:A:LEU:HD22	1:577:A:LEU:HD21	11	0.24
(1,545)	1:577:A:LEU:HD22	1:577:A:LEU:HD23	12	0.24
(1,545)	1:577:A:LEU:HD22	1:577:A:LEU:HD21	13	0.24
(1,545)	1:577:A:LEU:HD22	1:577:A:LEU:HD23	14	0.24
(1,545)	1:577:A:LEU:HD21	1:577:A:LEU:HD23	15	0.24
(1,545)	1:577:A:LEU:HD22	1:577:A:LEU:HD23	16	0.24
(1,545)	1:577:A:LEU:HD22	1:577:A:LEU:HD21	17	0.24
(1,545)	1:577:A:LEU:HD22	1:577:A:LEU:HD23	18	0.24
(1,545)	1:577:A:LEU:HD22	1:577:A:LEU:HD23	19	0.24
(1,545)	1:577:A:LEU:HD22	1:577:A:LEU:HD23	20	0.24
(1,542)	1:625:A:TRP:HE1	1:629:A:GLU:HG3	18	0.24
(1,369)	1:609:A:ALA:H	1:608:A:LEU:HD12	4	0.24
(1,369)	1:609:A:ALA:H	1:608:A:LEU:HD11	18	0.24
(1,339)	1:605:A:GLN:H	1:604:A:THR:HG21	4	0.24
(1,339)	1:605:A:GLN:H	1:604:A:THR:HG23	12	0.24
(1,339)	1:605:A:GLN:H	1:604:A:THR:HG21	18	0.24
(1,65)	1:595:A:SER:H	1:593:A:ASP:HB3	3	0.24
(1,2163)	1:567:A:GLN:HA	1:570:A:LEU:HD11	17	0.23
(1,2151)	1:628:A:LEU:HB3	1:625:A:TRP:HA	10	0.23
(1,2146)	1:615:A:GLU:HG2	1:584:A:LEU:HG	4	0.23
(1,2146)	1:615:A:GLU:HG2	1:584:A:LEU:HG	16	0.23
(1,2135)	1:567:A:GLN:HA	1:570:A:LEU:HD11	17	0.23
(1,2124)	1:612:A:ALA:HA	1:611:A:MET:HE3	18	0.23
(1,2109)	1:608:A:LEU:HD11	1:591:A:VAL:HG11	14	0.23
(1,2027)	1:564:A:TYR:HB3	1:567:A:GLN:HB2	2	0.23
(1,2027)	1:564:A:TYR:HB3	1:567:A:GLN:HB2	7	0.23
(1,2027)	1:564:A:TYR:HB3	1:567:A:GLN:HB2	14	0.23
(1,1961)	1:610:A:ASP:HB3	1:587:A:LEU:HB3	9	0.23
(1,1951)	1:615:A:GLU:HG2	1:584:A:LEU:HG	4	0.23
(1,1951)	1:615:A:GLU:HG2	1:584:A:LEU:HG	16	0.23
(1,1940)	1:620:A:GLN:HG2	1:621:A:ALA:HB2	9	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1907)	1:591:A:VAL:HA	1:608:A:LEU:HD21	2	0.23
(1,1895)	1:570:A:LEU:HG	1:573:A:LEU:HB2	6	0.23
(1,1874)	1:632:A:LYS:HG2	1:562:A:LEU:HD23	13	0.23
(1,1874)	1:632:A:LYS:HG2	1:562:A:LEU:HD22	19	0.23
(1,1853)	1:554:A:THR:HB	1:555:A:VAL:HG23	9	0.23
(1,1806)	1:577:A:LEU:HA	1:581:A:GLU:HB2	5	0.23
(1,1796)	1:580:A:LEU:HA	1:580:A:LEU:HD22	13	0.23
(1,1796)	1:580:A:LEU:HA	1:580:A:LEU:HD22	14	0.23
(1,1789)	1:556:A:LYS:HA	1:555:A:VAL:HG11	1	0.23
(1,1759)	1:609:A:ALA:HB3	1:605:A:GLN:HA	9	0.23
(1,1736)	1:607:A:VAL:HG11	1:608:A:LEU:HG	10	0.23
(1,1731)	1:607:A:VAL:HG22	1:603:A:GLN:HB3	20	0.23
(1,1719)	1:604:A:THR:HG21	1:599:A:GLN:HG2	17	0.23
(1,1706)	1:625:A:TRP:HD1	1:628:A:LEU:HB2	6	0.23
(1,1706)	1:625:A:TRP:HD1	1:628:A:LEU:HB2	16	0.23
(1,1693)	1:627:A:TYR:HD1	1:631:A:LEU:HD12	4	0.23
(1,1693)	1:627:A:TYR:HD1	1:631:A:LEU:HD13	6	0.23
(1,1693)	1:627:A:TYR:HD1	1:631:A:LEU:HD13	8	0.23
(1,1693)	1:627:A:TYR:HD1	1:631:A:LEU:HD13	15	0.23
(1,1670)	1:633:A:ASN:H	1:631:A:LEU:HB2	11	0.23
(1,1635)	1:623:A:GLU:H	1:622:A:PHE:HD1	12	0.23
(1,1608)	1:616:A:GLN:H	1:612:A:ALA:HA	9	0.23
(1,1594)	1:614:A:ALA:H	1:615:A:GLU:HG3	14	0.23
(1,1591)	1:583:A:LYS:H	1:583:A:LYS:HG3	7	0.23
(1,1591)	1:583:A:LYS:H	1:583:A:LYS:HG3	12	0.23
(1,1591)	1:583:A:LYS:H	1:583:A:LYS:HG3	18	0.23
(1,1577)	1:609:A:ALA:H	1:608:A:LEU:HG	15	0.23
(1,1569)	1:607:A:VAL:H	1:608:A:LEU:HD22	8	0.23
(1,1568)	1:607:A:VAL:H	1:606:A:LYS:HG2	15	0.23
(1,1568)	1:607:A:VAL:H	1:606:A:LYS:HG2	16	0.23
(1,1563)	1:605:A:GLN:H	1:605:A:GLN:HE22	9	0.23
(1,1546)	1:568:A:ARG:H	1:567:A:GLN:HG3	12	0.23
(1,1520)	1:577:A:LEU:H	1:574:A:PRO:HB2	20	0.23
(1,1509)	1:581:A:GLU:H	1:580:A:LEU:HG	13	0.23
(1,1503)	1:582:A:ALA:H	1:581:A:GLU:HB2	4	0.23
(1,1503)	1:582:A:ALA:H	1:581:A:GLU:HB2	11	0.23
(1,1503)	1:582:A:ALA:H	1:581:A:GLU:HB2	17	0.23
(1,1503)	1:582:A:ALA:H	1:581:A:GLU:HB2	18	0.23
(1,1491)	1:585:A:GLU:H	1:584:A:LEU:HG	12	0.23
(1,1491)	1:585:A:GLU:H	1:584:A:LEU:HG	15	0.23
(1,1484)	1:587:A:LEU:H	1:588:A:GLN:HG2	3	0.23
(1,1474)	1:589:A:THR:H	1:586:A:ALA:HA	17	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1461)	1:593:A:ASP:H	1:591:A:VAL:H	1	0.23
(1,1459)	1:593:A:ASP:H	1:594:A:ALA:H	4	0.23
(1,1459)	1:593:A:ASP:H	1:594:A:ALA:H	5	0.23
(1,1459)	1:593:A:ASP:H	1:594:A:ALA:H	6	0.23
(1,1443)	1:564:A:TYR:HE1	1:564:A:TYR:HA	8	0.23
(1,1443)	1:564:A:TYR:HE1	1:564:A:TYR:HA	12	0.23
(1,1430)	1:596:A:PHE:HD2	1:608:A:LEU:HD22	9	0.23
(1,1430)	1:596:A:PHE:HD2	1:608:A:LEU:HD21	13	0.23
(1,1430)	1:596:A:PHE:HD2	1:608:A:LEU:HD23	15	0.23
(1,1430)	1:596:A:PHE:HD2	1:608:A:LEU:HD22	18	0.23
(1,1422)	1:627:A:TYR:HD1	1:631:A:LEU:HD11	5	0.23
(1,1422)	1:627:A:TYR:HD1	1:631:A:LEU:HD13	11	0.23
(1,1422)	1:627:A:TYR:HD1	1:631:A:LEU:HD13	18	0.23
(1,1422)	1:627:A:TYR:HD1	1:631:A:LEU:HD13	19	0.23
(1,1420)	1:627:A:TYR:HE1	1:631:A:LEU:HD21	1	0.23
(1,1420)	1:627:A:TYR:HE1	1:631:A:LEU:HD22	6	0.23
(1,1420)	1:627:A:TYR:HE1	1:631:A:LEU:HD21	7	0.23
(1,1420)	1:627:A:TYR:HE1	1:631:A:LEU:HD23	10	0.23
(1,1412)	1:584:A:LEU:HD21	1:615:A:GLU:HB2	10	0.23
(1,1402)	1:606:A:LYS:HB2	1:606:A:LYS:HE2	14	0.23
(1,1401)	1:606:A:LYS:HB3	1:606:A:LYS:HE2	19	0.23
(1,1398)	1:587:A:LEU:HD22	1:583:A:LYS:HG2	12	0.23
(1,1398)	1:587:A:LEU:HD22	1:583:A:LYS:HG2	14	0.23
(1,1384)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	2	0.23
(1,1378)	1:624:A:ARG:HD3	1:573:A:LEU:HD13	17	0.23
(1,1374)	1:577:A:LEU:HD11	1:625:A:TRP:HB3	2	0.23
(1,1370)	1:604:A:THR:HG23	1:607:A:VAL:HB	3	0.23
(1,1335)	1:566:A:LEU:HG	1:562:A:LEU:HD23	9	0.23
(1,1333)	1:573:A:LEU:HD11	1:624:A:ARG:HD2	3	0.23
(1,1262)	1:570:A:LEU:HB3	1:567:A:GLN:HA	10	0.23
(1,1218)	1:606:A:LYS:HD3	1:606:A:LYS:HA	5	0.23
(1,1210)	1:606:A:LYS:HA	1:605:A:GLN:HB2	8	0.23
(1,1152)	1:565:A:LYS:HB2	1:565:A:LYS:HE3	3	0.23
(1,1063)	1:610:A:ASP:HB2	1:587:A:LEU:HD11	7	0.23
(1,1056)	1:622:A:PHE:HB2	1:577:A:LEU:HD21	4	0.23
(1,1056)	1:622:A:PHE:HB2	1:577:A:LEU:HD21	18	0.23
(1,1040)	1:629:A:GLU:HG3	1:570:A:LEU:HD13	16	0.23
(1,1024)	1:590:A:GLN:HG3	1:589:A:THR:HG21	11	0.23
(1,1019)	1:604:A:THR:HG21	1:599:A:GLN:HG2	17	0.23
(1,990)	1:591:A:VAL:HG21	1:611:A:MET:HG2	19	0.23
(1,985)	1:591:A:VAL:HB	1:608:A:LEU:HD21	15	0.23
(1,850)	1:604:A:THR:HA	1:607:A:VAL:HG12	16	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,850)	1:604:A:THR:HA	1:607:A:VAL:HG13	18	0.23
(1,820)	1:601:A:HIS:HA	1:605:A:GLN:HB2	7	0.23
(1,820)	1:601:A:HIS:HA	1:605:A:GLN:HB2	11	0.23
(1,745)	1:562:A:LEU:HA	1:562:A:LEU:HD21	5	0.23
(1,745)	1:562:A:LEU:HA	1:562:A:LEU:HD23	11	0.23
(1,745)	1:562:A:LEU:HA	1:562:A:LEU:HD21	19	0.23
(1,665)	1:631:A:LEU:HD21	1:631:A:LEU:HA	12	0.23
(1,665)	1:631:A:LEU:HD21	1:631:A:LEU:HA	17	0.23
(1,621)	1:577:A:LEU:HD23	1:573:A:LEU:HA	6	0.23
(1,621)	1:577:A:LEU:HD22	1:573:A:LEU:HA	8	0.23
(1,599)	1:601:A:HIS:HD2	1:602:A:GLU:HG3	3	0.23
(1,596)	1:564:A:TYR:HD2	1:564:A:TYR:HA	3	0.23
(1,586)	1:625:A:TRP:HD1	1:577:A:LEU:HD21	10	0.23
(1,585)	1:596:A:PHE:HZ	1:607:A:VAL:HG13	8	0.23
(1,585)	1:596:A:PHE:HZ	1:607:A:VAL:HG12	9	0.23
(1,554)	1:627:A:TYR:HE2	1:628:A:LEU:HD22	7	0.23
(1,552)	1:596:A:PHE:HD1	1:607:A:VAL:HG22	10	0.23
(1,552)	1:596:A:PHE:HD1	1:607:A:VAL:HG22	13	0.23
(1,550)	1:596:A:PHE:HD1	1:604:A:THR:HG22	7	0.23
(1,507)	1:629:A:GLU:H	1:570:A:LEU:HD23	13	0.23
(1,307)	1:566:A:LEU:H	1:566:A:LEU:HD11	11	0.23
(1,249)	1:573:A:LEU:H	1:573:A:LEU:HG	1	0.23
(1,248)	1:573:A:LEU:H	1:572:A:GLN:HB2	2	0.23
(1,173)	1:612:A:ALA:H	1:611:A:MET:HB2	9	0.23
(1,173)	1:612:A:ALA:H	1:611:A:MET:HB2	11	0.23
(1,173)	1:612:A:ALA:H	1:611:A:MET:HB2	20	0.23
(1,162)	1:584:A:LEU:H	1:583:A:LYS:HG3	9	0.23
(1,58)	1:596:A:PHE:H	1:594:A:ALA:HB1	3	0.23
(1,18)	1:599:A:GLN:H	1:596:A:PHE:HD1	9	0.23
(1,2146)	1:615:A:GLU:HG2	1:584:A:LEU:HG	1	0.22
(1,2124)	1:612:A:ALA:HA	1:611:A:MET:HE1	2	0.22
(1,2105)	1:566:A:LEU:HD21	1:628:A:LEU:HG	18	0.22
(1,2092)	1:562:A:LEU:HD12	1:570:A:LEU:HB2	1	0.22
(1,2034)	1:618:A:LEU:HG	1:615:A:GLU:HA	5	0.22
(1,2027)	1:564:A:TYR:HB3	1:567:A:GLN:HB2	15	0.22
(1,1995)	1:557:A:ARG:HD2	1:555:A:VAL:HG12	19	0.22
(1,1987)	1:614:A:ALA:HB2	1:587:A:LEU:HB2	16	0.22
(1,1986)	1:568:A:ARG:HD3	1:567:A:GLN:HG3	18	0.22
(1,1959)	1:622:A:PHE:HB2	1:619:A:GLU:HB2	17	0.22
(1,1957)	1:622:A:PHE:HB2	1:619:A:GLU:HB2	17	0.22
(1,1951)	1:615:A:GLU:HG2	1:584:A:LEU:HG	1	0.22
(1,1940)	1:620:A:GLN:HG2	1:621:A:ALA:HB2	13	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1937)	1:616:A:GLN:HG3	1:613:A:ALA:HB1	9	0.22
(1,1937)	1:616:A:GLN:HG3	1:613:A:ALA:HB1	10	0.22
(1,1920)	1:613:A:ALA:HB2	1:617:A:GLU:HB2	17	0.22
(1,1895)	1:618:A:LEU:HG	1:619:A:GLU:HB3	8	0.22
(1,1894)	1:576:A:LEU:HG	1:617:A:GLU:HG3	3	0.22
(1,1867)	1:564:A:TYR:HA	1:567:A:GLN:HA	19	0.22
(1,1828)	1:601:A:HIS:HA	1:602:A:GLU:HG2	15	0.22
(1,1795)	1:579:A:ASP:HA	1:583:A:LYS:HB2	10	0.22
(1,1779)	1:614:A:ALA:HA	1:580:A:LEU:HD12	20	0.22
(1,1778)	1:612:A:ALA:HA	1:584:A:LEU:HD22	19	0.22
(1,1756)	1:614:A:ALA:HB2	1:587:A:LEU:HB2	16	0.22
(1,1749)	1:613:A:ALA:HB2	1:617:A:GLU:HB2	17	0.22
(1,1736)	1:607:A:VAL:HG13	1:608:A:LEU:HG	11	0.22
(1,1718)	1:604:A:THR:HG22	1:599:A:GLN:HG3	11	0.22
(1,1709)	1:625:A:TRP:HD1	1:573:A:LEU:HB2	3	0.22
(1,1709)	1:625:A:TRP:HD1	1:573:A:LEU:HB2	12	0.22
(1,1706)	1:625:A:TRP:HD1	1:628:A:LEU:HB2	17	0.22
(1,1700)	1:622:A:PHE:HZ	1:618:A:LEU:HD12	6	0.22
(1,1700)	1:622:A:PHE:HZ	1:618:A:LEU:HD11	10	0.22
(1,1700)	1:622:A:PHE:HZ	1:618:A:LEU:HD13	18	0.22
(1,1698)	1:564:A:TYR:HD1	1:567:A:GLN:HB2	10	0.22
(1,1689)	1:596:A:PHE:HD1	1:599:A:GLN:HG3	7	0.22
(1,1683)	1:622:A:PHE:HE2	1:618:A:LEU:HD21	1	0.22
(1,1625)	1:620:A:GLN:H	1:621:A:ALA:HB1	8	0.22
(1,1608)	1:616:A:GLN:H	1:612:A:ALA:HA	12	0.22
(1,1591)	1:583:A:LYS:H	1:583:A:LYS:HG3	4	0.22
(1,1591)	1:583:A:LYS:H	1:583:A:LYS:HG3	13	0.22
(1,1577)	1:609:A:ALA:H	1:608:A:LEU:HG	1	0.22
(1,1577)	1:609:A:ALA:H	1:608:A:LEU:HG	4	0.22
(1,1577)	1:609:A:ALA:H	1:608:A:LEU:HG	17	0.22
(1,1568)	1:607:A:VAL:H	1:606:A:LYS:HG2	13	0.22
(1,1567)	1:607:A:VAL:H	1:606:A:LYS:HB2	5	0.22
(1,1567)	1:607:A:VAL:H	1:606:A:LYS:HB2	11	0.22
(1,1565)	1:607:A:VAL:H	1:610:A:ASP:HB2	17	0.22
(1,1549)	1:567:A:GLN:H	1:563:A:SER:HB3	18	0.22
(1,1546)	1:568:A:ARG:H	1:567:A:GLN:HG3	11	0.22
(1,1515)	1:579:A:ASP:H	1:576:A:LEU:HD11	11	0.22
(1,1503)	1:582:A:ALA:H	1:581:A:GLU:HB2	6	0.22
(1,1503)	1:582:A:ALA:H	1:581:A:GLU:HB2	12	0.22
(1,1503)	1:582:A:ALA:H	1:581:A:GLU:HB2	13	0.22
(1,1491)	1:585:A:GLU:H	1:584:A:LEU:HG	7	0.22
(1,1487)	1:587:A:LEU:H	1:587:A:LEU:HD21	16	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1461)	1:593:A:ASP:H	1:591:A:VAL:H	4	0.22
(1,1459)	1:593:A:ASP:H	1:594:A:ALA:H	12	0.22
(1,1459)	1:593:A:ASP:H	1:594:A:ALA:H	16	0.22
(1,1422)	1:627:A:TYR:HD1	1:631:A:LEU:HD13	1	0.22
(1,1422)	1:627:A:TYR:HD1	1:631:A:LEU:HD11	7	0.22
(1,1422)	1:627:A:TYR:HD1	1:631:A:LEU:HD13	13	0.22
(1,1422)	1:627:A:TYR:HD1	1:631:A:LEU:HD13	14	0.22
(1,1420)	1:627:A:TYR:HE1	1:631:A:LEU:HD21	2	0.22
(1,1402)	1:606:A:LYS:HB2	1:606:A:LYS:HE3	9	0.22
(1,1391)	1:614:A:ALA:HA	1:583:A:LYS:HE3	1	0.22
(1,1384)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	20	0.22
(1,1382)	1:573:A:LEU:HD12	1:624:A:ARG:HG2	15	0.22
(1,1370)	1:604:A:THR:HG22	1:607:A:VAL:HB	18	0.22
(1,1365)	1:631:A:LEU:HD21	1:566:A:LEU:HD12	13	0.22
(1,1363)	1:562:A:LEU:HD23	1:631:A:LEU:HB2	11	0.22
(1,1325)	1:628:A:LEU:HD13	1:569:A:GLU:HA	9	0.22
(1,1210)	1:606:A:LYS:HA	1:605:A:GLN:HB2	2	0.22
(1,1210)	1:606:A:LYS:HA	1:605:A:GLN:HB2	18	0.22
(1,1190)	1:562:A:LEU:HB3	1:632:A:LYS:HA	16	0.22
(1,1136)	1:600:A:PRO:HD3	1:603:A:GLN:HB3	16	0.22
(1,1136)	1:600:A:PRO:HD3	1:603:A:GLN:HB2	19	0.22
(1,1061)	1:610:A:ASP:HB3	1:607:A:VAL:HG12	6	0.22
(1,1020)	1:604:A:THR:HG22	1:599:A:GLN:HG3	11	0.22
(1,998)	1:583:A:LYS:HB3	1:587:A:LEU:HD12	2	0.22
(1,990)	1:591:A:VAL:HG23	1:611:A:MET:HG2	2	0.22
(1,985)	1:591:A:VAL:HB	1:608:A:LEU:HD21	16	0.22
(1,928)	1:583:A:LYS:HG3	1:587:A:LEU:HD22	14	0.22
(1,859)	1:604:A:THR:HB	1:608:A:LEU:HD22	7	0.22
(1,820)	1:601:A:HIS:HA	1:605:A:GLN:HB2	15	0.22
(1,810)	1:608:A:LEU:HA	1:608:A:LEU:HD11	9	0.22
(1,805)	1:629:A:GLU:HA	1:570:A:LEU:HD21	3	0.22
(1,774)	1:610:A:ASP:HA	1:587:A:LEU:HD11	4	0.22
(1,717)	1:621:A:ALA:HB2	1:577:A:LEU:HD22	2	0.22
(1,712)	1:594:A:ALA:HB2	1:593:A:ASP:HA	19	0.22
(1,665)	1:631:A:LEU:HD21	1:631:A:LEU:HA	3	0.22
(1,665)	1:631:A:LEU:HD23	1:631:A:LEU:HA	11	0.22
(1,658)	1:591:A:VAL:HG22	1:596:A:PHE:HB3	2	0.22
(1,658)	1:591:A:VAL:HG23	1:596:A:PHE:HB3	19	0.22
(1,650)	1:591:A:VAL:HG13	1:588:A:GLN:HA	1	0.22
(1,642)	1:604:A:THR:HG23	1:596:A:PHE:HA	3	0.22
(1,621)	1:577:A:LEU:HD23	1:573:A:LEU:HA	18	0.22
(1,603)	1:622:A:PHE:HD1	1:626:A:GLU:HG2	12	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,602)	1:597:A:PHE:HZ	1:608:A:LEU:HD13	4	0.22
(1,602)	1:597:A:PHE:HZ	1:608:A:LEU:HD11	11	0.22
(1,585)	1:596:A:PHE:HZ	1:607:A:VAL:HG11	7	0.22
(1,554)	1:627:A:TYR:HE2	1:628:A:LEU:HD23	14	0.22
(1,552)	1:596:A:PHE:HD1	1:607:A:VAL:HG23	5	0.22
(1,552)	1:596:A:PHE:HD1	1:607:A:VAL:HG22	6	0.22
(1,544)	1:625:A:TRP:HE1	1:570:A:LEU:HD13	16	0.22
(1,429)	1:618:A:LEU:H	1:617:A:GLU:HB2	13	0.22
(1,339)	1:605:A:GLN:H	1:604:A:THR:HG23	8	0.22
(1,162)	1:584:A:LEU:H	1:583:A:LYS:HG3	15	0.22
(1,162)	1:584:A:LEU:H	1:583:A:LYS:HG3	18	0.22
(1,110)	1:590:A:GLN:H	1:590:A:GLN:HG3	10	0.22
(1,58)	1:596:A:PHE:H	1:594:A:ALA:HB3	1	0.22
(1,2167)	1:606:A:LYS:HB3	1:606:A:LYS:HE3	7	0.21
(1,2167)	1:606:A:LYS:HB3	1:606:A:LYS:HE3	13	0.21
(1,2146)	1:615:A:GLU:HG2	1:584:A:LEU:HG	9	0.21
(1,2085)	1:580:A:LEU:HD22	1:617:A:GLU:HG3	19	0.21
(1,1978)	1:632:A:LYS:HE2	1:570:A:LEU:HD21	12	0.21
(1,1959)	1:622:A:PHE:HB2	1:619:A:GLU:HB2	20	0.21
(1,1957)	1:622:A:PHE:HB2	1:619:A:GLU:HB2	20	0.21
(1,1951)	1:615:A:GLU:HG2	1:584:A:LEU:HG	9	0.21
(1,1950)	1:615:A:GLU:HG3	1:612:A:ALA:HB3	1	0.21
(1,1937)	1:616:A:GLN:HG3	1:613:A:ALA:HB2	19	0.21
(1,1933)	1:611:A:MET:HB2	1:584:A:LEU:HD23	11	0.21
(1,1911)	1:581:A:GLU:HB3	1:618:A:LEU:HD13	6	0.21
(1,1907)	1:591:A:VAL:HA	1:608:A:LEU:HD22	6	0.21
(1,1907)	1:591:A:VAL:HA	1:608:A:LEU:HD23	17	0.21
(1,1901)	1:613:A:ALA:HB2	1:616:A:GLN:HB2	15	0.21
(1,1855)	1:572:A:GLN:HA	1:571:A:GLU:HA	2	0.21
(1,1845)	1:554:A:THR:HA	1:555:A:VAL:HG23	9	0.21
(1,1828)	1:601:A:HIS:HA	1:602:A:GLU:HG3	17	0.21
(1,1813)	1:588:A:GLN:HA	1:584:A:LEU:HD21	3	0.21
(1,1795)	1:579:A:ASP:HA	1:583:A:LYS:HB2	16	0.21
(1,1778)	1:612:A:ALA:HA	1:584:A:LEU:HD23	7	0.21
(1,1778)	1:612:A:ALA:HA	1:584:A:LEU:HD21	10	0.21
(1,1740)	1:628:A:LEU:HD21	1:631:A:LEU:HB2	4	0.21
(1,1736)	1:607:A:VAL:HG11	1:608:A:LEU:HG	2	0.21
(1,1736)	1:607:A:VAL:HG13	1:608:A:LEU:HG	7	0.21
(1,1731)	1:607:A:VAL:HG21	1:603:A:GLN:HB3	15	0.21
(1,1700)	1:622:A:PHE:HZ	1:618:A:LEU:HD13	19	0.21
(1,1693)	1:627:A:TYR:HD1	1:631:A:LEU:HD12	3	0.21
(1,1683)	1:622:A:PHE:HE2	1:618:A:LEU:HD23	19	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1682)	1:622:A:PHE:HD2	1:577:A:LEU:HD11	6	0.21
(1,1669)	1:633:A:ASN:H	1:631:A:LEU:HB3	10	0.21
(1,1633)	1:622:A:PHE:H	1:619:A:GLU:HB3	6	0.21
(1,1608)	1:616:A:GLN:H	1:612:A:ALA:HA	17	0.21
(1,1591)	1:583:A:LYS:H	1:583:A:LYS:HG3	15	0.21
(1,1577)	1:609:A:ALA:H	1:608:A:LEU:HG	10	0.21
(1,1577)	1:609:A:ALA:H	1:608:A:LEU:HG	14	0.21
(1,1569)	1:607:A:VAL:H	1:587:A:LEU:HD21	2	0.21
(1,1515)	1:579:A:ASP:H	1:576:A:LEU:HD12	4	0.21
(1,1509)	1:581:A:GLU:H	1:580:A:LEU:HG	11	0.21
(1,1509)	1:581:A:GLU:H	1:580:A:LEU:HG	14	0.21
(1,1503)	1:582:A:ALA:H	1:581:A:GLU:HB2	3	0.21
(1,1503)	1:582:A:ALA:H	1:581:A:GLU:HB2	9	0.21
(1,1491)	1:585:A:GLU:H	1:584:A:LEU:HG	17	0.21
(1,1487)	1:587:A:LEU:H	1:587:A:LEU:HD23	14	0.21
(1,1480)	1:588:A:GLN:H	1:586:A:ALA:HB1	12	0.21
(1,1459)	1:593:A:ASP:H	1:594:A:ALA:H	2	0.21
(1,1459)	1:593:A:ASP:H	1:594:A:ALA:H	8	0.21
(1,1459)	1:593:A:ASP:H	1:594:A:ALA:H	11	0.21
(1,1459)	1:593:A:ASP:H	1:594:A:ALA:H	14	0.21
(1,1456)	1:597:A:PHE:H	1:595:A:SER:HA	15	0.21
(1,1431)	1:622:A:PHE:HE2	1:618:A:LEU:HD21	1	0.21
(1,1431)	1:622:A:PHE:HE2	1:618:A:LEU:HD23	19	0.21
(1,1426)	1:627:A:TYR:HD2	1:628:A:LEU:HD23	15	0.21
(1,1422)	1:627:A:TYR:HD1	1:631:A:LEU:HD12	4	0.21
(1,1422)	1:627:A:TYR:HD1	1:631:A:LEU:HD13	6	0.21
(1,1422)	1:627:A:TYR:HD1	1:631:A:LEU:HD13	8	0.21
(1,1422)	1:627:A:TYR:HD1	1:631:A:LEU:HD13	15	0.21
(1,1412)	1:584:A:LEU:HD23	1:615:A:GLU:HB2	6	0.21
(1,1401)	1:606:A:LYS:HB3	1:606:A:LYS:HE3	7	0.21
(1,1401)	1:606:A:LYS:HB3	1:606:A:LYS:HE3	13	0.21
(1,1384)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	17	0.21
(1,1370)	1:604:A:THR:HG21	1:607:A:VAL:HB	5	0.21
(1,1365)	1:631:A:LEU:HD22	1:566:A:LEU:HD12	8	0.21
(1,1364)	1:628:A:LEU:HD21	1:631:A:LEU:HB2	4	0.21
(1,1363)	1:562:A:LEU:HD22	1:631:A:LEU:HB2	12	0.21
(1,1340)	1:573:A:LEU:HA	1:576:A:LEU:HG	18	0.21
(1,1328)	1:573:A:LEU:HD11	1:574:A:PRO:HD3	5	0.21
(1,1309)	1:573:A:LEU:HD23	1:576:A:LEU:HB2	16	0.21
(1,1265)	1:593:A:ASP:HB3	1:595:A:SER:HB2	8	0.21
(1,1265)	1:593:A:ASP:HB3	1:595:A:SER:HB2	17	0.21
(1,1244)	1:569:A:GLU:HG3	1:566:A:LEU:HA	11	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1210)	1:606:A:LYS:HA	1:605:A:GLN:HB3	15	0.21
(1,1170)	1:629:A:GLU:HG2	1:626:A:GLU:HA	6	0.21
(1,1164)	1:601:A:HIS:HB3	1:605:A:GLN:HG2	18	0.21
(1,1114)	1:567:A:GLN:HG2	1:562:A:LEU:HB2	2	0.21
(1,1063)	1:610:A:ASP:HB2	1:587:A:LEU:HD11	4	0.21
(1,1056)	1:622:A:PHE:HB2	1:577:A:LEU:HD23	11	0.21
(1,1040)	1:629:A:GLU:HG3	1:570:A:LEU:HD13	1	0.21
(1,1024)	1:590:A:GLN:HG3	1:589:A:THR:HG22	17	0.21
(1,1023)	1:590:A:GLN:HG3	1:587:A:LEU:HD23	10	0.21
(1,989)	1:611:A:MET:HG2	1:587:A:LEU:HD12	14	0.21
(1,956)	1:605:A:GLN:HB3	1:608:A:LEU:HD11	1	0.21
(1,938)	1:631:A:LEU:HG	1:562:A:LEU:HD22	16	0.21
(1,850)	1:604:A:THR:HA	1:607:A:VAL:HG12	4	0.21
(1,848)	1:622:A:PHE:HA	1:573:A:LEU:HD21	1	0.21
(1,820)	1:601:A:HIS:HA	1:605:A:GLN:HB2	5	0.21
(1,820)	1:601:A:HIS:HA	1:605:A:GLN:HB2	10	0.21
(1,774)	1:610:A:ASP:HA	1:587:A:LEU:HD13	16	0.21
(1,717)	1:621:A:ALA:HB3	1:577:A:LEU:HD22	9	0.21
(1,712)	1:594:A:ALA:HB2	1:593:A:ASP:HA	5	0.21
(1,712)	1:594:A:ALA:HB3	1:593:A:ASP:HA	8	0.21
(1,712)	1:594:A:ALA:HB1	1:593:A:ASP:HA	10	0.21
(1,665)	1:631:A:LEU:HD22	1:631:A:LEU:HA	14	0.21
(1,652)	1:591:A:VAL:HG11	1:608:A:LEU:HA	20	0.21
(1,650)	1:591:A:VAL:HG11	1:588:A:GLN:HA	8	0.21
(1,642)	1:604:A:THR:HG21	1:596:A:PHE:HA	5	0.21
(1,602)	1:597:A:PHE:HZ	1:608:A:LEU:HD11	14	0.21
(1,600)	1:601:A:HIS:HD2	1:602:A:GLU:HB3	13	0.21
(1,584)	1:625:A:TRP:HD1	1:570:A:LEU:HD22	14	0.21
(1,554)	1:627:A:TYR:HE2	1:628:A:LEU:HD22	1	0.21
(1,369)	1:609:A:ALA:H	1:608:A:LEU:HD13	6	0.21
(1,339)	1:605:A:GLN:H	1:604:A:THR:HG23	17	0.21
(1,273)	1:570:A:LEU:H	1:569:A:GLU:HB2	11	0.21
(1,248)	1:573:A:LEU:H	1:572:A:GLN:HB2	17	0.21
(1,248)	1:573:A:LEU:H	1:572:A:GLN:HB2	18	0.21
(1,173)	1:612:A:ALA:H	1:611:A:MET:HB2	2	0.21
(1,173)	1:612:A:ALA:H	1:611:A:MET:HB2	5	0.21
(1,173)	1:612:A:ALA:H	1:611:A:MET:HB2	6	0.21
(1,173)	1:612:A:ALA:H	1:611:A:MET:HB2	15	0.21
(1,173)	1:612:A:ALA:H	1:611:A:MET:HB2	19	0.21
(1,162)	1:584:A:LEU:H	1:583:A:LYS:HG3	7	0.21
(1,162)	1:584:A:LEU:H	1:583:A:LYS:HG3	11	0.21
(1,18)	1:599:A:GLN:H	1:596:A:PHE:HD2	5	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2167)	1:606:A:LYS:HB3	1:606:A:LYS:HE3	2	0.2
(1,2167)	1:606:A:LYS:HB3	1:606:A:LYS:HE3	6	0.2
(1,2167)	1:606:A:LYS:HB3	1:606:A:LYS:HE3	8	0.2
(1,2146)	1:615:A:GLU:HG2	1:584:A:LEU:HG	2	0.2
(1,2124)	1:612:A:ALA:HA	1:611:A:MET:HE3	7	0.2
(1,2092)	1:567:A:GLN:HB3	1:562:A:LEU:HD12	16	0.2
(1,2056)	1:572:A:GLN:HG3	1:569:A:GLU:HA	9	0.2
(1,2043)	1:583:A:LYS:HD2	1:583:A:LYS:HA	2	0.2
(1,2027)	1:564:A:TYR:HB3	1:567:A:GLN:HB2	3	0.2
(1,2027)	1:564:A:TYR:HB3	1:567:A:GLN:HB2	9	0.2
(1,1951)	1:615:A:GLU:HG2	1:584:A:LEU:HG	2	0.2
(1,1940)	1:572:A:GLN:HG2	1:568:A:ARG:HG2	15	0.2
(1,1926)	1:632:A:LYS:HB3	1:562:A:LEU:HD23	18	0.2
(1,1920)	1:613:A:ALA:HB1	1:617:A:GLU:HB2	9	0.2
(1,1911)	1:581:A:GLU:HB3	1:618:A:LEU:HD11	20	0.2
(1,1907)	1:591:A:VAL:HA	1:608:A:LEU:HD22	10	0.2
(1,1900)	1:567:A:GLN:HB3	1:562:A:LEU:HD12	16	0.2
(1,1894)	1:576:A:LEU:HG	1:617:A:GLU:HG3	13	0.2
(1,1874)	1:632:A:LYS:HG2	1:562:A:LEU:HD21	8	0.2
(1,1867)	1:564:A:TYR:HA	1:567:A:GLN:HA	4	0.2
(1,1828)	1:601:A:HIS:HA	1:602:A:GLU:HG3	1	0.2
(1,1795)	1:579:A:ASP:HA	1:583:A:LYS:HB2	5	0.2
(1,1779)	1:614:A:ALA:HA	1:580:A:LEU:HD11	5	0.2
(1,1778)	1:612:A:ALA:HA	1:584:A:LEU:HD22	5	0.2
(1,1763)	1:621:A:ALA:HB1	1:617:A:GLU:HG2	16	0.2
(1,1749)	1:613:A:ALA:HB1	1:617:A:GLU:HB2	9	0.2
(1,1723)	1:591:A:VAL:HG13	1:611:A:MET:HG3	14	0.2
(1,1718)	1:604:A:THR:HG21	1:599:A:GLN:HG3	7	0.2
(1,1718)	1:604:A:THR:HG22	1:599:A:GLN:HG3	10	0.2
(1,1718)	1:604:A:THR:HG21	1:599:A:GLN:HG3	18	0.2
(1,1706)	1:625:A:TRP:HD1	1:628:A:LEU:HB2	4	0.2
(1,1706)	1:625:A:TRP:HD1	1:628:A:LEU:HB2	7	0.2
(1,1694)	1:564:A:TYR:HD2	1:568:A:ARG:HG3	7	0.2
(1,1682)	1:622:A:PHE:HD2	1:577:A:LEU:HD13	3	0.2
(1,1670)	1:633:A:ASN:H	1:631:A:LEU:HB2	14	0.2
(1,1608)	1:616:A:GLN:H	1:612:A:ALA:HA	2	0.2
(1,1608)	1:616:A:GLN:H	1:612:A:ALA:HA	3	0.2
(1,1608)	1:616:A:GLN:H	1:612:A:ALA:HA	6	0.2
(1,1591)	1:583:A:LYS:H	1:583:A:LYS:HG3	9	0.2
(1,1577)	1:609:A:ALA:H	1:608:A:LEU:HG	12	0.2
(1,1568)	1:607:A:VAL:H	1:606:A:LYS:HG2	8	0.2
(1,1549)	1:567:A:GLN:H	1:563:A:SER:HB3	16	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1546)	1:568:A:ARG:H	1:567:A:GLN:HG3	8	0.2
(1,1535)	1:572:A:GLN:H	1:573:A:LEU:HD12	8	0.2
(1,1533)	1:572:A:GLN:H	1:571:A:GLU:HB2	2	0.2
(1,1530)	1:573:A:LEU:H	1:572:A:GLN:HB3	10	0.2
(1,1515)	1:579:A:ASP:H	1:576:A:LEU:HD12	17	0.2
(1,1509)	1:625:A:TRP:H	1:624:A:ARG:HG2	3	0.2
(1,1509)	1:581:A:GLU:H	1:580:A:LEU:HG	5	0.2
(1,1509)	1:581:A:GLU:H	1:580:A:LEU:HG	19	0.2
(1,1503)	1:582:A:ALA:H	1:581:A:GLU:HB2	16	0.2
(1,1503)	1:582:A:ALA:H	1:581:A:GLU:HB2	19	0.2
(1,1491)	1:585:A:GLU:H	1:584:A:LEU:HG	11	0.2
(1,1491)	1:585:A:GLU:H	1:584:A:LEU:HG	19	0.2
(1,1487)	1:587:A:LEU:H	1:587:A:LEU:HD22	1	0.2
(1,1484)	1:587:A:LEU:H	1:588:A:GLN:HG2	6	0.2
(1,1468)	1:592:A:ALA:H	1:593:A:ASP:HB3	8	0.2
(1,1451)	1:599:A:GLN:H	1:600:A:PRO:HD3	10	0.2
(1,1437)	1:564:A:TYR:HD2	1:568:A:ARG:HG3	7	0.2
(1,1430)	1:596:A:PHE:HD2	1:608:A:LEU:HD22	4	0.2
(1,1430)	1:596:A:PHE:HD2	1:608:A:LEU:HD23	17	0.2
(1,1430)	1:596:A:PHE:HD2	1:608:A:LEU:HD22	19	0.2
(1,1420)	1:627:A:TYR:HE1	1:631:A:LEU:HD21	16	0.2
(1,1418)	1:596:A:PHE:HE2	1:591:A:VAL:HG23	1	0.2
(1,1418)	1:596:A:PHE:HE2	1:591:A:VAL:HG21	13	0.2
(1,1412)	1:584:A:LEU:HD22	1:615:A:GLU:HB2	18	0.2
(1,1401)	1:606:A:LYS:HB3	1:606:A:LYS:HE3	2	0.2
(1,1401)	1:606:A:LYS:HB3	1:606:A:LYS:HE3	6	0.2
(1,1401)	1:606:A:LYS:HB3	1:606:A:LYS:HE3	8	0.2
(1,1401)	1:606:A:LYS:HB3	1:606:A:LYS:HE2	11	0.2
(1,1384)	1:602:A:GLU:HG2	1:601:A:HIS:HB2	15	0.2
(1,1340)	1:573:A:LEU:HA	1:576:A:LEU:HG	6	0.2
(1,1340)	1:573:A:LEU:HA	1:576:A:LEU:HG	8	0.2
(1,1328)	1:573:A:LEU:HD11	1:574:A:PRO:HD3	10	0.2
(1,1307)	1:566:A:LEU:HD13	1:565:A:LYS:HA	9	0.2
(1,1216)	1:606:A:LYS:HD2	1:606:A:LYS:HA	11	0.2
(1,1210)	1:606:A:LYS:HA	1:605:A:GLN:HB3	17	0.2
(1,1056)	1:622:A:PHE:HB2	1:577:A:LEU:HD21	7	0.2
(1,1040)	1:629:A:GLU:HG3	1:570:A:LEU:HD11	10	0.2
(1,1025)	1:590:A:GLN:HG2	1:591:A:VAL:HG22	11	0.2
(1,1020)	1:604:A:THR:HG21	1:599:A:GLN:HG3	7	0.2
(1,1020)	1:604:A:THR:HG22	1:599:A:GLN:HG3	10	0.2
(1,1020)	1:604:A:THR:HG21	1:599:A:GLN:HG3	18	0.2
(1,1016)	1:588:A:GLN:HG2	1:584:A:LEU:HG	8	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,998)	1:583:A:LYS:HB3	1:587:A:LEU:HD11	3	0.2
(1,998)	1:583:A:LYS:HB3	1:587:A:LEU:HD13	10	0.2
(1,985)	1:591:A:VAL:HB	1:608:A:LEU:HD23	10	0.2
(1,985)	1:591:A:VAL:HB	1:608:A:LEU:HD23	11	0.2
(1,985)	1:591:A:VAL:HB	1:608:A:LEU:HD23	18	0.2
(1,972)	1:629:A:GLU:HB2	1:570:A:LEU:HD13	16	0.2
(1,928)	1:583:A:LYS:HG3	1:587:A:LEU:HD22	4	0.2
(1,851)	1:604:A:THR:HA	1:608:A:LEU:HD13	14	0.2
(1,851)	1:604:A:THR:HA	1:608:A:LEU:HD11	16	0.2
(1,851)	1:604:A:THR:HA	1:608:A:LEU:HD11	18	0.2
(1,820)	1:601:A:HIS:HA	1:605:A:GLN:HB2	1	0.2
(1,820)	1:601:A:HIS:HA	1:605:A:GLN:HB2	16	0.2
(1,774)	1:610:A:ASP:HA	1:587:A:LEU:HD12	13	0.2
(1,750)	1:604:A:THR:HG23	1:599:A:GLN:HA	9	0.2
(1,750)	1:604:A:THR:HG22	1:599:A:GLN:HA	13	0.2
(1,745)	1:562:A:LEU:HA	1:562:A:LEU:HD23	2	0.2
(1,745)	1:562:A:LEU:HA	1:562:A:LEU:HD21	14	0.2
(1,712)	1:594:A:ALA:HB1	1:593:A:ASP:HA	6	0.2
(1,712)	1:594:A:ALA:HB3	1:593:A:ASP:HA	13	0.2
(1,665)	1:631:A:LEU:HD23	1:631:A:LEU:HA	10	0.2
(1,664)	1:631:A:LEU:HD21	1:566:A:LEU:HB2	17	0.2
(1,652)	1:591:A:VAL:HG12	1:608:A:LEU:HA	13	0.2
(1,650)	1:591:A:VAL:HG11	1:588:A:GLN:HA	6	0.2
(1,642)	1:604:A:THR:HG23	1:596:A:PHE:HA	16	0.2
(1,642)	1:604:A:THR:HG22	1:596:A:PHE:HA	18	0.2
(1,603)	1:622:A:PHE:HD1	1:626:A:GLU:HG2	18	0.2
(1,585)	1:596:A:PHE:HZ	1:607:A:VAL:HG12	10	0.2
(1,585)	1:596:A:PHE:HZ	1:607:A:VAL:HG12	12	0.2
(1,585)	1:596:A:PHE:HZ	1:607:A:VAL:HG12	19	0.2
(1,584)	1:625:A:TRP:HD1	1:570:A:LEU:HD22	4	0.2
(1,554)	1:627:A:TYR:HE2	1:628:A:LEU:HD23	19	0.2
(1,544)	1:625:A:TRP:HE1	1:570:A:LEU:HD12	11	0.2
(1,538)	1:635:A:GLY:H	1:631:A:LEU:HD11	15	0.2
(1,507)	1:629:A:GLU:H	1:570:A:LEU:HD22	9	0.2
(1,507)	1:629:A:GLU:H	1:570:A:LEU:HD21	14	0.2
(1,507)	1:629:A:GLU:H	1:570:A:LEU:HD22	20	0.2
(1,369)	1:609:A:ALA:H	1:608:A:LEU:HD13	10	0.2
(1,274)	1:570:A:LEU:H	1:569:A:GLU:HG2	9	0.2
(1,182)	1:581:A:GLU:H	1:580:A:LEU:HD11	14	0.2
(1,173)	1:612:A:ALA:H	1:611:A:MET:HB2	1	0.2
(1,162)	1:584:A:LEU:H	1:583:A:LYS:HG3	5	0.2
(1,162)	1:584:A:LEU:H	1:583:A:LYS:HG3	12	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	1:586:A:ALA:H	1:589:A:THR:HG23	3	0.2
(1,58)	1:596:A:PHE:H	1:594:A:ALA:HB3	2	0.2
(1,58)	1:596:A:PHE:H	1:594:A:ALA:HB3	4	0.2
(1,2121)	1:581:A:GLU:HG2	1:618:A:LEU:HD23	5	0.19
(1,2105)	1:566:A:LEU:HD22	1:628:A:LEU:HG	17	0.19
(1,2081)	1:608:A:LEU:HD23	1:607:A:VAL:HB	12	0.19
(1,2059)	1:615:A:GLU:HA	1:619:A:GLU:HG2	3	0.19
(1,2027)	1:564:A:TYR:HB3	1:567:A:GLN:HB2	11	0.19
(1,2027)	1:564:A:TYR:HB3	1:567:A:GLN:HB2	17	0.19
(1,1992)	1:562:A:LEU:HB2	1:632:A:LYS:HG2	17	0.19
(1,1963)	1:596:A:PHE:HB3	1:591:A:VAL:HG12	20	0.19
(1,1961)	1:610:A:ASP:HB3	1:587:A:LEU:HB3	4	0.19
(1,1959)	1:622:A:PHE:HB2	1:619:A:GLU:HB2	8	0.19
(1,1959)	1:622:A:PHE:HB2	1:619:A:GLU:HB2	14	0.19
(1,1957)	1:622:A:PHE:HB2	1:619:A:GLU:HB2	8	0.19
(1,1957)	1:622:A:PHE:HB2	1:619:A:GLU:HB2	14	0.19
(1,1946)	1:581:A:GLU:HG2	1:618:A:LEU:HD23	5	0.19
(1,1923)	1:614:A:ALA:HB2	1:611:A:MET:HG3	3	0.19
(1,1868)	1:569:A:GLU:HA	1:566:A:LEU:HA	1	0.19
(1,1867)	1:564:A:TYR:HA	1:567:A:GLN:HA	3	0.19
(1,1813)	1:588:A:GLN:HA	1:584:A:LEU:HD23	1	0.19
(1,1813)	1:588:A:GLN:HA	1:584:A:LEU:HD23	2	0.19
(1,1813)	1:588:A:GLN:HA	1:584:A:LEU:HD22	14	0.19
(1,1813)	1:588:A:GLN:HA	1:584:A:LEU:HD22	17	0.19
(1,1790)	1:557:A:ARG:HA	1:555:A:VAL:HG22	8	0.19
(1,1790)	1:557:A:ARG:HA	1:555:A:VAL:HG12	19	0.19
(1,1789)	1:556:A:LYS:HA	1:555:A:VAL:HG12	19	0.19
(1,1776)	1:600:A:PRO:HG2	1:599:A:GLN:HA	15	0.19
(1,1752)	1:614:A:ALA:HB2	1:611:A:MET:HG3	3	0.19
(1,1740)	1:628:A:LEU:HD23	1:631:A:LEU:HB2	9	0.19
(1,1736)	1:607:A:VAL:HG11	1:608:A:LEU:HG	15	0.19
(1,1718)	1:604:A:THR:HG22	1:599:A:GLN:HG3	3	0.19
(1,1710)	1:577:A:LEU:HD21	1:574:A:PRO:HG3	3	0.19
(1,1709)	1:625:A:TRP:HD1	1:573:A:LEU:HB2	5	0.19
(1,1708)	1:625:A:TRP:HD1	1:628:A:LEU:HD11	9	0.19
(1,1708)	1:625:A:TRP:HD1	1:628:A:LEU:HD12	18	0.19
(1,1706)	1:625:A:TRP:HD1	1:628:A:LEU:HB2	15	0.19
(1,1693)	1:627:A:TYR:HD1	1:631:A:LEU:HD11	16	0.19
(1,1689)	1:596:A:PHE:HD1	1:607:A:VAL:HB	3	0.19
(1,1670)	1:633:A:ASN:H	1:631:A:LEU:HB2	19	0.19
(1,1617)	1:617:A:GLU:H	1:580:A:LEU:HD21	1	0.19
(1,1617)	1:617:A:GLU:H	1:580:A:LEU:HD23	16	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1617)	1:617:A:GLU:H	1:580:A:LEU:HD23	18	0.19
(1,1604)	1:628:A:LEU:H	1:570:A:LEU:HG	8	0.19
(1,1594)	1:614:A:ALA:H	1:615:A:GLU:HG3	9	0.19
(1,1588)	1:583:A:LYS:H	1:581:A:GLU:HG2	18	0.19
(1,1569)	1:607:A:VAL:H	1:608:A:LEU:HD21	15	0.19
(1,1568)	1:607:A:VAL:H	1:606:A:LYS:HG2	4	0.19
(1,1553)	1:566:A:LEU:H	1:566:A:LEU:HG	3	0.19
(1,1546)	1:568:A:ARG:H	1:567:A:GLN:HG3	5	0.19
(1,1546)	1:568:A:ARG:H	1:567:A:GLN:HG3	16	0.19
(1,1520)	1:577:A:LEU:H	1:578:A:GLU:HG3	15	0.19
(1,1515)	1:579:A:ASP:H	1:576:A:LEU:HD13	5	0.19
(1,1515)	1:579:A:ASP:H	1:576:A:LEU:HD11	7	0.19
(1,1515)	1:579:A:ASP:H	1:576:A:LEU:HD13	20	0.19
(1,1509)	1:581:A:GLU:H	1:580:A:LEU:HG	1	0.19
(1,1509)	1:581:A:GLU:H	1:580:A:LEU:HG	10	0.19
(1,1503)	1:582:A:ALA:H	1:581:A:GLU:HB2	15	0.19
(1,1491)	1:585:A:GLU:H	1:584:A:LEU:HG	10	0.19
(1,1488)	1:586:A:ALA:H	1:585:A:GLU:HA	5	0.19
(1,1459)	1:593:A:ASP:H	1:594:A:ALA:H	7	0.19
(1,1459)	1:593:A:ASP:H	1:594:A:ALA:H	19	0.19
(1,1456)	1:597:A:PHE:H	1:595:A:SER:HA	9	0.19
(1,1451)	1:599:A:GLN:H	1:600:A:PRO:HD3	18	0.19
(1,1451)	1:599:A:GLN:H	1:600:A:PRO:HD3	19	0.19
(1,1430)	1:596:A:PHE:HD2	1:608:A:LEU:HD23	1	0.19
(1,1430)	1:596:A:PHE:HD2	1:608:A:LEU:HD21	5	0.19
(1,1430)	1:596:A:PHE:HD2	1:608:A:LEU:HD21	8	0.19
(1,1430)	1:596:A:PHE:HD2	1:608:A:LEU:HD23	14	0.19
(1,1430)	1:596:A:PHE:HD2	1:608:A:LEU:HD23	16	0.19
(1,1422)	1:627:A:TYR:HD1	1:631:A:LEU:HD12	3	0.19
(1,1418)	1:596:A:PHE:HE2	1:591:A:VAL:HG23	6	0.19
(1,1418)	1:596:A:PHE:HE2	1:591:A:VAL:HG22	9	0.19
(1,1384)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	1	0.19
(1,1384)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	11	0.19
(1,1370)	1:604:A:THR:HG23	1:607:A:VAL:HB	16	0.19
(1,1364)	1:628:A:LEU:HD23	1:631:A:LEU:HB2	9	0.19
(1,1340)	1:573:A:LEU:HA	1:576:A:LEU:HG	12	0.19
(1,1326)	1:566:A:LEU:HD22	1:563:A:SER:HB3	15	0.19
(1,1325)	1:628:A:LEU:HD12	1:569:A:GLU:HA	1	0.19
(1,1216)	1:606:A:LYS:HD2	1:606:A:LYS:HA	5	0.19
(1,1136)	1:600:A:PRO:HD3	1:603:A:GLN:HB2	17	0.19
(1,1110)	1:628:A:LEU:HB2	1:570:A:LEU:HD21	2	0.19
(1,1110)	1:628:A:LEU:HB2	1:570:A:LEU:HD22	5	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1094)	1:632:A:LYS:HE2	1:570:A:LEU:HD13	11	0.19
(1,1040)	1:629:A:GLU:HG3	1:570:A:LEU:HD11	12	0.19
(1,1023)	1:590:A:GLN:HG3	1:587:A:LEU:HD22	3	0.19
(1,1020)	1:604:A:THR:HG22	1:599:A:GLN:HG3	3	0.19
(1,998)	1:583:A:LYS:HB3	1:587:A:LEU:HD13	1	0.19
(1,998)	1:583:A:LYS:HB3	1:587:A:LEU:HD12	7	0.19
(1,998)	1:583:A:LYS:HB3	1:587:A:LEU:HD12	20	0.19
(1,922)	1:612:A:ALA:HB1	1:611:A:MET:HE3	13	0.19
(1,858)	1:604:A:THR:HB	1:607:A:VAL:HB	8	0.19
(1,850)	1:604:A:THR:HA	1:607:A:VAL:HG13	12	0.19
(1,850)	1:604:A:THR:HA	1:607:A:VAL:HG12	19	0.19
(1,820)	1:601:A:HIS:HA	1:605:A:GLN:HB2	17	0.19
(1,810)	1:608:A:LEU:HA	1:608:A:LEU:HD11	13	0.19
(1,774)	1:610:A:ASP:HA	1:587:A:LEU:HD13	6	0.19
(1,774)	1:610:A:ASP:HA	1:587:A:LEU:HD12	10	0.19
(1,774)	1:610:A:ASP:HA	1:587:A:LEU:HD11	14	0.19
(1,712)	1:594:A:ALA:HB1	1:593:A:ASP:HA	16	0.19
(1,672)	1:607:A:VAL:HG22	1:606:A:LYS:HE3	5	0.19
(1,642)	1:604:A:THR:HG23	1:596:A:PHE:HA	6	0.19
(1,600)	1:601:A:HIS:HD2	1:602:A:GLU:HB3	9	0.19
(1,581)	1:601:A:HIS:HD2	1:605:A:GLN:HG3	8	0.19
(1,550)	1:596:A:PHE:HD1	1:604:A:THR:HG21	12	0.19
(1,369)	1:609:A:ALA:H	1:608:A:LEU:HD11	7	0.19
(1,339)	1:605:A:GLN:H	1:604:A:THR:HG23	9	0.19
(1,182)	1:581:A:GLU:H	1:580:A:LEU:HD12	5	0.19
(1,162)	1:584:A:LEU:H	1:583:A:LYS:HG3	3	0.19
(1,162)	1:584:A:LEU:H	1:583:A:LYS:HG3	13	0.19
(1,123)	1:589:A:THR:H	1:592:A:ALA:HB1	3	0.19
(1,58)	1:596:A:PHE:H	1:594:A:ALA:HB3	14	0.19
(1,35)	1:598:A:SER:H	1:599:A:GLN:HB3	8	0.19
(1,2165)	1:606:A:LYS:HA	1:610:A:ASP:HB2	5	0.18
(1,2163)	1:567:A:GLN:HA	1:570:A:LEU:HD13	8	0.18
(1,2162)	1:568:A:ARG:HD2	1:565:A:LYS:HA	5	0.18
(1,2157)	1:612:A:ALA:HB3	1:611:A:MET:HB3	14	0.18
(1,2156)	1:634:A:GLY:HA3	1:633:A:ASN:HB2	1	0.18
(1,2146)	1:615:A:GLU:HG2	1:584:A:LEU:HG	8	0.18
(1,2135)	1:567:A:GLN:HA	1:570:A:LEU:HD13	8	0.18
(1,2124)	1:612:A:ALA:HA	1:611:A:MET:HE3	9	0.18
(1,2105)	1:566:A:LEU:HD21	1:628:A:LEU:HG	14	0.18
(1,2081)	1:608:A:LEU:HD21	1:607:A:VAL:HB	1	0.18
(1,2059)	1:615:A:GLU:HA	1:619:A:GLU:HG2	9	0.18
(1,2051)	1:603:A:GLN:HG2	1:600:A:PRO:HA	11	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2048)	1:611:A:MET:HG3	1:584:A:LEU:HA	13	0.18
(1,2027)	1:564:A:TYR:HB3	1:567:A:GLN:HB2	4	0.18
(1,1987)	1:614:A:ALA:HB3	1:587:A:LEU:HB2	20	0.18
(1,1961)	1:610:A:ASP:HB3	1:587:A:LEU:HB3	7	0.18
(1,1959)	1:622:A:PHE:HB2	1:619:A:GLU:HB2	10	0.18
(1,1957)	1:622:A:PHE:HB2	1:619:A:GLU:HB2	10	0.18
(1,1951)	1:615:A:GLU:HG2	1:584:A:LEU:HG	8	0.18
(1,1950)	1:615:A:GLU:HG3	1:612:A:ALA:HB1	14	0.18
(1,1944)	1:585:A:GLU:HG3	1:586:A:ALA:HB1	7	0.18
(1,1933)	1:611:A:MET:HB2	1:584:A:LEU:HD21	18	0.18
(1,1871)	1:594:A:ALA:HB1	1:595:A:SER:HB2	12	0.18
(1,1806)	1:577:A:LEU:HA	1:581:A:GLU:HB2	20	0.18
(1,1795)	1:579:A:ASP:HA	1:583:A:LYS:HB2	1	0.18
(1,1779)	1:614:A:ALA:HA	1:580:A:LEU:HD12	16	0.18
(1,1778)	1:612:A:ALA:HA	1:584:A:LEU:HD21	14	0.18
(1,1760)	1:594:A:ALA:HB1	1:595:A:SER:HB2	12	0.18
(1,1759)	1:609:A:ALA:HB3	1:605:A:GLN:HA	10	0.18
(1,1756)	1:614:A:ALA:HB3	1:587:A:LEU:HB2	20	0.18
(1,1740)	1:628:A:LEU:HD21	1:631:A:LEU:HB2	3	0.18
(1,1736)	1:607:A:VAL:HG11	1:608:A:LEU:HG	20	0.18
(1,1730)	1:607:A:VAL:HG22	1:587:A:LEU:HD21	11	0.18
(1,1718)	1:604:A:THR:HG21	1:599:A:GLN:HG3	12	0.18
(1,1706)	1:625:A:TRP:HD1	1:628:A:LEU:HB2	5	0.18
(1,1698)	1:564:A:TYR:HD1	1:567:A:GLN:HB2	5	0.18
(1,1694)	1:564:A:TYR:HD2	1:568:A:ARG:HG2	5	0.18
(1,1683)	1:622:A:PHE:HE2	1:618:A:LEU:HD21	8	0.18
(1,1669)	1:633:A:ASN:H	1:632:A:LYS:HG3	13	0.18
(1,1635)	1:623:A:GLU:H	1:622:A:PHE:HD1	16	0.18
(1,1588)	1:583:A:LYS:H	1:581:A:GLU:HG2	6	0.18
(1,1569)	1:607:A:VAL:H	1:608:A:LEU:HD23	20	0.18
(1,1568)	1:607:A:VAL:H	1:606:A:LYS:HG2	3	0.18
(1,1568)	1:607:A:VAL:H	1:606:A:LYS:HG2	7	0.18
(1,1567)	1:607:A:VAL:H	1:606:A:LYS:HB2	16	0.18
(1,1562)	1:604:A:THR:H	1:599:A:GLN:HB2	11	0.18
(1,1546)	1:568:A:ARG:H	1:567:A:GLN:HG3	2	0.18
(1,1534)	1:572:A:GLN:H	1:571:A:GLU:HB3	13	0.18
(1,1491)	1:585:A:GLU:H	1:584:A:LEU:HG	1	0.18
(1,1491)	1:585:A:GLU:H	1:584:A:LEU:HG	16	0.18
(1,1491)	1:585:A:GLU:H	1:584:A:LEU:HG	20	0.18
(1,1488)	1:586:A:ALA:H	1:585:A:GLU:HA	15	0.18
(1,1487)	1:587:A:LEU:H	1:587:A:LEU:HD22	20	0.18
(1,1474)	1:589:A:THR:H	1:586:A:ALA:HA	18	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1451)	1:599:A:GLN:H	1:600:A:PRO:HD3	4	0.18
(1,1451)	1:599:A:GLN:H	1:600:A:PRO:HD3	5	0.18
(1,1451)	1:599:A:GLN:H	1:600:A:PRO:HD3	14	0.18
(1,1448)	1:603:A:GLN:H	1:601:A:HIS:HA	16	0.18
(1,1446)	1:568:A:ARG:HD3	1:564:A:TYR:HE2	7	0.18
(1,1437)	1:564:A:TYR:HD2	1:568:A:ARG:HG2	5	0.18
(1,1430)	1:596:A:PHE:HD2	1:608:A:LEU:HD23	3	0.18
(1,1430)	1:596:A:PHE:HD2	1:608:A:LEU:HD22	10	0.18
(1,1430)	1:596:A:PHE:HD2	1:608:A:LEU:HD22	11	0.18
(1,1430)	1:596:A:PHE:HD2	1:608:A:LEU:HD22	20	0.18
(1,1384)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	13	0.18
(1,1377)	1:565:A:LYS:HD2	1:563:A:SER:HB2	9	0.18
(1,1365)	1:631:A:LEU:HD21	1:566:A:LEU:HD11	12	0.18
(1,1364)	1:628:A:LEU:HD21	1:631:A:LEU:HB2	3	0.18
(1,1363)	1:562:A:LEU:HD23	1:631:A:LEU:HB2	2	0.18
(1,1340)	1:573:A:LEU:HA	1:576:A:LEU:HG	2	0.18
(1,1340)	1:573:A:LEU:HA	1:576:A:LEU:HG	13	0.18
(1,1335)	1:566:A:LEU:HG	1:562:A:LEU:HD23	12	0.18
(1,1328)	1:573:A:LEU:HD12	1:574:A:PRO:HD3	6	0.18
(1,1324)	1:628:A:LEU:HA	1:628:A:LEU:HD12	1	0.18
(1,1292)	1:577:A:LEU:HD21	1:573:A:LEU:HD11	18	0.18
(1,1278)	1:632:A:LYS:HG2	1:562:A:LEU:HD11	14	0.18
(1,1265)	1:593:A:ASP:HB3	1:595:A:SER:HB3	5	0.18
(1,1220)	1:551:A:LYS:HD2	1:551:A:LYS:HA	10	0.18
(1,1218)	1:606:A:LYS:HD3	1:606:A:LYS:HA	11	0.18
(1,1210)	1:606:A:LYS:HA	1:605:A:GLN:HB3	10	0.18
(1,1136)	1:600:A:PRO:HD3	1:603:A:GLN:HB2	8	0.18
(1,1063)	1:610:A:ASP:HB2	1:587:A:LEU:HD12	5	0.18
(1,1063)	1:610:A:ASP:HB2	1:587:A:LEU:HD13	8	0.18
(1,1063)	1:610:A:ASP:HB2	1:587:A:LEU:HD11	14	0.18
(1,1056)	1:622:A:PHE:HB2	1:577:A:LEU:HD21	6	0.18
(1,1056)	1:622:A:PHE:HB2	1:577:A:LEU:HD22	19	0.18
(1,1020)	1:604:A:THR:HG21	1:599:A:GLN:HG3	12	0.18
(1,920)	1:604:A:THR:HB	1:601:A:HIS:HA	8	0.18
(1,859)	1:604:A:THR:HB	1:608:A:LEU:HD23	17	0.18
(1,820)	1:601:A:HIS:HA	1:605:A:GLN:HB2	8	0.18
(1,820)	1:601:A:HIS:HA	1:605:A:GLN:HB2	12	0.18
(1,810)	1:608:A:LEU:HA	1:608:A:LEU:HD11	12	0.18
(1,810)	1:608:A:LEU:HA	1:608:A:LEU:HD13	17	0.18
(1,774)	1:610:A:ASP:HA	1:587:A:LEU:HD13	11	0.18
(1,774)	1:610:A:ASP:HA	1:587:A:LEU:HD12	15	0.18
(1,750)	1:604:A:THR:HG21	1:599:A:GLN:HA	4	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,745)	1:562:A:LEU:HA	1:562:A:LEU:HD22	16	0.18
(1,730)	1:600:A:PRO:HD3	1:603:A:GLN:HG2	2	0.18
(1,712)	1:594:A:ALA:HB1	1:593:A:ASP:HA	1	0.18
(1,712)	1:594:A:ALA:HB2	1:593:A:ASP:HA	11	0.18
(1,672)	1:607:A:VAL:HG21	1:606:A:LYS:HE2	4	0.18
(1,665)	1:631:A:LEU:HD21	1:631:A:LEU:HA	18	0.18
(1,642)	1:604:A:THR:HG22	1:596:A:PHE:HA	4	0.18
(1,634)	1:577:A:LEU:HD13	1:574:A:PRO:HA	14	0.18
(1,585)	1:596:A:PHE:HZ	1:607:A:VAL:HG12	2	0.18
(1,584)	1:625:A:TRP:HD1	1:570:A:LEU:HD22	2	0.18
(1,584)	1:625:A:TRP:HD1	1:570:A:LEU:HD23	20	0.18
(1,564)	1:597:A:PHE:HE2	1:591:A:VAL:HG13	19	0.18
(1,471)	1:623:A:GLU:H	1:623:A:GLU:HG3	13	0.18
(1,429)	1:618:A:LEU:H	1:617:A:GLU:HB2	11	0.18
(1,339)	1:605:A:GLN:H	1:604:A:THR:HG22	1	0.18
(1,339)	1:605:A:GLN:H	1:604:A:THR:HG21	11	0.18
(1,258)	1:572:A:GLN:H	1:572:A:GLN:HG3	1	0.18
(1,182)	1:581:A:GLU:H	1:580:A:LEU:HD12	1	0.18
(1,182)	1:581:A:GLU:H	1:580:A:LEU:HD11	18	0.18
(1,162)	1:584:A:LEU:H	1:583:A:LYS:HG3	2	0.18
(1,162)	1:584:A:LEU:H	1:583:A:LYS:HG3	6	0.18
(1,2165)	1:606:A:LYS:HA	1:610:A:ASP:HB2	19	0.17
(1,2124)	1:612:A:ALA:HA	1:611:A:MET:HE1	1	0.17
(1,2081)	1:608:A:LEU:HD21	1:607:A:VAL:HB	16	0.17
(1,1963)	1:596:A:PHE:HB3	1:591:A:VAL:HG11	9	0.17
(1,1959)	1:622:A:PHE:HB2	1:619:A:GLU:HB2	13	0.17
(1,1957)	1:622:A:PHE:HB2	1:619:A:GLU:HB2	13	0.17
(1,1911)	1:581:A:GLU:HB3	1:618:A:LEU:HD11	2	0.17
(1,1907)	1:591:A:VAL:HA	1:608:A:LEU:HD22	18	0.17
(1,1874)	1:632:A:LYS:HG2	1:562:A:LEU:HD22	14	0.17
(1,1849)	1:604:A:THR:HA	1:599:A:GLN:HB2	16	0.17
(1,1828)	1:601:A:HIS:HA	1:602:A:GLU:HG3	16	0.17
(1,1806)	1:577:A:LEU:HA	1:581:A:GLU:HB2	4	0.17
(1,1795)	1:579:A:ASP:HA	1:583:A:LYS:HB2	4	0.17
(1,1785)	1:586:A:ALA:HA	1:585:A:GLU:HB3	7	0.17
(1,1779)	1:614:A:ALA:HA	1:580:A:LEU:HD12	3	0.17
(1,1779)	1:614:A:ALA:HA	1:580:A:LEU:HD13	10	0.17
(1,1779)	1:614:A:ALA:HA	1:580:A:LEU:HD13	18	0.17
(1,1729)	1:631:A:LEU:HD22	1:561:A:LYS:HA	1	0.17
(1,1710)	1:577:A:LEU:HD23	1:574:A:PRO:HG3	12	0.17
(1,1710)	1:577:A:LEU:HD23	1:574:A:PRO:HG3	17	0.17
(1,1708)	1:625:A:TRP:HD1	1:628:A:LEU:HD13	7	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1698)	1:564:A:TYR:HD1	1:567:A:GLN:HB2	18	0.17
(1,1694)	1:564:A:TYR:HD2	1:565:A:LYS:HG2	10	0.17
(1,1694)	1:564:A:TYR:HD2	1:568:A:ARG:HG2	12	0.17
(1,1689)	1:596:A:PHE:HD1	1:607:A:VAL:HB	13	0.17
(1,1635)	1:623:A:GLU:H	1:622:A:PHE:HD1	18	0.17
(1,1632)	1:622:A:PHE:H	1:619:A:GLU:HB2	20	0.17
(1,1594)	1:614:A:ALA:H	1:616:A:GLN:HB2	6	0.17
(1,1594)	1:614:A:ALA:H	1:615:A:GLU:HG3	8	0.17
(1,1591)	1:583:A:LYS:H	1:583:A:LYS:HG3	1	0.17
(1,1577)	1:609:A:ALA:H	1:608:A:LEU:HG	19	0.17
(1,1569)	1:607:A:VAL:H	1:608:A:LEU:HD23	9	0.17
(1,1563)	1:605:A:GLN:H	1:605:A:GLN:HE22	4	0.17
(1,1562)	1:604:A:THR:H	1:599:A:GLN:HB2	3	0.17
(1,1562)	1:604:A:THR:H	1:599:A:GLN:HB2	17	0.17
(1,1549)	1:567:A:GLN:H	1:563:A:SER:HB3	11	0.17
(1,1509)	1:581:A:GLU:H	1:580:A:LEU:HG	18	0.17
(1,1491)	1:585:A:GLU:H	1:584:A:LEU:HG	13	0.17
(1,1487)	1:587:A:LEU:H	1:587:A:LEU:HD23	11	0.17
(1,1474)	1:589:A:THR:H	1:586:A:ALA:HA	10	0.17
(1,1474)	1:589:A:THR:H	1:586:A:ALA:HA	12	0.17
(1,1446)	1:568:A:ARG:HD3	1:564:A:TYR:HE2	9	0.17
(1,1437)	1:564:A:TYR:HD2	1:568:A:ARG:HG2	12	0.17
(1,1431)	1:622:A:PHE:HE2	1:618:A:LEU:HD21	8	0.17
(1,1430)	1:596:A:PHE:HD2	1:608:A:LEU:HD22	6	0.17
(1,1430)	1:596:A:PHE:HD2	1:608:A:LEU:HD22	7	0.17
(1,1430)	1:596:A:PHE:HD2	1:608:A:LEU:HD22	12	0.17
(1,1426)	1:627:A:TYR:HD2	1:628:A:LEU:HD21	6	0.17
(1,1426)	1:627:A:TYR:HD2	1:628:A:LEU:HD23	13	0.17
(1,1422)	1:627:A:TYR:HD1	1:631:A:LEU:HD11	16	0.17
(1,1420)	1:627:A:TYR:HE1	1:631:A:LEU:HD22	15	0.17
(1,1412)	1:584:A:LEU:HD22	1:615:A:GLU:HB2	1	0.17
(1,1384)	1:602:A:GLU:HG2	1:601:A:HIS:HB2	8	0.17
(1,1384)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	16	0.17
(1,1377)	1:565:A:LYS:HD2	1:563:A:SER:HB2	6	0.17
(1,1340)	1:573:A:LEU:HA	1:576:A:LEU:HG	16	0.17
(1,1326)	1:566:A:LEU:HD22	1:563:A:SER:HB3	7	0.17
(1,1325)	1:628:A:LEU:HD12	1:569:A:GLU:HA	12	0.17
(1,1324)	1:628:A:LEU:HA	1:628:A:LEU:HD12	8	0.17
(1,1309)	1:573:A:LEU:HD23	1:576:A:LEU:HB2	5	0.17
(1,1292)	1:577:A:LEU:HD21	1:573:A:LEU:HD11	5	0.17
(1,1292)	1:577:A:LEU:HD21	1:573:A:LEU:HD13	12	0.17
(1,1244)	1:569:A:GLU:HG3	1:566:A:LEU:HA	20	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1165)	1:601:A:HIS:HB2	1:605:A:GLN:HG2	17	0.17
(1,1061)	1:610:A:ASP:HB3	1:607:A:VAL:HG11	14	0.17
(1,1056)	1:622:A:PHE:HB2	1:577:A:LEU:HD22	15	0.17
(1,1014)	1:605:A:GLN:HG2	1:608:A:LEU:HD13	10	0.17
(1,998)	1:583:A:LYS:HB3	1:587:A:LEU:HD11	6	0.17
(1,998)	1:583:A:LYS:HB3	1:587:A:LEU:HD11	8	0.17
(1,998)	1:583:A:LYS:HB3	1:587:A:LEU:HD13	13	0.17
(1,998)	1:583:A:LYS:HB3	1:587:A:LEU:HD11	16	0.17
(1,985)	1:591:A:VAL:HB	1:608:A:LEU:HD22	13	0.17
(1,970)	1:632:A:LYS:HD2	1:570:A:LEU:HD12	14	0.17
(1,956)	1:605:A:GLN:HB3	1:608:A:LEU:HD13	2	0.17
(1,928)	1:583:A:LYS:HG3	1:587:A:LEU:HD22	12	0.17
(1,881)	1:568:A:ARG:HA	1:568:A:ARG:HD2	2	0.17
(1,859)	1:604:A:THR:HB	1:608:A:LEU:HD23	1	0.17
(1,848)	1:622:A:PHE:HA	1:573:A:LEU:HD23	10	0.17
(1,820)	1:601:A:HIS:HA	1:605:A:GLN:HB2	2	0.17
(1,811)	1:618:A:LEU:HA	1:618:A:LEU:HD21	17	0.17
(1,810)	1:608:A:LEU:HA	1:608:A:LEU:HD13	1	0.17
(1,810)	1:608:A:LEU:HA	1:608:A:LEU:HD12	6	0.17
(1,810)	1:608:A:LEU:HA	1:608:A:LEU:HD11	20	0.17
(1,774)	1:610:A:ASP:HA	1:587:A:LEU:HD11	2	0.17
(1,774)	1:610:A:ASP:HA	1:587:A:LEU:HD11	20	0.17
(1,750)	1:604:A:THR:HG21	1:599:A:GLN:HA	18	0.17
(1,717)	1:621:A:ALA:HB1	1:577:A:LEU:HD23	12	0.17
(1,712)	1:594:A:ALA:HB1	1:593:A:ASP:HA	2	0.17
(1,712)	1:594:A:ALA:HB1	1:593:A:ASP:HA	9	0.17
(1,712)	1:594:A:ALA:HB2	1:593:A:ASP:HA	12	0.17
(1,710)	1:594:A:ALA:HB1	1:595:A:SER:HA	11	0.17
(1,708)	1:592:A:ALA:HB3	1:593:A:ASP:HA	3	0.17
(1,658)	1:591:A:VAL:HG23	1:596:A:PHE:HB3	3	0.17
(1,585)	1:596:A:PHE:HZ	1:607:A:VAL:HG12	18	0.17
(1,585)	1:596:A:PHE:HZ	1:607:A:VAL:HG12	20	0.17
(1,584)	1:625:A:TRP:HD1	1:570:A:LEU:HD23	7	0.17
(1,584)	1:625:A:TRP:HD1	1:570:A:LEU:HD23	18	0.17
(1,559)	1:596:A:PHE:HE1	1:604:A:THR:HG21	12	0.17
(1,446)	1:620:A:GLN:H	1:619:A:GLU:HG3	12	0.17
(1,429)	1:618:A:LEU:H	1:617:A:GLU:HB2	16	0.17
(1,369)	1:609:A:ALA:H	1:608:A:LEU:HD11	5	0.17
(1,307)	1:566:A:LEU:H	1:566:A:LEU:HD12	2	0.17
(1,262)	1:571:A:GLU:H	1:571:A:GLU:HG2	6	0.17
(1,258)	1:572:A:GLN:H	1:572:A:GLN:HG3	15	0.17
(1,182)	1:581:A:GLU:H	1:580:A:LEU:HD13	9	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,182)	1:581:A:GLU:H	1:580:A:LEU:HD11	11	0.17
(1,162)	1:584:A:LEU:H	1:583:A:LYS:HG3	14	0.17
(1,162)	1:584:A:LEU:H	1:583:A:LYS:HG3	20	0.17
(1,110)	1:590:A:GLN:H	1:590:A:GLN:HG3	9	0.17
(1,2175)	1:597:A:PHE:HD1	1:604:A:THR:HB	5	0.16
(1,2124)	1:612:A:ALA:HA	1:611:A:MET:HE1	8	0.16
(1,2081)	1:608:A:LEU:HD23	1:607:A:VAL:HB	7	0.16
(1,2059)	1:615:A:GLU:HA	1:619:A:GLU:HG2	1	0.16
(1,2059)	1:615:A:GLU:HA	1:619:A:GLU:HG2	12	0.16
(1,1987)	1:614:A:ALA:HB1	1:587:A:LEU:HB2	13	0.16
(1,1961)	1:610:A:ASP:HB3	1:587:A:LEU:HB3	13	0.16
(1,1952)	1:580:A:LEU:HD22	1:617:A:GLU:HG3	7	0.16
(1,1935)	1:567:A:GLN:HG2	1:562:A:LEU:HG	2	0.16
(1,1889)	1:568:A:ARG:HG2	1:569:A:GLU:HB2	3	0.16
(1,1889)	1:568:A:ARG:HG3	1:571:A:GLU:HB2	5	0.16
(1,1889)	1:568:A:ARG:HG2	1:569:A:GLU:HB2	16	0.16
(1,1867)	1:564:A:TYR:HA	1:567:A:GLN:HA	15	0.16
(1,1849)	1:604:A:THR:HA	1:599:A:GLN:HB2	18	0.16
(1,1813)	1:588:A:GLN:HA	1:584:A:LEU:HD21	20	0.16
(1,1778)	1:612:A:ALA:HA	1:584:A:LEU:HD22	1	0.16
(1,1756)	1:614:A:ALA:HB1	1:587:A:LEU:HB2	13	0.16
(1,1706)	1:625:A:TRP:HD1	1:628:A:LEU:HB2	11	0.16
(1,1706)	1:625:A:TRP:HD1	1:628:A:LEU:HB2	14	0.16
(1,1698)	1:564:A:TYR:HD2	1:567:A:GLN:HB2	14	0.16
(1,1683)	1:622:A:PHE:HE2	1:618:A:LEU:HD22	3	0.16
(1,1682)	1:622:A:PHE:HD2	1:577:A:LEU:HD11	20	0.16
(1,1669)	1:633:A:ASN:H	1:631:A:LEU:HB3	8	0.16
(1,1669)	1:633:A:ASN:H	1:631:A:LEU:HB3	17	0.16
(1,1629)	1:621:A:ALA:H	1:620:A:GLN:HG3	2	0.16
(1,1617)	1:617:A:GLU:H	1:580:A:LEU:HD23	3	0.16
(1,1617)	1:617:A:GLU:H	1:580:A:LEU:HD22	9	0.16
(1,1577)	1:609:A:ALA:H	1:608:A:LEU:HG	20	0.16
(1,1546)	1:568:A:ARG:H	1:567:A:GLN:HG3	10	0.16
(1,1530)	1:573:A:LEU:H	1:572:A:GLN:HB3	12	0.16
(1,1515)	1:579:A:ASP:H	1:576:A:LEU:HD12	2	0.16
(1,1509)	1:581:A:GLU:H	1:580:A:LEU:HG	2	0.16
(1,1509)	1:581:A:GLU:H	1:580:A:LEU:HG	6	0.16
(1,1509)	1:581:A:GLU:H	1:580:A:LEU:HG	9	0.16
(1,1509)	1:581:A:GLU:H	1:580:A:LEU:HG	16	0.16
(1,1491)	1:585:A:GLU:H	1:584:A:LEU:HG	14	0.16
(1,1474)	1:589:A:THR:H	1:586:A:ALA:HA	7	0.16
(1,1460)	1:606:A:LYS:H	1:608:A:LEU:H	8	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1460)	1:606:A:LYS:H	1:608:A:LEU:H	16	0.16
(1,1446)	1:568:A:ARG:HD3	1:564:A:TYR:HE2	17	0.16
(1,1437)	1:564:A:TYR:HD2	1:568:A:ARG:HG3	9	0.16
(1,1431)	1:622:A:PHE:HE2	1:618:A:LEU:HD22	3	0.16
(1,1398)	1:587:A:LEU:HD22	1:583:A:LYS:HG2	19	0.16
(1,1377)	1:565:A:LYS:HD3	1:563:A:SER:HB2	20	0.16
(1,1370)	1:604:A:THR:HG22	1:607:A:VAL:HB	14	0.16
(1,1340)	1:573:A:LEU:HA	1:576:A:LEU:HG	20	0.16
(1,1335)	1:566:A:LEU:HG	1:562:A:LEU:HD22	8	0.16
(1,1307)	1:566:A:LEU:HD12	1:565:A:LYS:HA	14	0.16
(1,1266)	1:596:A:PHE:HA	1:593:A:ASP:HB3	13	0.16
(1,1244)	1:569:A:GLU:HG3	1:566:A:LEU:HA	9	0.16
(1,1210)	1:606:A:LYS:HA	1:605:A:GLN:HB2	16	0.16
(1,1147)	1:565:A:LYS:HA	1:565:A:LYS:HD3	9	0.16
(1,1110)	1:628:A:LEU:HB2	1:570:A:LEU:HD23	8	0.16
(1,1056)	1:622:A:PHE:HB2	1:577:A:LEU:HD22	2	0.16
(1,1023)	1:590:A:GLN:HG3	1:587:A:LEU:HD21	13	0.16
(1,998)	1:583:A:LYS:HB3	1:587:A:LEU:HD11	18	0.16
(1,979)	1:583:A:LYS:HD3	1:587:A:LEU:HD11	12	0.16
(1,972)	1:629:A:GLU:HB2	1:570:A:LEU:HD12	11	0.16
(1,928)	1:583:A:LYS:HG3	1:587:A:LEU:HD22	2	0.16
(1,928)	1:583:A:LYS:HG3	1:587:A:LEU:HD21	9	0.16
(1,922)	1:612:A:ALA:HB3	1:611:A:MET:HE3	4	0.16
(1,820)	1:601:A:HIS:HA	1:605:A:GLN:HB2	4	0.16
(1,820)	1:601:A:HIS:HA	1:605:A:GLN:HB2	18	0.16
(1,820)	1:601:A:HIS:HA	1:605:A:GLN:HB2	20	0.16
(1,810)	1:608:A:LEU:HA	1:608:A:LEU:HD13	3	0.16
(1,810)	1:608:A:LEU:HA	1:608:A:LEU:HD13	5	0.16
(1,810)	1:608:A:LEU:HA	1:608:A:LEU:HD12	11	0.16
(1,774)	1:610:A:ASP:HA	1:587:A:LEU:HD12	1	0.16
(1,717)	1:621:A:ALA:HB3	1:577:A:LEU:HD23	13	0.16
(1,712)	1:594:A:ALA:HB2	1:593:A:ASP:HA	7	0.16
(1,712)	1:594:A:ALA:HB1	1:593:A:ASP:HA	14	0.16
(1,712)	1:594:A:ALA:HB1	1:593:A:ASP:HA	15	0.16
(1,712)	1:594:A:ALA:HB1	1:593:A:ASP:HA	17	0.16
(1,710)	1:594:A:ALA:HB2	1:595:A:SER:HA	13	0.16
(1,664)	1:631:A:LEU:HD21	1:566:A:LEU:HB2	3	0.16
(1,652)	1:591:A:VAL:HG13	1:608:A:LEU:HA	9	0.16
(1,642)	1:604:A:THR:HG21	1:596:A:PHE:HA	20	0.16
(1,621)	1:577:A:LEU:HD23	1:573:A:LEU:HA	7	0.16
(1,600)	1:601:A:HIS:HD2	1:602:A:GLU:HB3	12	0.16
(1,596)	1:564:A:TYR:HD2	1:564:A:TYR:HA	4	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,587)	1:596:A:PHE:HZ	1:604:A:THR:HG21	9	0.16
(1,584)	1:625:A:TRP:HD1	1:570:A:LEU:HD22	3	0.16
(1,584)	1:625:A:TRP:HD1	1:570:A:LEU:HD22	6	0.16
(1,584)	1:625:A:TRP:HD1	1:570:A:LEU:HD21	11	0.16
(1,564)	1:597:A:PHE:HE2	1:591:A:VAL:HG11	12	0.16
(1,559)	1:596:A:PHE:HE1	1:604:A:THR:HG22	7	0.16
(1,471)	1:623:A:GLU:H	1:623:A:GLU:HG3	9	0.16
(1,274)	1:570:A:LEU:H	1:569:A:GLU:HG2	14	0.16
(1,273)	1:570:A:LEU:H	1:569:A:GLU:HB2	20	0.16
(1,262)	1:571:A:GLU:H	1:571:A:GLU:HG2	19	0.16
(1,182)	1:581:A:GLU:H	1:580:A:LEU:HD13	4	0.16
(1,173)	1:612:A:ALA:H	1:611:A:MET:HB2	3	0.16
(1,162)	1:584:A:LEU:H	1:583:A:LYS:HG3	8	0.16
(1,135)	1:588:A:GLN:H	1:591:A:VAL:HG21	12	0.16
(1,2171)	1:591:A:VAL:HG21	1:597:A:PHE:HZ	4	0.15
(1,2165)	1:606:A:LYS:HA	1:606:A:LYS:HE3	7	0.15
(1,2146)	1:615:A:GLU:HG2	1:584:A:LEU:HG	12	0.15
(1,2124)	1:612:A:ALA:HA	1:611:A:MET:HE2	11	0.15
(1,2052)	1:603:A:GLN:HG3	1:599:A:GLN:HA	12	0.15
(1,2051)	1:603:A:GLN:HG2	1:600:A:PRO:HA	2	0.15
(1,1996)	1:624:A:ARG:HD3	1:628:A:LEU:HD22	7	0.15
(1,1978)	1:583:A:LYS:HE3	1:587:A:LEU:HD22	4	0.15
(1,1957)	1:622:A:PHE:HB2	1:619:A:GLU:HB3	9	0.15
(1,1951)	1:615:A:GLU:HG2	1:584:A:LEU:HG	12	0.15
(1,1950)	1:615:A:GLU:HG3	1:612:A:ALA:HB1	18	0.15
(1,1935)	1:567:A:GLN:HG2	1:562:A:LEU:HB2	11	0.15
(1,1933)	1:611:A:MET:HB2	1:608:A:LEU:HD22	2	0.15
(1,1923)	1:614:A:ALA:HB3	1:611:A:MET:HG3	10	0.15
(1,1920)	1:613:A:ALA:HB2	1:617:A:GLU:HB2	2	0.15
(1,1920)	1:613:A:ALA:HB3	1:617:A:GLU:HB2	7	0.15
(1,1895)	1:618:A:LEU:HG	1:619:A:GLU:HB3	20	0.15
(1,1868)	1:569:A:GLU:HA	1:566:A:LEU:HA	5	0.15
(1,1868)	1:569:A:GLU:HA	1:566:A:LEU:HA	16	0.15
(1,1828)	1:601:A:HIS:HA	1:602:A:GLU:HG3	11	0.15
(1,1806)	1:577:A:LEU:HA	1:581:A:GLU:HB2	8	0.15
(1,1806)	1:577:A:LEU:HA	1:581:A:GLU:HB2	17	0.15
(1,1797)	1:628:A:LEU:HD23	1:624:A:ARG:HA	3	0.15
(1,1787)	1:621:A:ALA:HA	1:620:A:GLN:HB3	2	0.15
(1,1752)	1:614:A:ALA:HB3	1:611:A:MET:HG3	10	0.15
(1,1749)	1:613:A:ALA:HB2	1:617:A:GLU:HB2	2	0.15
(1,1745)	1:614:A:ALA:HB3	1:580:A:LEU:HD22	9	0.15
(1,1741)	1:628:A:LEU:HD23	1:624:A:ARG:HA	3	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1711)	1:577:A:LEU:HD23	1:626:A:GLU:HG3	13	0.15
(1,1709)	1:625:A:TRP:HD1	1:573:A:LEU:HB2	9	0.15
(1,1698)	1:564:A:TYR:HD2	1:567:A:GLN:HB2	3	0.15
(1,1683)	1:622:A:PHE:HE2	1:618:A:LEU:HD23	20	0.15
(1,1633)	1:622:A:PHE:H	1:619:A:GLU:HB3	18	0.15
(1,1617)	1:617:A:GLU:H	1:580:A:LEU:HD22	19	0.15
(1,1577)	1:609:A:ALA:H	1:608:A:LEU:HG	2	0.15
(1,1568)	1:607:A:VAL:H	1:606:A:LYS:HG2	17	0.15
(1,1562)	1:604:A:THR:H	1:599:A:GLN:HB2	9	0.15
(1,1546)	1:568:A:ARG:H	1:567:A:GLN:HG3	3	0.15
(1,1538)	1:571:A:GLU:H	1:570:A:LEU:HD12	5	0.15
(1,1535)	1:572:A:GLN:H	1:573:A:LEU:HD12	18	0.15
(1,1509)	1:581:A:GLU:H	1:580:A:LEU:HG	8	0.15
(1,1484)	1:587:A:LEU:H	1:588:A:GLN:HG2	2	0.15
(1,1451)	1:599:A:GLN:H	1:600:A:PRO:HD3	13	0.15
(1,1446)	1:568:A:ARG:HD3	1:564:A:TYR:HE1	3	0.15
(1,1446)	1:568:A:ARG:HD3	1:564:A:TYR:HE2	16	0.15
(1,1431)	1:622:A:PHE:HE2	1:618:A:LEU:HD23	20	0.15
(1,1425)	1:596:A:PHE:HE1	1:607:A:VAL:HG13	3	0.15
(1,1418)	1:596:A:PHE:HE2	1:591:A:VAL:HG23	11	0.15
(1,1412)	1:584:A:LEU:HD22	1:615:A:GLU:HB2	3	0.15
(1,1391)	1:614:A:ALA:HA	1:583:A:LYS:HE2	11	0.15
(1,1384)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	3	0.15
(1,1377)	1:565:A:LYS:HD2	1:563:A:SER:HB2	8	0.15
(1,1374)	1:577:A:LEU:HD11	1:625:A:TRP:HB3	18	0.15
(1,1370)	1:604:A:THR:HG23	1:607:A:VAL:HB	6	0.15
(1,1370)	1:604:A:THR:HG23	1:607:A:VAL:HB	13	0.15
(1,1340)	1:573:A:LEU:HA	1:576:A:LEU:HG	1	0.15
(1,1340)	1:573:A:LEU:HA	1:576:A:LEU:HG	5	0.15
(1,1340)	1:573:A:LEU:HA	1:576:A:LEU:HG	7	0.15
(1,1335)	1:566:A:LEU:HG	1:562:A:LEU:HD21	3	0.15
(1,1328)	1:573:A:LEU:HD13	1:574:A:PRO:HD3	2	0.15
(1,1328)	1:573:A:LEU:HD11	1:574:A:PRO:HD3	18	0.15
(1,1292)	1:577:A:LEU:HD21	1:573:A:LEU:HD11	7	0.15
(1,1266)	1:596:A:PHE:HA	1:593:A:ASP:HB3	1	0.15
(1,1266)	1:596:A:PHE:HA	1:593:A:ASP:HB3	2	0.15
(1,1210)	1:606:A:LYS:HA	1:605:A:GLN:HB3	11	0.15
(1,1190)	1:562:A:LEU:HB2	1:632:A:LYS:HA	3	0.15
(1,1174)	1:623:A:GLU:HG2	1:622:A:PHE:HB2	8	0.15
(1,1163)	1:599:A:GLN:HG3	1:600:A:PRO:HD3	19	0.15
(1,1114)	1:567:A:GLN:HG2	1:562:A:LEU:HB2	11	0.15
(1,1111)	1:631:A:LEU:HD23	1:562:A:LEU:HB2	19	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1035)	1:628:A:LEU:HD12	1:569:A:GLU:HG3	2	0.15
(1,1034)	1:569:A:GLU:HG2	1:573:A:LEU:HD12	8	0.15
(1,998)	1:583:A:LYS:HB3	1:587:A:LEU:HD11	11	0.15
(1,990)	1:591:A:VAL:HG22	1:611:A:MET:HG2	5	0.15
(1,858)	1:604:A:THR:HB	1:607:A:VAL:HB	18	0.15
(1,811)	1:618:A:LEU:HA	1:618:A:LEU:HD22	5	0.15
(1,811)	1:618:A:LEU:HA	1:618:A:LEU:HD22	13	0.15
(1,811)	1:618:A:LEU:HA	1:618:A:LEU:HD22	20	0.15
(1,810)	1:608:A:LEU:HA	1:608:A:LEU:HD12	2	0.15
(1,810)	1:608:A:LEU:HA	1:608:A:LEU:HD13	7	0.15
(1,810)	1:608:A:LEU:HA	1:608:A:LEU:HD13	8	0.15
(1,810)	1:608:A:LEU:HA	1:608:A:LEU:HD13	15	0.15
(1,774)	1:610:A:ASP:HA	1:587:A:LEU:HD13	18	0.15
(1,757)	1:562:A:LEU:HA	1:566:A:LEU:HB2	2	0.15
(1,712)	1:594:A:ALA:HB1	1:593:A:ASP:HA	20	0.15
(1,710)	1:594:A:ALA:HB1	1:595:A:SER:HA	12	0.15
(1,710)	1:594:A:ALA:HB3	1:595:A:SER:HA	18	0.15
(1,708)	1:592:A:ALA:HB1	1:593:A:ASP:HA	8	0.15
(1,636)	1:577:A:LEU:HD11	1:621:A:ALA:HA	5	0.15
(1,621)	1:577:A:LEU:HD21	1:573:A:LEU:HA	2	0.15
(1,621)	1:577:A:LEU:HD23	1:573:A:LEU:HA	20	0.15
(1,603)	1:622:A:PHE:HD1	1:626:A:GLU:HG2	4	0.15
(1,600)	1:601:A:HIS:HD2	1:602:A:GLU:HB3	14	0.15
(1,558)	1:564:A:TYR:HE2	1:568:A:ARG:HB2	13	0.15
(1,554)	1:627:A:TYR:HE2	1:628:A:LEU:HD21	4	0.15
(1,507)	1:629:A:GLU:H	1:570:A:LEU:HD21	15	0.15
(1,429)	1:618:A:LEU:H	1:617:A:GLU:HB2	20	0.15
(1,339)	1:605:A:GLN:H	1:604:A:THR:HG22	19	0.15
(1,321)	1:604:A:THR:H	1:596:A:PHE:HE1	15	0.15
(1,274)	1:570:A:LEU:H	1:569:A:GLU:HG2	8	0.15
(1,274)	1:570:A:LEU:H	1:569:A:GLU:HG2	13	0.15
(1,182)	1:581:A:GLU:H	1:580:A:LEU:HD13	3	0.15
(1,135)	1:588:A:GLN:H	1:591:A:VAL:HG21	2	0.15
(1,135)	1:588:A:GLN:H	1:591:A:VAL:HG22	10	0.15
(1,135)	1:588:A:GLN:H	1:591:A:VAL:HG23	15	0.15
(1,64)	1:595:A:SER:H	1:596:A:PHE:HB2	1	0.15
(1,18)	1:599:A:GLN:H	1:596:A:PHE:HD1	2	0.15
(1,2175)	1:597:A:PHE:HD1	1:604:A:THR:HB	10	0.14
(1,2163)	1:567:A:GLN:HA	1:570:A:LEU:HD13	20	0.14
(1,2160)	1:630:A:ALA:HB2	1:627:A:TYR:HB2	19	0.14
(1,2135)	1:567:A:GLN:HA	1:570:A:LEU:HD13	20	0.14
(1,1987)	1:614:A:ALA:HB2	1:587:A:LEU:HB2	17	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1963)	1:596:A:PHE:HB3	1:591:A:VAL:HG11	2	0.14
(1,1963)	1:596:A:PHE:HB3	1:591:A:VAL:HG11	12	0.14
(1,1937)	1:616:A:GLN:HG3	1:612:A:ALA:HB3	1	0.14
(1,1933)	1:611:A:MET:HB2	1:608:A:LEU:HD23	4	0.14
(1,1933)	1:611:A:MET:HB2	1:608:A:LEU:HD23	10	0.14
(1,1933)	1:611:A:MET:HB2	1:608:A:LEU:HD21	17	0.14
(1,1907)	1:591:A:VAL:HA	1:608:A:LEU:HD22	11	0.14
(1,1907)	1:591:A:VAL:HA	1:608:A:LEU:HD23	16	0.14
(1,1906)	1:590:A:GLN:HB2	1:607:A:VAL:HG12	2	0.14
(1,1867)	1:564:A:TYR:HA	1:567:A:GLN:HA	9	0.14
(1,1849)	1:604:A:THR:HA	1:599:A:GLN:HB2	13	0.14
(1,1813)	1:588:A:GLN:HA	1:584:A:LEU:HD22	6	0.14
(1,1806)	1:577:A:LEU:HA	1:581:A:GLU:HB2	13	0.14
(1,1806)	1:577:A:LEU:HA	1:581:A:GLU:HB2	19	0.14
(1,1787)	1:621:A:ALA:HA	1:620:A:GLN:HB2	10	0.14
(1,1756)	1:614:A:ALA:HB2	1:587:A:LEU:HB2	17	0.14
(1,1730)	1:607:A:VAL:HG23	1:587:A:LEU:HD23	20	0.14
(1,1721)	1:604:A:THR:HG21	1:601:A:HIS:HA	18	0.14
(1,1711)	1:577:A:LEU:HD23	1:626:A:GLU:HG3	8	0.14
(1,1709)	1:625:A:TRP:HD1	1:573:A:LEU:HB2	11	0.14
(1,1708)	1:625:A:TRP:HD1	1:628:A:LEU:HD12	14	0.14
(1,1700)	1:622:A:PHE:HZ	1:618:A:LEU:HD12	7	0.14
(1,1700)	1:622:A:PHE:HZ	1:618:A:LEU:HD13	8	0.14
(1,1694)	1:564:A:TYR:HD2	1:568:A:ARG:HG2	20	0.14
(1,1682)	1:622:A:PHE:HD2	1:577:A:LEU:HD12	10	0.14
(1,1669)	1:633:A:ASN:H	1:631:A:LEU:HB3	3	0.14
(1,1660)	1:631:A:LEU:H	1:631:A:LEU:HD13	19	0.14
(1,1632)	1:622:A:PHE:H	1:619:A:GLU:HB2	9	0.14
(1,1620)	1:619:A:GLU:H	1:615:A:GLU:HA	11	0.14
(1,1594)	1:614:A:ALA:H	1:615:A:GLU:HG3	17	0.14
(1,1549)	1:567:A:GLN:H	1:563:A:SER:HB3	20	0.14
(1,1515)	1:579:A:ASP:H	1:576:A:LEU:HD11	15	0.14
(1,1509)	1:581:A:GLU:H	1:580:A:LEU:HG	4	0.14
(1,1509)	1:581:A:GLU:H	1:580:A:LEU:HG	12	0.14
(1,1503)	1:582:A:ALA:H	1:581:A:GLU:HB2	20	0.14
(1,1484)	1:587:A:LEU:H	1:588:A:GLN:HG2	15	0.14
(1,1484)	1:587:A:LEU:H	1:588:A:GLN:HG2	18	0.14
(1,1474)	1:589:A:THR:H	1:586:A:ALA:HA	11	0.14
(1,1459)	1:593:A:ASP:H	1:594:A:ALA:H	3	0.14
(1,1456)	1:597:A:PHE:H	1:595:A:SER:HA	4	0.14
(1,1456)	1:597:A:PHE:H	1:595:A:SER:HA	12	0.14
(1,1446)	1:568:A:ARG:HD3	1:564:A:TYR:HE2	11	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1437)	1:564:A:TYR:HD2	1:568:A:ARG:HG2	20	0.14
(1,1430)	1:596:A:PHE:HD2	1:608:A:LEU:HD21	2	0.14
(1,1426)	1:627:A:TYR:HD2	1:628:A:LEU:HD21	5	0.14
(1,1418)	1:596:A:PHE:HE2	1:591:A:VAL:HG21	4	0.14
(1,1412)	1:584:A:LEU:HD21	1:615:A:GLU:HB2	17	0.14
(1,1398)	1:587:A:LEU:HD22	1:583:A:LYS:HG2	15	0.14
(1,1384)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	7	0.14
(1,1377)	1:565:A:LYS:HD2	1:563:A:SER:HB2	18	0.14
(1,1374)	1:577:A:LEU:HD12	1:625:A:TRP:HB3	16	0.14
(1,1370)	1:604:A:THR:HG21	1:607:A:VAL:HB	12	0.14
(1,1365)	1:631:A:LEU:HD21	1:566:A:LEU:HD13	3	0.14
(1,1340)	1:573:A:LEU:HA	1:576:A:LEU:HG	9	0.14
(1,1292)	1:577:A:LEU:HD23	1:573:A:LEU:HD11	8	0.14
(1,1292)	1:577:A:LEU:HD22	1:573:A:LEU:HD11	19	0.14
(1,1266)	1:596:A:PHE:HA	1:593:A:ASP:HB3	3	0.14
(1,1244)	1:569:A:GLU:HG3	1:566:A:LEU:HA	18	0.14
(1,1147)	1:565:A:LYS:HA	1:565:A:LYS:HD3	14	0.14
(1,1114)	1:567:A:GLN:HG2	1:562:A:LEU:HB3	8	0.14
(1,1110)	1:628:A:LEU:HB2	1:570:A:LEU:HD23	13	0.14
(1,1061)	1:610:A:ASP:HB3	1:607:A:VAL:HG13	2	0.14
(1,1009)	1:603:A:GLN:HG2	1:599:A:GLN:HB3	16	0.14
(1,1006)	1:567:A:GLN:HG3	1:562:A:LEU:HD12	15	0.14
(1,989)	1:611:A:MET:HG2	1:587:A:LEU:HD13	13	0.14
(1,985)	1:591:A:VAL:HB	1:608:A:LEU:HD21	1	0.14
(1,985)	1:591:A:VAL:HB	1:608:A:LEU:HD22	2	0.14
(1,985)	1:591:A:VAL:HB	1:608:A:LEU:HD22	5	0.14
(1,985)	1:591:A:VAL:HB	1:608:A:LEU:HD23	19	0.14
(1,920)	1:604:A:THR:HB	1:601:A:HIS:HA	18	0.14
(1,858)	1:604:A:THR:HB	1:607:A:VAL:HB	17	0.14
(1,851)	1:604:A:THR:HA	1:608:A:LEU:HD11	15	0.14
(1,820)	1:601:A:HIS:HA	1:605:A:GLN:HB2	3	0.14
(1,819)	1:604:A:THR:HG21	1:601:A:HIS:HA	18	0.14
(1,811)	1:618:A:LEU:HA	1:618:A:LEU:HD21	10	0.14
(1,811)	1:618:A:LEU:HA	1:618:A:LEU:HD22	19	0.14
(1,810)	1:608:A:LEU:HA	1:608:A:LEU:HD12	14	0.14
(1,810)	1:608:A:LEU:HA	1:608:A:LEU:HD13	16	0.14
(1,810)	1:608:A:LEU:HA	1:608:A:LEU:HD11	19	0.14
(1,782)	1:579:A:ASP:HA	1:578:A:GLU:HB2	2	0.14
(1,782)	1:579:A:ASP:HA	1:578:A:GLU:HB2	16	0.14
(1,774)	1:610:A:ASP:HA	1:587:A:LEU:HD13	3	0.14
(1,774)	1:610:A:ASP:HA	1:587:A:LEU:HD11	7	0.14
(1,717)	1:621:A:ALA:HB3	1:577:A:LEU:HD21	7	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,710)	1:594:A:ALA:HB3	1:595:A:SER:HA	9	0.14
(1,664)	1:631:A:LEU:HD21	1:566:A:LEU:HB2	6	0.14
(1,650)	1:591:A:VAL:HG12	1:588:A:GLN:HA	17	0.14
(1,603)	1:622:A:PHE:HD1	1:626:A:GLU:HG2	8	0.14
(1,601)	1:601:A:HIS:HD2	1:605:A:GLN:HB2	10	0.14
(1,601)	1:601:A:HIS:HD2	1:605:A:GLN:HB2	15	0.14
(1,600)	1:601:A:HIS:HD2	1:602:A:GLU:HB3	2	0.14
(1,596)	1:564:A:TYR:HD2	1:564:A:TYR:HA	14	0.14
(1,584)	1:625:A:TRP:HD1	1:570:A:LEU:HD23	1	0.14
(1,584)	1:625:A:TRP:HD1	1:570:A:LEU:HD23	9	0.14
(1,580)	1:625:A:TRP:HE3	1:626:A:GLU:HG3	16	0.14
(1,564)	1:597:A:PHE:HE2	1:591:A:VAL:HG12	14	0.14
(1,557)	1:564:A:TYR:HE2	1:568:A:ARG:HG3	2	0.14
(1,552)	1:596:A:PHE:HD1	1:607:A:VAL:HG22	16	0.14
(1,550)	1:596:A:PHE:HD1	1:604:A:THR:HG23	10	0.14
(1,429)	1:618:A:LEU:H	1:617:A:GLU:HB2	6	0.14
(1,429)	1:618:A:LEU:H	1:617:A:GLU:HB2	9	0.14
(1,249)	1:573:A:LEU:H	1:573:A:LEU:HG	10	0.14
(1,162)	1:584:A:LEU:H	1:583:A:LYS:HG3	1	0.14
(1,162)	1:584:A:LEU:H	1:583:A:LYS:HG3	19	0.14
(1,135)	1:588:A:GLN:H	1:591:A:VAL:HG22	11	0.14
(1,135)	1:588:A:GLN:H	1:591:A:VAL:HG22	20	0.14
(1,78)	1:593:A:ASP:H	1:589:A:THR:HA	5	0.14
(1,18)	1:599:A:GLN:H	1:596:A:PHE:HD1	14	0.14
(1,2169)	1:576:A:LEU:HD12	1:617:A:GLU:HG3	16	0.13
(1,2146)	1:615:A:GLU:HG2	1:584:A:LEU:HG	6	0.13
(1,2146)	1:615:A:GLU:HG2	1:584:A:LEU:HG	13	0.13
(1,2136)	1:573:A:LEU:HA	1:573:A:LEU:HD13	14	0.13
(1,2088)	1:576:A:LEU:HD12	1:617:A:GLU:HG3	16	0.13
(1,2059)	1:615:A:GLU:HA	1:619:A:GLU:HG2	18	0.13
(1,2022)	1:599:A:GLN:HG3	1:600:A:PRO:HD2	3	0.13
(1,2022)	1:599:A:GLN:HG3	1:600:A:PRO:HD2	11	0.13
(1,2022)	1:599:A:GLN:HG3	1:600:A:PRO:HD2	12	0.13
(1,1987)	1:614:A:ALA:HB3	1:587:A:LEU:HB2	11	0.13
(1,1987)	1:614:A:ALA:HB1	1:587:A:LEU:HB2	19	0.13
(1,1951)	1:615:A:GLU:HG2	1:584:A:LEU:HG	6	0.13
(1,1951)	1:615:A:GLU:HG2	1:584:A:LEU:HG	13	0.13
(1,1940)	1:572:A:GLN:HG2	1:568:A:ARG:HG3	10	0.13
(1,1917)	1:585:A:GLU:HB2	1:584:A:LEU:HD12	7	0.13
(1,1894)	1:562:A:LEU:HG	1:567:A:GLN:HG3	8	0.13
(1,1828)	1:601:A:HIS:HA	1:602:A:GLU:HG3	4	0.13
(1,1828)	1:601:A:HIS:HA	1:603:A:GLN:HG3	10	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1795)	1:579:A:ASP:HA	1:583:A:LYS:HB2	6	0.13
(1,1756)	1:614:A:ALA:HB3	1:587:A:LEU:HB2	11	0.13
(1,1756)	1:614:A:ALA:HB1	1:587:A:LEU:HB2	19	0.13
(1,1736)	1:607:A:VAL:HG13	1:608:A:LEU:HG	6	0.13
(1,1721)	1:604:A:THR:HG22	1:601:A:HIS:HA	16	0.13
(1,1718)	1:604:A:THR:HG22	1:599:A:GLN:HG3	15	0.13
(1,1682)	1:622:A:PHE:HD2	1:577:A:LEU:HD11	8	0.13
(1,1669)	1:633:A:ASN:H	1:631:A:LEU:HB3	6	0.13
(1,1669)	1:633:A:ASN:H	1:632:A:LYS:HG3	19	0.13
(1,1668)	1:633:A:ASN:H	1:629:A:GLU:HA	10	0.13
(1,1660)	1:631:A:LEU:H	1:631:A:LEU:HD11	18	0.13
(1,1635)	1:623:A:GLU:H	1:622:A:PHE:HD1	5	0.13
(1,1635)	1:623:A:GLU:H	1:622:A:PHE:HD1	6	0.13
(1,1635)	1:623:A:GLU:H	1:622:A:PHE:HD1	7	0.13
(1,1635)	1:623:A:GLU:H	1:622:A:PHE:HD1	8	0.13
(1,1617)	1:617:A:GLU:H	1:580:A:LEU:HD23	13	0.13
(1,1594)	1:614:A:ALA:H	1:616:A:GLN:HB2	18	0.13
(1,1584)	1:611:A:MET:H	1:587:A:LEU:HD21	12	0.13
(1,1584)	1:611:A:MET:H	1:587:A:LEU:HD22	13	0.13
(1,1568)	1:607:A:VAL:H	1:606:A:LYS:HG2	12	0.13
(1,1549)	1:567:A:GLN:H	1:563:A:SER:HB3	8	0.13
(1,1546)	1:568:A:ARG:H	1:567:A:GLN:HG3	20	0.13
(1,1530)	1:573:A:LEU:H	1:572:A:GLN:HB3	16	0.13
(1,1509)	1:625:A:TRP:H	1:624:A:ARG:HG2	20	0.13
(1,1474)	1:589:A:THR:H	1:586:A:ALA:HA	5	0.13
(1,1456)	1:597:A:PHE:H	1:595:A:SER:HA	1	0.13
(1,1446)	1:568:A:ARG:HD3	1:564:A:TYR:HE2	15	0.13
(1,1425)	1:596:A:PHE:HE1	1:607:A:VAL:HG13	8	0.13
(1,1419)	1:596:A:PHE:HZ	1:591:A:VAL:HG21	4	0.13
(1,1418)	1:596:A:PHE:HE2	1:591:A:VAL:HG23	3	0.13
(1,1418)	1:596:A:PHE:HE2	1:591:A:VAL:HG23	10	0.13
(1,1418)	1:596:A:PHE:HE2	1:591:A:VAL:HG21	18	0.13
(1,1412)	1:584:A:LEU:HD22	1:615:A:GLU:HB2	19	0.13
(1,1399)	1:583:A:LYS:HG2	1:580:A:LEU:HD22	6	0.13
(1,1398)	1:587:A:LEU:HD21	1:583:A:LYS:HG2	20	0.13
(1,1390)	1:599:A:GLN:HG3	1:600:A:PRO:HD2	3	0.13
(1,1390)	1:599:A:GLN:HG3	1:600:A:PRO:HD2	11	0.13
(1,1390)	1:599:A:GLN:HG3	1:600:A:PRO:HD2	12	0.13
(1,1384)	1:602:A:GLU:HG3	1:601:A:HIS:HB2	4	0.13
(1,1382)	1:573:A:LEU:HD13	1:624:A:ARG:HG2	1	0.13
(1,1381)	1:573:A:LEU:HD13	1:624:A:ARG:HB2	4	0.13
(1,1367)	1:570:A:LEU:HD23	1:628:A:LEU:HB3	11	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1340)	1:573:A:LEU:HA	1:576:A:LEU:HG	3	0.13
(1,1340)	1:573:A:LEU:HA	1:576:A:LEU:HG	4	0.13
(1,1324)	1:628:A:LEU:HA	1:628:A:LEU:HD12	12	0.13
(1,1292)	1:577:A:LEU:HD21	1:573:A:LEU:HD13	16	0.13
(1,1266)	1:596:A:PHE:HA	1:593:A:ASP:HB3	8	0.13
(1,1244)	1:569:A:GLU:HG3	1:566:A:LEU:HA	12	0.13
(1,1210)	1:606:A:LYS:HA	1:605:A:GLN:HB2	4	0.13
(1,1165)	1:601:A:HIS:HB2	1:605:A:GLN:HG2	8	0.13
(1,1136)	1:600:A:PRO:HD3	1:603:A:GLN:HB2	4	0.13
(1,1056)	1:622:A:PHE:HB2	1:577:A:LEU:HD22	10	0.13
(1,1040)	1:629:A:GLU:HG3	1:570:A:LEU:HD11	5	0.13
(1,1040)	1:629:A:GLU:HG3	1:570:A:LEU:HD12	11	0.13
(1,1040)	1:629:A:GLU:HG3	1:570:A:LEU:HD13	15	0.13
(1,1020)	1:604:A:THR:HG22	1:599:A:GLN:HG3	15	0.13
(1,998)	1:583:A:LYS:HB3	1:587:A:LEU:HD13	5	0.13
(1,977)	1:617:A:GLU:HB2	1:580:A:LEU:HD11	15	0.13
(1,972)	1:629:A:GLU:HB2	1:570:A:LEU:HD12	18	0.13
(1,966)	1:591:A:VAL:HA	1:608:A:LEU:HD22	9	0.13
(1,928)	1:583:A:LYS:HG3	1:587:A:LEU:HD22	10	0.13
(1,881)	1:568:A:ARG:HA	1:568:A:ARG:HD2	15	0.13
(1,859)	1:604:A:THR:HB	1:608:A:LEU:HD23	14	0.13
(1,858)	1:604:A:THR:HB	1:607:A:VAL:HB	4	0.13
(1,851)	1:604:A:THR:HA	1:608:A:LEU:HD12	19	0.13
(1,819)	1:604:A:THR:HG22	1:601:A:HIS:HA	16	0.13
(1,811)	1:618:A:LEU:HA	1:618:A:LEU:HD23	1	0.13
(1,811)	1:618:A:LEU:HA	1:618:A:LEU:HD21	7	0.13
(1,782)	1:579:A:ASP:HA	1:578:A:GLU:HB2	4	0.13
(1,774)	1:610:A:ASP:HA	1:587:A:LEU:HD13	8	0.13
(1,774)	1:610:A:ASP:HA	1:587:A:LEU:HD12	9	0.13
(1,717)	1:621:A:ALA:HB3	1:577:A:LEU:HD21	15	0.13
(1,708)	1:592:A:ALA:HB2	1:593:A:ASP:HA	12	0.13
(1,708)	1:592:A:ALA:HB1	1:593:A:ASP:HA	13	0.13
(1,708)	1:592:A:ALA:HB3	1:593:A:ASP:HA	14	0.13
(1,708)	1:592:A:ALA:HB1	1:593:A:ASP:HA	18	0.13
(1,664)	1:631:A:LEU:HD23	1:566:A:LEU:HB2	19	0.13
(1,652)	1:591:A:VAL:HG13	1:608:A:LEU:HA	12	0.13
(1,650)	1:591:A:VAL:HG13	1:588:A:GLN:HA	14	0.13
(1,634)	1:577:A:LEU:HD13	1:574:A:PRO:HA	8	0.13
(1,599)	1:601:A:HIS:HD2	1:602:A:GLU:HG2	8	0.13
(1,599)	1:601:A:HIS:HD2	1:602:A:GLU:HG2	15	0.13
(1,585)	1:596:A:PHE:HZ	1:607:A:VAL:HG12	17	0.13
(1,581)	1:601:A:HIS:HD2	1:605:A:GLN:HG3	17	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,507)	1:629:A:GLU:H	1:570:A:LEU:HD21	2	0.13
(1,429)	1:618:A:LEU:H	1:617:A:GLU:HB2	3	0.13
(1,429)	1:618:A:LEU:H	1:617:A:GLU:HB2	18	0.13
(1,369)	1:609:A:ALA:H	1:608:A:LEU:HD13	2	0.13
(1,369)	1:609:A:ALA:H	1:608:A:LEU:HD12	13	0.13
(1,369)	1:609:A:ALA:H	1:608:A:LEU:HD12	20	0.13
(1,307)	1:566:A:LEU:H	1:566:A:LEU:HD13	10	0.13
(1,182)	1:581:A:GLU:H	1:580:A:LEU:HD11	8	0.13
(1,182)	1:581:A:GLU:H	1:580:A:LEU:HD13	16	0.13
(1,182)	1:581:A:GLU:H	1:580:A:LEU:HD12	19	0.13
(1,162)	1:584:A:LEU:H	1:583:A:LYS:HG3	17	0.13
(1,149)	1:586:A:ALA:H	1:589:A:THR:HG21	16	0.13
(1,135)	1:588:A:GLN:H	1:591:A:VAL:HG21	9	0.13
(1,123)	1:589:A:THR:H	1:592:A:ALA:HB1	14	0.13
(1,110)	1:590:A:GLN:H	1:590:A:GLN:HG3	15	0.13
(2,12)	1:583:A:LYS:N	1:579:A:ASP:O	6	0.12
(2,2)	1:577:A:LEU:N	1:573:A:LEU:O	6	0.12
(1,2175)	1:597:A:PHE:HD1	1:604:A:THR:HB	7	0.12
(1,2169)	1:576:A:LEU:HD12	1:617:A:GLU:HG3	14	0.12
(1,2124)	1:612:A:ALA:HA	1:611:A:MET:HE2	20	0.12
(1,2118)	1:583:A:LYS:HE2	1:580:A:LEU:HD22	9	0.12
(1,2088)	1:576:A:LEU:HD12	1:617:A:GLU:HG3	14	0.12
(1,2051)	1:603:A:GLN:HG2	1:600:A:PRO:HA	20	0.12
(1,2036)	1:561:A:LYS:HD3	1:561:A:LYS:HA	11	0.12
(1,2036)	1:561:A:LYS:HD2	1:561:A:LYS:HA	20	0.12
(1,2022)	1:599:A:GLN:HG3	1:600:A:PRO:HD2	9	0.12
(1,1987)	1:614:A:ALA:HB2	1:587:A:LEU:HB2	6	0.12
(1,1963)	1:596:A:PHE:HB3	1:591:A:VAL:HG12	6	0.12
(1,1933)	1:611:A:MET:HB2	1:584:A:LEU:HD21	12	0.12
(1,1933)	1:611:A:MET:HB2	1:608:A:LEU:HD23	19	0.12
(1,1907)	1:591:A:VAL:HA	1:608:A:LEU:HD23	1	0.12
(1,1889)	1:568:A:ARG:HG3	1:571:A:GLU:HB2	6	0.12
(1,1828)	1:601:A:HIS:HA	1:602:A:GLU:HG3	3	0.12
(1,1813)	1:588:A:GLN:HA	1:584:A:LEU:HD23	11	0.12
(1,1756)	1:614:A:ALA:HB2	1:587:A:LEU:HB2	6	0.12
(1,1745)	1:614:A:ALA:HB1	1:580:A:LEU:HD23	16	0.12
(1,1736)	1:607:A:VAL:HG12	1:608:A:LEU:HG	18	0.12
(1,1731)	1:607:A:VAL:HG21	1:603:A:GLN:HB3	2	0.12
(1,1718)	1:604:A:THR:HG21	1:599:A:GLN:HG3	4	0.12
(1,1710)	1:577:A:LEU:HD23	1:574:A:PRO:HG3	7	0.12
(1,1710)	1:577:A:LEU:HD21	1:574:A:PRO:HG3	15	0.12
(1,1709)	1:625:A:TRP:HD1	1:573:A:LEU:HB2	2	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1709)	1:625:A:TRP:HD1	1:573:A:LEU:HB2	4	0.12
(1,1702)	1:622:A:PHE:HD1	1:626:A:GLU:HG3	15	0.12
(1,1700)	1:622:A:PHE:HZ	1:618:A:LEU:HD11	13	0.12
(1,1698)	1:564:A:TYR:HD1	1:567:A:GLN:HB2	6	0.12
(1,1683)	1:622:A:PHE:HE2	1:618:A:LEU:HD23	5	0.12
(1,1670)	1:633:A:ASN:H	1:631:A:LEU:HB2	16	0.12
(1,1660)	1:631:A:LEU:H	1:631:A:LEU:HD11	20	0.12
(1,1635)	1:623:A:GLU:H	1:622:A:PHE:HD1	2	0.12
(1,1635)	1:623:A:GLU:H	1:622:A:PHE:HD1	9	0.12
(1,1632)	1:622:A:PHE:H	1:619:A:GLU:HB2	13	0.12
(1,1588)	1:583:A:LYS:H	1:581:A:GLU:HG2	14	0.12
(1,1586)	1:613:A:ALA:H	1:612:A:ALA:HA	2	0.12
(1,1586)	1:613:A:ALA:H	1:612:A:ALA:HA	20	0.12
(1,1577)	1:609:A:ALA:H	1:608:A:LEU:HG	8	0.12
(1,1569)	1:607:A:VAL:H	1:608:A:LEU:HD23	19	0.12
(1,1562)	1:604:A:THR:H	1:599:A:GLN:HB2	2	0.12
(1,1546)	1:568:A:ARG:H	1:567:A:GLN:HG3	4	0.12
(1,1546)	1:568:A:ARG:H	1:567:A:GLN:HG3	9	0.12
(1,1534)	1:572:A:GLN:H	1:572:A:GLN:HB3	7	0.12
(1,1520)	1:577:A:LEU:H	1:578:A:GLU:HG3	9	0.12
(1,1488)	1:586:A:ALA:H	1:583:A:LYS:HA	3	0.12
(1,1488)	1:586:A:ALA:H	1:583:A:LYS:HA	7	0.12
(1,1488)	1:586:A:ALA:H	1:583:A:LYS:HA	9	0.12
(1,1488)	1:586:A:ALA:H	1:583:A:LYS:HA	12	0.12
(1,1487)	1:587:A:LEU:H	1:587:A:LEU:HD23	6	0.12
(1,1484)	1:587:A:LEU:H	1:588:A:GLN:HG2	8	0.12
(1,1484)	1:587:A:LEU:H	1:588:A:GLN:HG2	19	0.12
(1,1474)	1:589:A:THR:H	1:586:A:ALA:HA	4	0.12
(1,1456)	1:597:A:PHE:H	1:595:A:SER:HA	19	0.12
(1,1451)	1:599:A:GLN:H	1:600:A:PRO:HD3	8	0.12
(1,1451)	1:599:A:GLN:H	1:600:A:PRO:HD3	16	0.12
(1,1446)	1:568:A:ARG:HD3	1:564:A:TYR:HE1	4	0.12
(1,1420)	1:627:A:TYR:HE1	1:631:A:LEU:HD23	9	0.12
(1,1414)	1:596:A:PHE:HD2	1:591:A:VAL:HG11	2	0.12
(1,1390)	1:599:A:GLN:HG3	1:600:A:PRO:HD2	9	0.12
(1,1365)	1:631:A:LEU:HD23	1:566:A:LEU:HD11	19	0.12
(1,1363)	1:562:A:LEU:HD22	1:631:A:LEU:HB2	17	0.12
(1,1317)	1:611:A:MET:HA	1:587:A:LEU:HD21	12	0.12
(1,1266)	1:596:A:PHE:HA	1:593:A:ASP:HB3	17	0.12
(1,1266)	1:596:A:PHE:HA	1:593:A:ASP:HB3	19	0.12
(1,1265)	1:593:A:ASP:HB3	1:595:A:SER:HB3	7	0.12
(1,1250)	1:626:A:GLU:HG2	1:623:A:GLU:HA	17	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1246)	1:582:A:ALA:HA	1:585:A:GLU:HG3	13	0.12
(1,1244)	1:569:A:GLU:HG3	1:566:A:LEU:HA	3	0.12
(1,1244)	1:569:A:GLU:HG3	1:566:A:LEU:HA	4	0.12
(1,1210)	1:606:A:LYS:HA	1:605:A:GLN:HB3	14	0.12
(1,1110)	1:628:A:LEU:HB2	1:570:A:LEU:HD22	18	0.12
(1,1023)	1:590:A:GLN:HG3	1:587:A:LEU:HD22	20	0.12
(1,1020)	1:604:A:THR:HG21	1:599:A:GLN:HG3	4	0.12
(1,922)	1:612:A:ALA:HB3	1:611:A:MET:HE2	17	0.12
(1,920)	1:604:A:THR:HB	1:601:A:HIS:HA	2	0.12
(1,920)	1:604:A:THR:HB	1:601:A:HIS:HA	11	0.12
(1,858)	1:604:A:THR:HB	1:607:A:VAL:HB	11	0.12
(1,858)	1:604:A:THR:HB	1:607:A:VAL:HB	16	0.12
(1,851)	1:604:A:THR:HA	1:608:A:LEU:HD11	5	0.12
(1,811)	1:618:A:LEU:HA	1:618:A:LEU:HD23	8	0.12
(1,810)	1:608:A:LEU:HA	1:608:A:LEU:HD11	4	0.12
(1,810)	1:608:A:LEU:HA	1:608:A:LEU:HD13	18	0.12
(1,805)	1:629:A:GLU:HA	1:570:A:LEU:HD22	18	0.12
(1,756)	1:630:A:ALA:HA	1:629:A:GLU:HB2	19	0.12
(1,730)	1:600:A:PRO:HD3	1:603:A:GLN:HG2	9	0.12
(1,712)	1:594:A:ALA:HB1	1:593:A:ASP:HA	18	0.12
(1,710)	1:594:A:ALA:HB3	1:595:A:SER:HA	6	0.12
(1,710)	1:594:A:ALA:HB3	1:595:A:SER:HA	10	0.12
(1,642)	1:604:A:THR:HG22	1:596:A:PHE:HA	7	0.12
(1,642)	1:604:A:THR:HG22	1:596:A:PHE:HA	11	0.12
(1,636)	1:577:A:LEU:HD12	1:621:A:ALA:HA	6	0.12
(1,601)	1:601:A:HIS:HD2	1:605:A:GLN:HB2	14	0.12
(1,600)	1:601:A:HIS:HD2	1:602:A:GLU:HB3	3	0.12
(1,600)	1:601:A:HIS:HD2	1:602:A:GLU:HB3	15	0.12
(1,592)	1:627:A:TYR:HE2	1:628:A:LEU:HG	4	0.12
(1,585)	1:596:A:PHE:HZ	1:607:A:VAL:HG12	4	0.12
(1,555)	1:627:A:TYR:HE2	1:566:A:LEU:HD22	1	0.12
(1,554)	1:627:A:TYR:HE2	1:628:A:LEU:HD21	2	0.12
(1,552)	1:596:A:PHE:HD1	1:607:A:VAL:HG22	9	0.12
(1,446)	1:620:A:GLN:H	1:619:A:GLU:HG3	6	0.12
(1,429)	1:618:A:LEU:H	1:617:A:GLU:HB2	10	0.12
(1,429)	1:618:A:LEU:H	1:617:A:GLU:HB2	17	0.12
(1,317)	1:563:A:SER:H	1:566:A:LEU:HD21	5	0.12
(1,314)	1:565:A:LYS:H	1:565:A:LYS:HG3	19	0.12
(1,273)	1:570:A:LEU:H	1:569:A:GLU:HB2	6	0.12
(1,262)	1:571:A:GLU:H	1:571:A:GLU:HG2	4	0.12
(1,262)	1:571:A:GLU:H	1:571:A:GLU:HG2	9	0.12
(1,248)	1:573:A:LEU:H	1:572:A:GLN:HB2	3	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,182)	1:581:A:GLU:H	1:580:A:LEU:HD12	12	0.12
(1,182)	1:581:A:GLU:H	1:580:A:LEU:HD11	13	0.12
(1,182)	1:581:A:GLU:H	1:580:A:LEU:HD13	20	0.12
(1,149)	1:586:A:ALA:H	1:589:A:THR:HG23	12	0.12
(1,74)	1:606:A:LYS:H	1:603:A:GLN:HA	9	0.12
(1,64)	1:595:A:SER:H	1:596:A:PHE:HB2	2	0.12
(1,64)	1:595:A:SER:H	1:596:A:PHE:HB2	3	0.12
(2,2)	1:577:A:LEU:N	1:573:A:LEU:O	13	0.11
(1,2163)	1:567:A:GLN:HA	1:570:A:LEU:HD12	12	0.11
(1,2151)	1:628:A:LEU:HB3	1:625:A:TRP:HA	14	0.11
(1,2136)	1:573:A:LEU:HA	1:573:A:LEU:HD13	11	0.11
(1,2135)	1:567:A:GLN:HA	1:570:A:LEU:HD12	12	0.11
(1,2124)	1:612:A:ALA:HA	1:611:A:MET:HE3	6	0.11
(1,2121)	1:581:A:GLU:HG2	1:618:A:LEU:HD21	8	0.11
(1,2042)	1:573:A:LEU:HG	1:570:A:LEU:HA	6	0.11
(1,2028)	1:564:A:TYR:HB2	1:567:A:GLN:HB2	10	0.11
(1,2025)	1:622:A:PHE:HB3	1:623:A:GLU:HG3	9	0.11
(1,2022)	1:599:A:GLN:HG3	1:600:A:PRO:HD2	2	0.11
(1,1987)	1:614:A:ALA:HB2	1:587:A:LEU:HB2	8	0.11
(1,1978)	1:583:A:LYS:HE3	1:587:A:LEU:HD22	14	0.11
(1,1963)	1:596:A:PHE:HB3	1:591:A:VAL:HG11	5	0.11
(1,1960)	1:622:A:PHE:HB3	1:623:A:GLU:HG3	9	0.11
(1,1946)	1:581:A:GLU:HG2	1:618:A:LEU:HD21	8	0.11
(1,1941)	1:616:A:GLN:HG2	1:613:A:ALA:HB2	20	0.11
(1,1933)	1:611:A:MET:HB2	1:584:A:LEU:HD23	8	0.11
(1,1911)	1:581:A:GLU:HB3	1:618:A:LEU:HD13	3	0.11
(1,1895)	1:618:A:LEU:HG	1:619:A:GLU:HB3	17	0.11
(1,1889)	1:568:A:ARG:HG3	1:571:A:GLU:HB2	8	0.11
(1,1889)	1:568:A:ARG:HG3	1:571:A:GLU:HB2	12	0.11
(1,1867)	1:564:A:TYR:HA	1:567:A:GLN:HA	7	0.11
(1,1790)	1:557:A:ARG:HA	1:555:A:VAL:HG22	5	0.11
(1,1787)	1:621:A:ALA:HA	1:620:A:GLN:HB3	1	0.11
(1,1781)	1:609:A:ALA:HA	1:608:A:LEU:HB2	10	0.11
(1,1781)	1:609:A:ALA:HA	1:608:A:LEU:HB2	18	0.11
(1,1779)	1:614:A:ALA:HA	1:580:A:LEU:HD13	8	0.11
(1,1756)	1:614:A:ALA:HB2	1:587:A:LEU:HB2	8	0.11
(1,1736)	1:607:A:VAL:HG12	1:608:A:LEU:HG	12	0.11
(1,1710)	1:577:A:LEU:HD23	1:574:A:PRO:HG3	4	0.11
(1,1710)	1:577:A:LEU:HD21	1:574:A:PRO:HG3	9	0.11
(1,1710)	1:577:A:LEU:HD21	1:574:A:PRO:HG3	10	0.11
(1,1700)	1:622:A:PHE:HZ	1:618:A:LEU:HD12	3	0.11
(1,1700)	1:622:A:PHE:HZ	1:618:A:LEU:HD13	12	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1700)	1:622:A:PHE:HZ	1:618:A:LEU:HD13	17	0.11
(1,1660)	1:631:A:LEU:H	1:631:A:LEU:HD11	15	0.11
(1,1617)	1:617:A:GLU:H	1:580:A:LEU:HD23	12	0.11
(1,1614)	1:617:A:GLU:H	1:617:A:GLU:HG2	2	0.11
(1,1586)	1:613:A:ALA:H	1:612:A:ALA:HA	3	0.11
(1,1586)	1:613:A:ALA:H	1:612:A:ALA:HA	8	0.11
(1,1586)	1:613:A:ALA:H	1:612:A:ALA:HA	10	0.11
(1,1586)	1:613:A:ALA:H	1:612:A:ALA:HA	13	0.11
(1,1586)	1:613:A:ALA:H	1:612:A:ALA:HA	14	0.11
(1,1586)	1:613:A:ALA:H	1:612:A:ALA:HA	17	0.11
(1,1577)	1:609:A:ALA:H	1:608:A:LEU:HG	13	0.11
(1,1569)	1:607:A:VAL:H	1:587:A:LEU:HD21	6	0.11
(1,1562)	1:604:A:THR:H	1:599:A:GLN:HB2	1	0.11
(1,1553)	1:566:A:LEU:H	1:565:A:LYS:HB3	16	0.11
(1,1549)	1:567:A:GLN:H	1:563:A:SER:HB3	12	0.11
(1,1538)	1:571:A:GLU:H	1:570:A:LEU:HD12	6	0.11
(1,1530)	1:573:A:LEU:H	1:572:A:GLN:HB3	2	0.11
(1,1488)	1:586:A:ALA:H	1:583:A:LYS:HA	13	0.11
(1,1487)	1:587:A:LEU:H	1:587:A:LEU:HD23	10	0.11
(1,1456)	1:597:A:PHE:H	1:595:A:SER:HA	14	0.11
(1,1446)	1:568:A:ARG:HD3	1:564:A:TYR:HE2	2	0.11
(1,1446)	1:568:A:ARG:HD3	1:564:A:TYR:HE2	19	0.11
(1,1431)	1:622:A:PHE:HE2	1:618:A:LEU:HD23	5	0.11
(1,1425)	1:596:A:PHE:HE1	1:607:A:VAL:HG12	15	0.11
(1,1418)	1:596:A:PHE:HE2	1:591:A:VAL:HG21	14	0.11
(1,1415)	1:596:A:PHE:HE2	1:591:A:VAL:HG11	2	0.11
(1,1414)	1:596:A:PHE:HD2	1:591:A:VAL:HG11	4	0.11
(1,1414)	1:596:A:PHE:HD2	1:591:A:VAL:HG13	10	0.11
(1,1414)	1:596:A:PHE:HD2	1:591:A:VAL:HG12	11	0.11
(1,1414)	1:596:A:PHE:HD2	1:591:A:VAL:HG11	14	0.11
(1,1398)	1:587:A:LEU:HD21	1:583:A:LYS:HG2	18	0.11
(1,1390)	1:599:A:GLN:HG3	1:600:A:PRO:HD2	2	0.11
(1,1378)	1:624:A:ARG:HD3	1:573:A:LEU:HD11	9	0.11
(1,1377)	1:565:A:LYS:HD2	1:563:A:SER:HB2	7	0.11
(1,1374)	1:577:A:LEU:HD11	1:625:A:TRP:HB3	1	0.11
(1,1374)	1:577:A:LEU:HD12	1:625:A:TRP:HB3	6	0.11
(1,1374)	1:577:A:LEU:HD11	1:625:A:TRP:HB3	19	0.11
(1,1340)	1:573:A:LEU:HA	1:576:A:LEU:HG	10	0.11
(1,1340)	1:573:A:LEU:HA	1:576:A:LEU:HG	17	0.11
(1,1333)	1:573:A:LEU:HD13	1:624:A:ARG:HD2	20	0.11
(1,1324)	1:628:A:LEU:HA	1:628:A:LEU:HD12	10	0.11
(1,1324)	1:628:A:LEU:HA	1:628:A:LEU:HD13	13	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1319)	1:567:A:GLN:HA	1:562:A:LEU:HD12	5	0.11
(1,1307)	1:566:A:LEU:HD12	1:565:A:LYS:HA	19	0.11
(1,1292)	1:577:A:LEU:HD22	1:573:A:LEU:HD12	3	0.11
(1,1292)	1:577:A:LEU:HD21	1:573:A:LEU:HD11	17	0.11
(1,1266)	1:596:A:PHE:HA	1:593:A:ASP:HB3	20	0.11
(1,1246)	1:582:A:ALA:HA	1:585:A:GLU:HG3	4	0.11
(1,1210)	1:606:A:LYS:HA	1:605:A:GLN:HB3	3	0.11
(1,1110)	1:628:A:LEU:HB2	1:570:A:LEU:HD22	20	0.11
(1,1062)	1:610:A:ASP:HB2	1:587:A:LEU:HD21	10	0.11
(1,990)	1:591:A:VAL:HG21	1:611:A:MET:HG2	3	0.11
(1,990)	1:591:A:VAL:HG23	1:611:A:MET:HG2	12	0.11
(1,990)	1:591:A:VAL:HG22	1:611:A:MET:HG2	18	0.11
(1,970)	1:632:A:LYS:HD3	1:570:A:LEU:HD12	2	0.11
(1,970)	1:632:A:LYS:HD3	1:570:A:LEU:HD13	11	0.11
(1,966)	1:591:A:VAL:HA	1:608:A:LEU:HD22	12	0.11
(1,966)	1:591:A:VAL:HA	1:608:A:LEU:HD21	13	0.11
(1,928)	1:583:A:LYS:HG3	1:587:A:LEU:HD21	1	0.11
(1,928)	1:583:A:LYS:HG3	1:587:A:LEU:HD22	11	0.11
(1,920)	1:604:A:THR:HB	1:601:A:HIS:HA	4	0.11
(1,920)	1:604:A:THR:HB	1:601:A:HIS:HA	9	0.11
(1,870)	1:556:A:LYS:HA	1:556:A:LYS:HE3	5	0.11
(1,858)	1:604:A:THR:HB	1:607:A:VAL:HB	9	0.11
(1,847)	1:622:A:PHE:HA	1:621:A:ALA:HB3	16	0.11
(1,811)	1:618:A:LEU:HA	1:618:A:LEU:HD23	4	0.11
(1,811)	1:618:A:LEU:HA	1:618:A:LEU:HD22	9	0.11
(1,811)	1:618:A:LEU:HA	1:618:A:LEU:HD22	11	0.11
(1,805)	1:629:A:GLU:HA	1:570:A:LEU:HD23	8	0.11
(1,805)	1:629:A:GLU:HA	1:570:A:LEU:HD21	10	0.11
(1,805)	1:629:A:GLU:HA	1:570:A:LEU:HD22	20	0.11
(1,782)	1:579:A:ASP:HA	1:578:A:GLU:HB2	10	0.11
(1,782)	1:579:A:ASP:HA	1:578:A:GLU:HB2	19	0.11
(1,710)	1:594:A:ALA:HB3	1:595:A:SER:HA	16	0.11
(1,710)	1:594:A:ALA:HB3	1:595:A:SER:HA	17	0.11
(1,668)	1:631:A:LEU:HD13	1:635:A:GLY:HA2	9	0.11
(1,650)	1:591:A:VAL:HG13	1:588:A:GLN:HA	4	0.11
(1,650)	1:591:A:VAL:HG12	1:588:A:GLN:HA	18	0.11
(1,621)	1:577:A:LEU:HD21	1:573:A:LEU:HA	9	0.11
(1,609)	1:625:A:TRP:HD1	1:573:A:LEU:HD13	13	0.11
(1,600)	1:601:A:HIS:HD2	1:602:A:GLU:HB3	20	0.11
(1,599)	1:601:A:HIS:HD2	1:602:A:GLU:HG3	7	0.11
(1,571)	1:622:A:PHE:HD2	1:619:A:GLU:HA	14	0.11
(1,554)	1:627:A:TYR:HE2	1:628:A:LEU:HD22	15	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,552)	1:596:A:PHE:HD1	1:607:A:VAL:HG22	19	0.11
(1,369)	1:609:A:ALA:H	1:608:A:LEU:HD13	14	0.11
(1,369)	1:609:A:ALA:H	1:608:A:LEU:HD11	16	0.11
(1,314)	1:565:A:LYS:H	1:565:A:LYS:HG3	9	0.11
(1,276)	1:570:A:LEU:H	1:570:A:LEU:HD23	9	0.11
(1,274)	1:570:A:LEU:H	1:569:A:GLU:HG2	4	0.11
(1,248)	1:573:A:LEU:H	1:572:A:GLN:HB2	4	0.11
(1,123)	1:589:A:THR:H	1:592:A:ALA:HB3	9	0.11
(1,123)	1:589:A:THR:H	1:592:A:ALA:HB2	19	0.11
(1,110)	1:590:A:GLN:H	1:590:A:GLN:HG3	12	0.11
(1,110)	1:590:A:GLN:H	1:590:A:GLN:HG3	20	0.11
(1,78)	1:593:A:ASP:H	1:589:A:THR:HA	20	0.11
(1,18)	1:599:A:GLN:H	1:596:A:PHE:HD1	6	0.11
(2,36)	1:621:A:ALA:N	1:617:A:GLU:O	2	0.1
(2,12)	1:583:A:LYS:N	1:579:A:ASP:O	1	0.1
(1,2155)	1:628:A:LEU:HD11	1:624:A:ARG:HB2	8	0.1
(1,2136)	1:573:A:LEU:HA	1:573:A:LEU:HD11	13	0.1
(1,2136)	1:573:A:LEU:HA	1:573:A:LEU:HD12	17	0.1
(1,2136)	1:573:A:LEU:HA	1:573:A:LEU:HD12	20	0.1
(1,2028)	1:564:A:TYR:HB2	1:567:A:GLN:HB2	5	0.1
(1,2022)	1:599:A:GLN:HG3	1:600:A:PRO:HD2	20	0.1
(1,1967)	1:579:A:ASP:HB3	1:576:A:LEU:HG	19	0.1
(1,1961)	1:610:A:ASP:HB3	1:587:A:LEU:HB3	18	0.1
(1,1949)	1:612:A:ALA:HB2	1:615:A:GLU:HG2	13	0.1
(1,1939)	1:572:A:GLN:HG3	1:568:A:ARG:HG2	14	0.1
(1,1895)	1:618:A:LEU:HG	1:619:A:GLU:HB3	7	0.1
(1,1789)	1:556:A:LYS:HA	1:555:A:VAL:HG22	13	0.1
(1,1789)	1:556:A:LYS:HA	1:555:A:VAL:HG11	16	0.1
(1,1781)	1:609:A:ALA:HA	1:608:A:LEU:HB2	12	0.1
(1,1779)	1:614:A:ALA:HA	1:580:A:LEU:HD13	11	0.1
(1,1755)	1:612:A:ALA:HB2	1:615:A:GLU:HG2	13	0.1
(1,1745)	1:614:A:ALA:HB3	1:580:A:LEU:HD23	15	0.1
(1,1698)	1:564:A:TYR:HD2	1:567:A:GLN:HB2	4	0.1
(1,1683)	1:622:A:PHE:HE2	1:618:A:LEU:HD23	9	0.1
(1,1586)	1:613:A:ALA:H	1:612:A:ALA:HA	5	0.1
(1,1569)	1:607:A:VAL:H	1:587:A:LEU:HD21	14	0.1
(1,1563)	1:605:A:GLN:H	1:605:A:GLN:HE22	10	0.1
(1,1530)	1:573:A:LEU:H	1:572:A:GLN:HB3	7	0.1
(1,1515)	1:579:A:ASP:H	1:576:A:LEU:HD12	18	0.1
(1,1487)	1:587:A:LEU:H	1:587:A:LEU:HD22	8	0.1
(1,1456)	1:597:A:PHE:H	1:595:A:SER:HA	10	0.1
(1,1446)	1:568:A:ARG:HD3	1:564:A:TYR:HE1	14	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1425)	1:596:A:PHE:HE1	1:607:A:VAL:HG11	11	0.1
(1,1390)	1:599:A:GLN:HG3	1:600:A:PRO:HD2	20	0.1
(1,1374)	1:577:A:LEU:HD13	1:625:A:TRP:HB3	11	0.1
(1,1292)	1:577:A:LEU:HD21	1:573:A:LEU:HD11	20	0.1
(1,1264)	1:568:A:ARG:HD2	1:564:A:TYR:HA	11	0.1
(1,1244)	1:569:A:GLU:HG3	1:566:A:LEU:HA	17	0.1
(1,1063)	1:610:A:ASP:HB2	1:587:A:LEU:HD13	18	0.1
(1,881)	1:568:A:ARG:HA	1:568:A:ARG:HD2	3	0.1
(1,859)	1:604:A:THR:HB	1:608:A:LEU:HD22	6	0.1
(1,858)	1:604:A:THR:HB	1:607:A:VAL:HB	15	0.1
(1,811)	1:618:A:LEU:HA	1:618:A:LEU:HD21	3	0.1
(1,708)	1:592:A:ALA:HB1	1:593:A:ASP:HA	20	0.1
(1,652)	1:591:A:VAL:HG13	1:608:A:LEU:HA	14	0.1
(1,642)	1:604:A:THR:HG21	1:596:A:PHE:HA	2	0.1
(1,507)	1:629:A:GLU:H	1:570:A:LEU:HD22	12	0.1
(1,446)	1:620:A:GLN:H	1:619:A:GLU:HG3	1	0.1
(1,276)	1:570:A:LEU:H	1:570:A:LEU:HD22	2	0.1
(1,276)	1:570:A:LEU:H	1:570:A:LEU:HD23	20	0.1
(1,214)	1:578:A:GLU:H	1:577:A:LEU:HD21	15	0.1
(1,162)	1:584:A:LEU:H	1:583:A:LYS:HG3	16	0.1
(1,156)	1:585:A:GLU:H	1:581:A:GLU:HG2	10	0.1
(1,135)	1:588:A:GLN:H	1:591:A:VAL:HG23	13	0.1
(1,134)	1:588:A:GLN:H	1:587:A:LEU:HD13	13	0.1
(1,123)	1:589:A:THR:H	1:592:A:ALA:HB3	2	0.1

10 Dihedral-angle violation analysis ⓘ

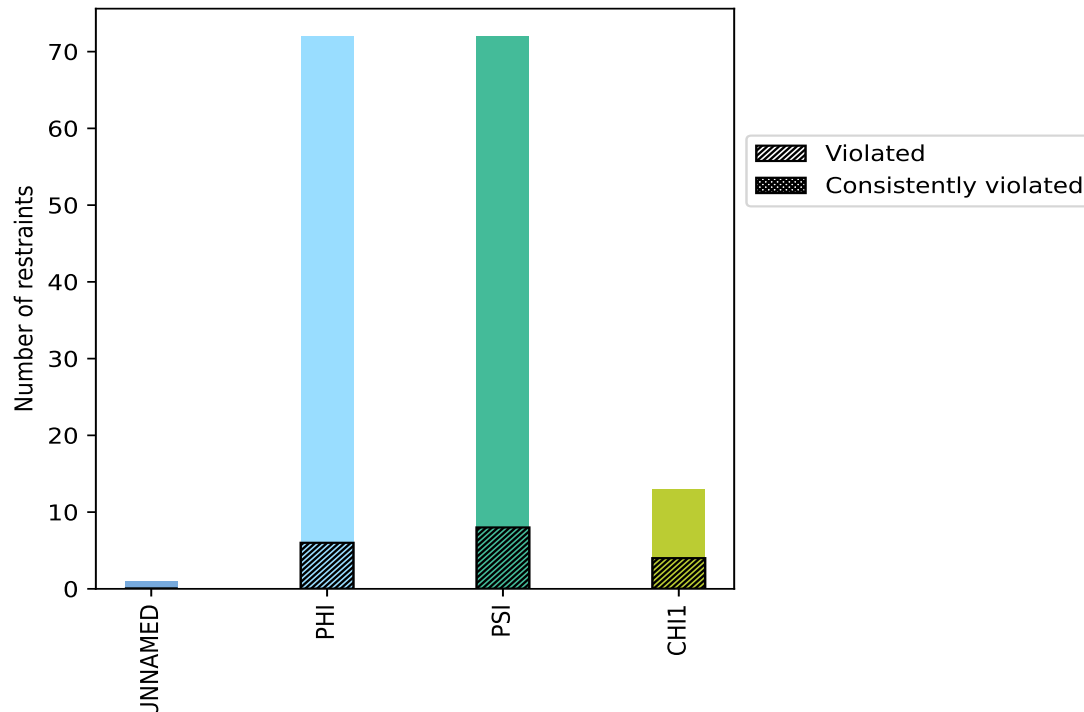
10.1 Summary of dihedral-angle violations ⓘ

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
UNNAMED	1	0.6	0	0.0	0.0	0	0.0	0.0
PHI	72	45.6	6	8.3	3.8	0	0.0	0.0
PSI	72	45.6	8	11.1	5.1	0	0.0	0.0
CHI1	13	8.2	4	30.8	2.5	0	0.0	0.0
Total	158	100.0	18	11.4	11.4	0	0.0	0.0

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

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



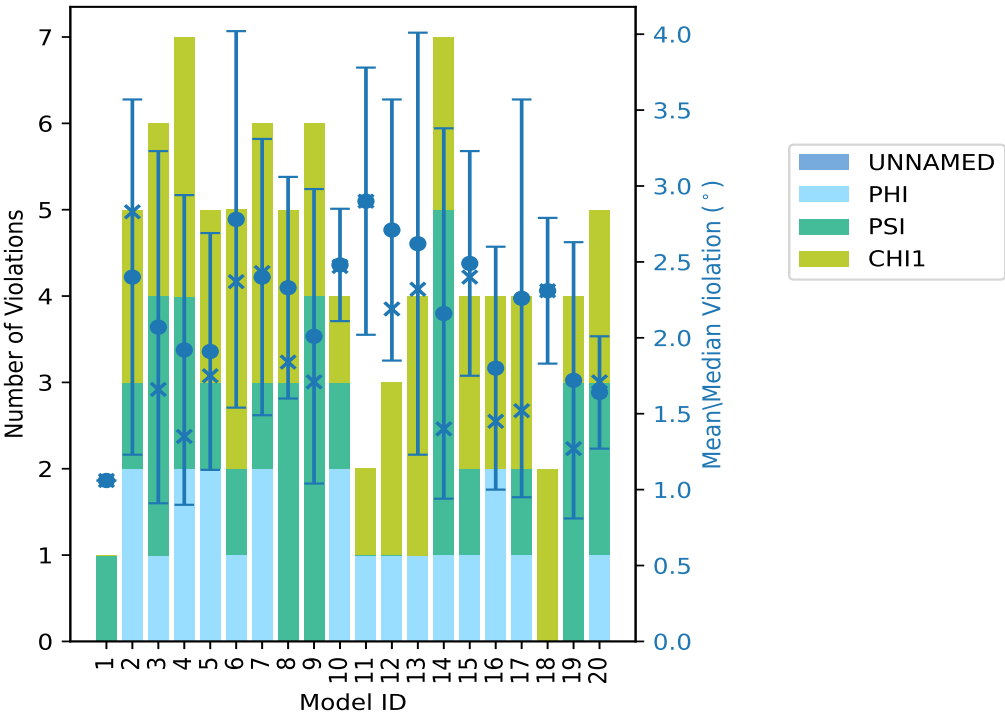
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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 (°)
	UNNAMED	PHI	PSI	CHI1	Total				
1	0	0	1	0	1	1.06	1.06	0.0	1.06
2	0	2	1	2	5	2.4	4.06	1.17	2.83
3	0	1	3	2	6	2.07	4.62	1.16	1.66
4	0	2	2	3	7	1.92	3.79	1.02	1.35
5	0	2	1	2	5	1.91	3.38	0.78	1.75
6	0	1	1	3	5	2.78	4.42	1.24	2.37
7	0	2	1	3	6	2.4	4.01	0.91	2.43
8	0	0	3	2	5	2.33	3.4	0.73	1.84
9	0	0	4	2	6	2.01	3.99	0.97	1.71
10	0	2	1	1	4	2.48	2.96	0.37	2.47
11	0	1	0	1	2	2.9	3.78	0.88	2.9
12	0	1	0	2	3	2.71	3.93	0.86	2.19
13	0	1	0	3	4	2.62	4.61	1.39	2.32
14	0	1	4	2	7	2.16	4.35	1.22	1.4
15	0	1	1	2	4	2.49	3.45	0.74	2.4
16	0	2	0	2	4	1.8	3.16	0.8	1.45
17	0	1	1	2	4	2.26	4.53	1.31	1.52
18	0	0	0	2	2	2.31	2.79	0.48	2.31
19	0	0	3	1	4	1.72	3.29	0.91	1.27
20	0	1	2	2	5	1.64	2.23	0.37	1.71

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	
UNNAMED	PHI	PSI	CHI1	Total	Count ¹	%
0	2	3	1	6	1	5.0
0	0	2	0	2	2	10.0
0	1	0	0	1	3	15.0
0	2	0	0	2	4	20.0
0	0	0	0	0	5	25.0
0	0	1	1	2	6	30.0
0	0	0	0	0	7	35.0
0	1	2	0	3	8	40.0
0	0	0	0	0	9	45.0
0	0	0	0	0	10	50.0
0	0	0	0	0	11	55.0

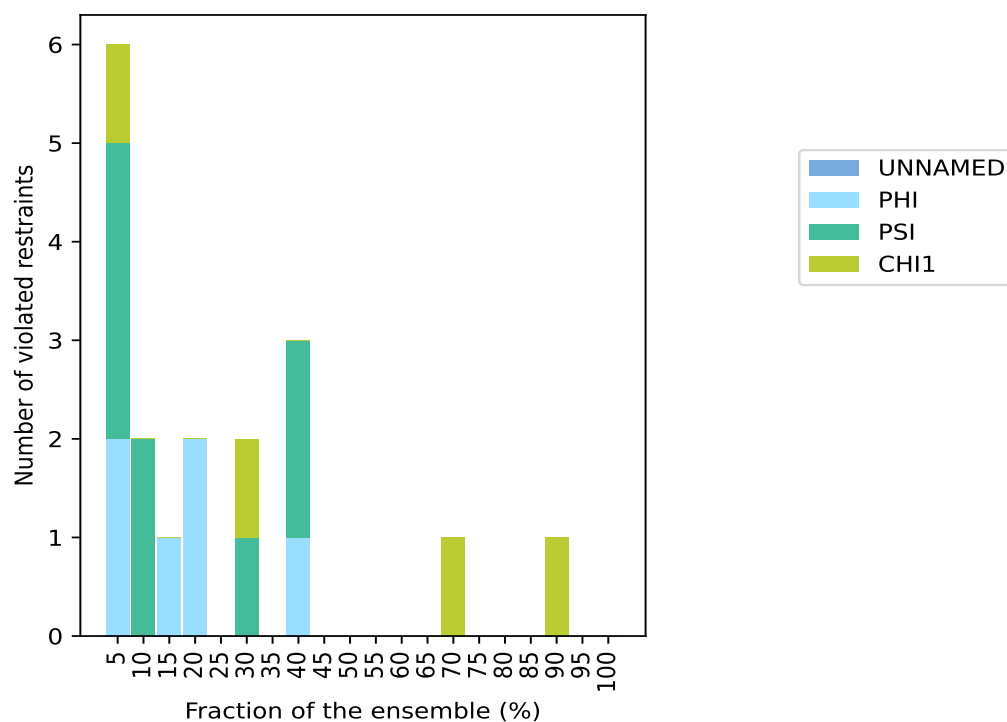
Continued on next page...

Continued from previous page...

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

¹ Number of models with violations

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

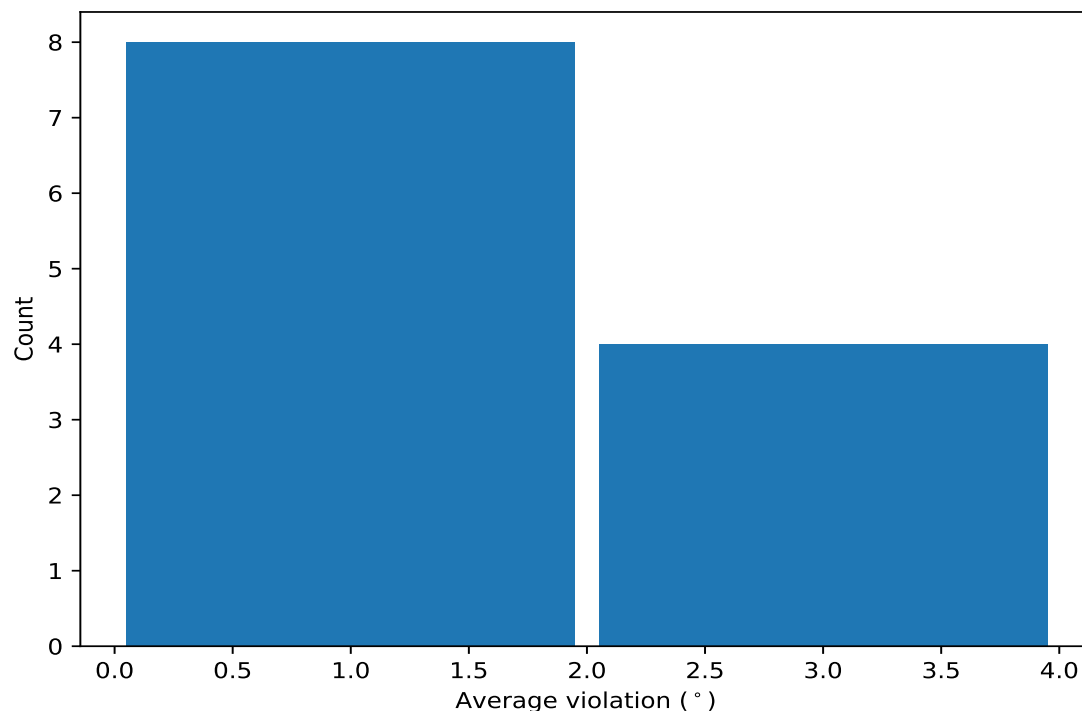


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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.

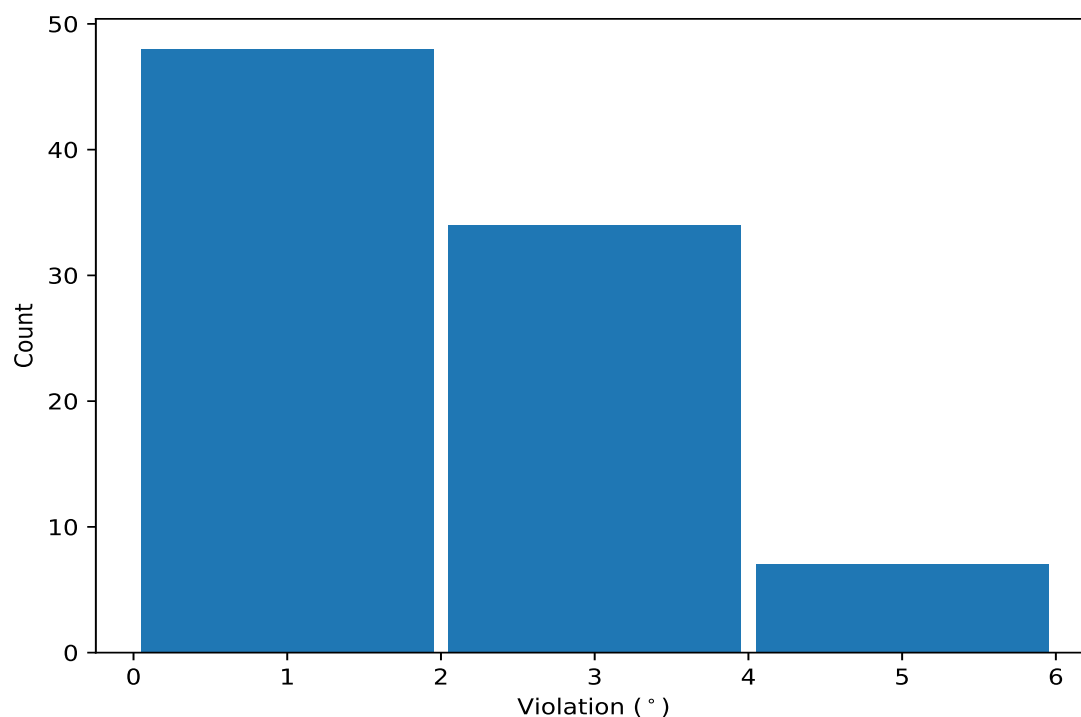
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,4)	1:573:A:LEU:N	1:573:A:LEU:CA	1:573:A:LEU:CB	1:573:A:LEU:CG	18	3.55	0.84	3.62
(1,5)	1:577:A:LEU:N	1:577:A:LEU:CA	1:577:A:LEU:CB	1:577:A:LEU:CG	14	2.15	0.55	2.2
(1,30)	1:570:A:LEU:N	1:570:A:LEU:CA	1:570:A:LEU:C	1:571:A:GLU:N	8	1.84	0.69	1.61
(1,95)	1:602:A:GLU:C	1:603:A:GLN:N	1:603:A:GLN:CA	1:603:A:GLN:C	8	1.63	0.4	1.64
(1,26)	1:568:A:ARG:N	1:568:A:ARG:CA	1:568:A:ARG:C	1:569:A:GLU:N	8	1.26	0.25	1.16
(1,7)	1:603:A:GLN:N	1:603:A:GLN:CA	1:603:A:GLN:CB	1:603:A:GLN:CG	6	3.19	0.89	3.5
(1,156)	1:633:A:ASN:N	1:633:A:ASN:CA	1:633:A:ASN:C	1:634:A:GLY:N	6	1.69	0.26	1.75
(1,21)	1:565:A:LYS:C	1:566:A:LEU:N	1:566:A:LEU:CA	1:566:A:LEU:C	4	2.68	0.95	2.57
(1,25)	1:567:A:GLN:C	1:568:A:ARG:N	1:568:A:ARG:CA	1:568:A:ARG:C	4	1.63	0.39	1.63
(1,157)	1:633:A:ASN:C	1:634:A:GLY:N	1:634:A:GLY:CA	1:634:A:GLY:C	3	1.31	0.19	1.35
(1,32)	1:571:A:GLU:N	1:571:A:GLU:CA	1:571:A:GLU:C	1:572:A:GLN:N	2	1.47	0.36	1.47
(1,158)	1:634:A:GLY:N	1:634:A:GLY:CA	1:634:A:GLY:C	1:635:A:GLY:N	2	1.36	0.04	1.36

¹ Number of violated models, ²Standard 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 (°)
(1,4)	1:573:A:LEU:N	1:573:A:LEU:CA	1:573:A:LEU:CB	1:573:A:LEU:CG	3	4.62
(1,4)	1:573:A:LEU:N	1:573:A:LEU:CA	1:573:A:LEU:CB	1:573:A:LEU:CG	13	4.61
(1,4)	1:573:A:LEU:N	1:573:A:LEU:CA	1:573:A:LEU:CB	1:573:A:LEU:CG	17	4.53
(1,4)	1:573:A:LEU:N	1:573:A:LEU:CA	1:573:A:LEU:CB	1:573:A:LEU:CG	6	4.42
(1,4)	1:573:A:LEU:N	1:573:A:LEU:CA	1:573:A:LEU:CB	1:573:A:LEU:CG	14	4.35
(1,21)	1:565:A:LYS:C	1:566:A:LEU:N	1:566:A:LEU:CA	1:566:A:LEU:C	2	4.06
(1,7)	1:603:A:GLN:N	1:603:A:GLN:CA	1:603:A:GLN:CB	1:603:A:GLN:CG	7	4.01
(1,7)	1:603:A:GLN:N	1:603:A:GLN:CA	1:603:A:GLN:CB	1:603:A:GLN:CG	6	3.99
(1,4)	1:573:A:LEU:N	1:573:A:LEU:CA	1:573:A:LEU:CB	1:573:A:LEU:CG	9	3.99
(1,4)	1:573:A:LEU:N	1:573:A:LEU:CA	1:573:A:LEU:CB	1:573:A:LEU:CG	12	3.93
(1,4)	1:573:A:LEU:N	1:573:A:LEU:CA	1:573:A:LEU:CB	1:573:A:LEU:CG	4	3.79
(1,4)	1:573:A:LEU:N	1:573:A:LEU:CA	1:573:A:LEU:CB	1:573:A:LEU:CG	11	3.78
(1,7)	1:603:A:GLN:N	1:603:A:GLN:CA	1:603:A:GLN:CB	1:603:A:GLN:CG	14	3.75
(1,4)	1:573:A:LEU:N	1:573:A:LEU:CA	1:573:A:LEU:CB	1:573:A:LEU:CG	15	3.45

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,4)	1:573:A:LEU:N	1:573:A:LEU:CA	1:573:A:LEU:CB	1:573:A:LEU:CG	8	3.4
(1,4)	1:573:A:LEU:N	1:573:A:LEU:CA	1:573:A:LEU:CB	1:573:A:LEU:CG	5	3.38
(1,4)	1:573:A:LEU:N	1:573:A:LEU:CA	1:573:A:LEU:CB	1:573:A:LEU:CG	19	3.29
(1,7)	1:603:A:GLN:N	1:603:A:GLN:CA	1:603:A:GLN:CB	1:603:A:GLN:CG	13	3.24
(1,4)	1:573:A:LEU:N	1:573:A:LEU:CA	1:573:A:LEU:CB	1:573:A:LEU:CG	16	3.16
(1,5)	1:577:A:LEU:N	1:577:A:LEU:CA	1:577:A:LEU:CB	1:577:A:LEU:CG	8	3.01
(1,4)	1:573:A:LEU:N	1:573:A:LEU:CA	1:573:A:LEU:CB	1:573:A:LEU:CG	2	3.0
(1,30)	1:570:A:LEU:N	1:570:A:LEU:CA	1:570:A:LEU:C	1:571:A:GLU:N	4	2.99
(1,30)	1:570:A:LEU:N	1:570:A:LEU:CA	1:570:A:LEU:C	1:571:A:GLU:N	10	2.96
(1,21)	1:565:A:LYS:C	1:566:A:LEU:N	1:566:A:LEU:CA	1:566:A:LEU:C	15	2.96
(1,5)	1:577:A:LEU:N	1:577:A:LEU:CA	1:577:A:LEU:CB	1:577:A:LEU:CG	2	2.83
(1,5)	1:577:A:LEU:N	1:577:A:LEU:CA	1:577:A:LEU:CB	1:577:A:LEU:CG	18	2.79
(1,5)	1:577:A:LEU:N	1:577:A:LEU:CA	1:577:A:LEU:CB	1:577:A:LEU:CG	7	2.77
(1,7)	1:603:A:GLN:N	1:603:A:GLN:CA	1:603:A:GLN:CB	1:603:A:GLN:CG	10	2.69
(1,4)	1:573:A:LEU:N	1:573:A:LEU:CA	1:573:A:LEU:CB	1:573:A:LEU:CG	7	2.68
(1,5)	1:577:A:LEU:N	1:577:A:LEU:CA	1:577:A:LEU:CB	1:577:A:LEU:CG	6	2.37
(1,95)	1:602:A:GLU:C	1:603:A:GLN:N	1:603:A:GLN:CA	1:603:A:GLN:C	10	2.26
(1,5)	1:577:A:LEU:N	1:577:A:LEU:CA	1:577:A:LEU:CB	1:577:A:LEU:CG	20	2.23
(1,5)	1:577:A:LEU:N	1:577:A:LEU:CA	1:577:A:LEU:CB	1:577:A:LEU:CG	9	2.21
(1,5)	1:577:A:LEU:N	1:577:A:LEU:CA	1:577:A:LEU:CB	1:577:A:LEU:CG	12	2.19
(1,21)	1:565:A:LYS:C	1:566:A:LEU:N	1:566:A:LEU:CA	1:566:A:LEU:C	7	2.18
(1,5)	1:577:A:LEU:N	1:577:A:LEU:CA	1:577:A:LEU:CB	1:577:A:LEU:CG	4	2.13
(1,95)	1:602:A:GLU:C	1:603:A:GLN:N	1:603:A:GLN:CA	1:603:A:GLN:C	6	2.06
(1,79)	1:594:A:ALA:C	1:595:A:SER:N	1:595:A:SER:CA	1:595:A:SER:C	11	2.03
(1,156)	1:633:A:ASN:N	1:633:A:ASN:CA	1:633:A:ASN:C	1:634:A:GLY:N	9	2.02
(1,25)	1:567:A:GLN:C	1:568:A:ARG:N	1:568:A:ARG:CA	1:568:A:ARG:C	12	2.02
(1,25)	1:567:A:GLN:C	1:568:A:ARG:N	1:568:A:ARG:CA	1:568:A:ARG:C	10	2.01
(1,156)	1:633:A:ASN:N	1:633:A:ASN:CA	1:633:A:ASN:C	1:634:A:GLY:N	3	1.88
(1,95)	1:602:A:GLU:C	1:603:A:GLN:N	1:603:A:GLN:CA	1:603:A:GLN:C	5	1.86
(1,26)	1:568:A:ARG:N	1:568:A:ARG:CA	1:568:A:ARG:C	1:569:A:GLU:N	8	1.84
(1,32)	1:571:A:GLU:N	1:571:A:GLU:CA	1:571:A:GLU:C	1:572:A:GLN:N	8	1.83
(1,5)	1:577:A:LEU:N	1:577:A:LEU:CA	1:577:A:LEU:CB	1:577:A:LEU:CG	15	1.83
(1,4)	1:573:A:LEU:N	1:573:A:LEU:CA	1:573:A:LEU:CB	1:573:A:LEU:CG	18	1.83
(1,30)	1:570:A:LEU:N	1:570:A:LEU:CA	1:570:A:LEU:C	1:571:A:GLU:N	14	1.81
(1,156)	1:633:A:ASN:N	1:633:A:ASN:CA	1:633:A:ASN:C	1:634:A:GLY:N	5	1.75
(1,156)	1:633:A:ASN:N	1:633:A:ASN:CA	1:633:A:ASN:C	1:634:A:GLY:N	20	1.75
(1,95)	1:602:A:GLU:C	1:603:A:GLN:N	1:603:A:GLN:CA	1:603:A:GLN:C	3	1.75
(1,30)	1:570:A:LEU:N	1:570:A:LEU:CA	1:570:A:LEU:C	1:571:A:GLU:N	15	1.71
(1,4)	1:573:A:LEU:N	1:573:A:LEU:CA	1:573:A:LEU:CB	1:573:A:LEU:CG	20	1.71
(1,84)	1:597:A:PHE:N	1:597:A:PHE:CA	1:597:A:PHE:C	1:598:A:SER:N	8	1.57
(1,5)	1:577:A:LEU:N	1:577:A:LEU:CA	1:577:A:LEU:CB	1:577:A:LEU:CG	3	1.56
(1,156)	1:633:A:ASN:N	1:633:A:ASN:CA	1:633:A:ASN:C	1:634:A:GLY:N	17	1.54
(1,95)	1:602:A:GLU:C	1:603:A:GLN:N	1:603:A:GLN:CA	1:603:A:GLN:C	7	1.54
(1,157)	1:633:A:ASN:C	1:634:A:GLY:N	1:634:A:GLY:CA	1:634:A:GLY:C	16	1.52
(1,30)	1:570:A:LEU:N	1:570:A:LEU:CA	1:570:A:LEU:C	1:571:A:GLU:N	3	1.51
(1,21)	1:565:A:LYS:C	1:566:A:LEU:N	1:566:A:LEU:CA	1:566:A:LEU:C	17	1.51
(1,7)	1:603:A:GLN:N	1:603:A:GLN:CA	1:603:A:GLN:CB	1:603:A:GLN:CG	5	1.48
(1,5)	1:577:A:LEU:N	1:577:A:LEU:CA	1:577:A:LEU:CB	1:577:A:LEU:CG	17	1.44
(1,158)	1:634:A:GLY:N	1:634:A:GLY:CA	1:634:A:GLY:C	1:635:A:GLY:N	9	1.4
(1,26)	1:568:A:ARG:N	1:568:A:ARG:CA	1:568:A:ARG:C	1:569:A:GLU:N	14	1.4
(1,5)	1:577:A:LEU:N	1:577:A:LEU:CA	1:577:A:LEU:CB	1:577:A:LEU:CG	13	1.39

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,5)	1:577:A:LEU:N	1:577:A:LEU:CA	1:577:A:LEU:CB	1:577:A:LEU:CG	16	1.38
(1,157)	1:633:A:ASN:C	1:634:A:GLY:N	1:634:A:GLY:CA	1:634:A:GLY:C	4	1.35
(1,95)	1:602:A:GLU:C	1:603:A:GLN:N	1:603:A:GLN:CA	1:603:A:GLN:C	14	1.35
(1,26)	1:568:A:ARG:N	1:568:A:ARG:CA	1:568:A:ARG:C	1:569:A:GLU:N	19	1.34
(1,158)	1:634:A:GLY:N	1:634:A:GLY:CA	1:634:A:GLY:C	1:635:A:GLY:N	14	1.32
(1,30)	1:570:A:LEU:N	1:570:A:LEU:CA	1:570:A:LEU:C	1:571:A:GLU:N	20	1.27
(1,25)	1:567:A:GLN:C	1:568:A:ARG:N	1:568:A:ARG:CA	1:568:A:ARG:C	13	1.26
(1,30)	1:570:A:LEU:N	1:570:A:LEU:CA	1:570:A:LEU:C	1:571:A:GLU:N	7	1.24
(1,30)	1:570:A:LEU:N	1:570:A:LEU:CA	1:570:A:LEU:C	1:571:A:GLU:N	9	1.22
(1,25)	1:567:A:GLN:C	1:568:A:ARG:N	1:568:A:ARG:CA	1:568:A:ARG:C	20	1.22
(1,156)	1:633:A:ASN:N	1:633:A:ASN:CA	1:633:A:ASN:C	1:634:A:GLY:N	19	1.21
(1,26)	1:568:A:ARG:N	1:568:A:ARG:CA	1:568:A:ARG:C	1:569:A:GLU:N	9	1.19
(1,154)	1:632:A:LYS:N	1:632:A:LYS:CA	1:632:A:LYS:C	1:633:A:ASN:N	14	1.13
(1,95)	1:602:A:GLU:C	1:603:A:GLN:N	1:603:A:GLN:CA	1:603:A:GLN:C	16	1.13
(1,26)	1:568:A:ARG:N	1:568:A:ARG:CA	1:568:A:ARG:C	1:569:A:GLU:N	3	1.12
(1,32)	1:571:A:GLU:N	1:571:A:GLU:CA	1:571:A:GLU:C	1:572:A:GLN:N	2	1.11
(1,26)	1:568:A:ARG:N	1:568:A:ARG:CA	1:568:A:ARG:C	1:569:A:GLU:N	6	1.08
(1,157)	1:633:A:ASN:C	1:634:A:GLY:N	1:634:A:GLY:CA	1:634:A:GLY:C	5	1.07
(1,95)	1:602:A:GLU:C	1:603:A:GLN:N	1:603:A:GLN:CA	1:603:A:GLN:C	4	1.07
(1,14)	1:627:A:TYR:N	1:627:A:TYR:CA	1:627:A:TYR:CB	1:627:A:TYR:CG	4	1.07
(1,26)	1:568:A:ARG:N	1:568:A:ARG:CA	1:568:A:ARG:C	1:569:A:GLU:N	1	1.06
(1,102)	1:606:A:LYS:N	1:606:A:LYS:CA	1:606:A:LYS:C	1:607:A:VAL:N	19	1.05
(1,26)	1:568:A:ARG:N	1:568:A:ARG:CA	1:568:A:ARG:C	1:569:A:GLU:N	4	1.03
(1,73)	1:591:A:VAL:C	1:592:A:ALA:N	1:592:A:ALA:CA	1:592:A:ALA:C	2	1.01