



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 01:26 PM UTC

PDB ID : 2M41 / pdb_00002m41
BMRB ID : 18982
Title : Solution Structure of the AXH domain of Ataxin-1 in complex with ligand peptide from Capicua
Authors : de Chiara, C.; Kelly, G.; Pastore, A.
Deposited on : 2013-01-28

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 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

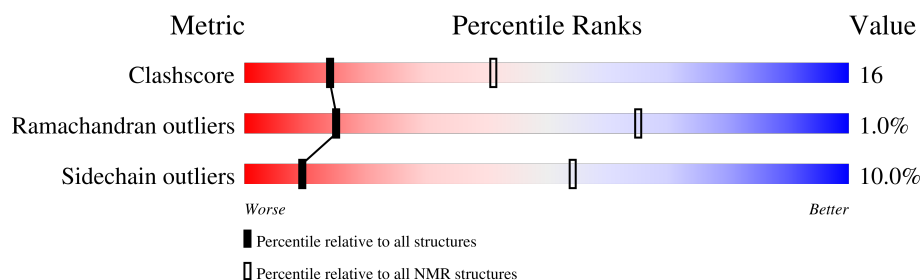
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 79%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	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	15	
2	B	126	

2 Ensemble composition and analysis

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

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:35-A:43, B:571-B:605, B:609-B:689 (125)	0.46	14

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

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

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

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

3 Entry composition

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

- Molecule 1 is a protein called Protein capicua homolog.

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

- Molecule 2 is a protein called Ataxin-1.

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

There are 3 discrepancies between the modelled and reference sequences:

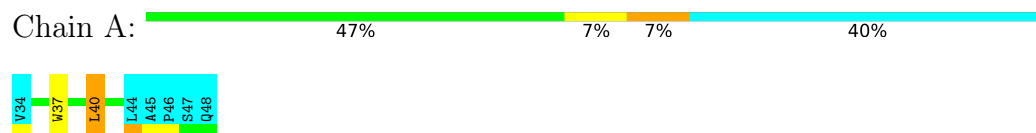
Chain	Residue	Modelled	Actual	Comment	Reference
B	564	GLY	-	expression tag	UNP P54253
B	565	ALA	-	expression tag	UNP P54253
B	566	MET	-	expression tag	UNP P54253

4 Residue-property plots

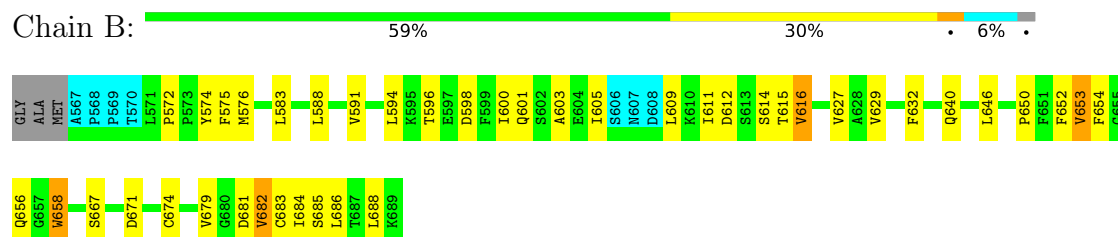
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Protein capicua homolog



- Molecule 2: Ataxin-1

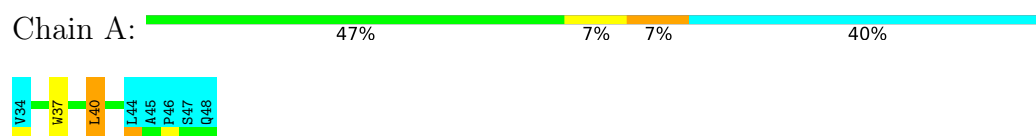


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Protein capicua homolog



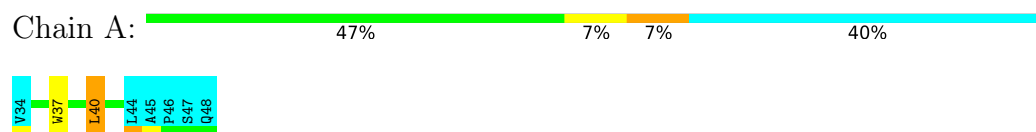
- Molecule 2: Ataxin-1



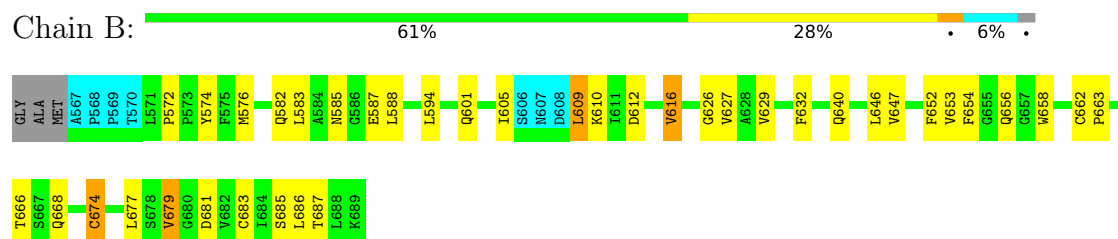


4.2.2 Score per residue for model 2

- Molecule 1: Protein capicua homolog

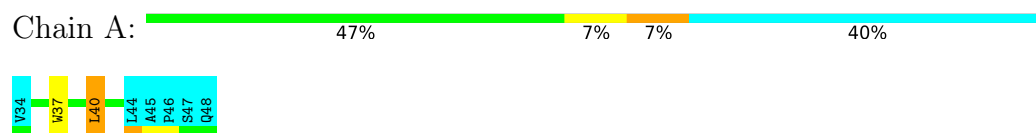


- Molecule 2: Ataxin-1

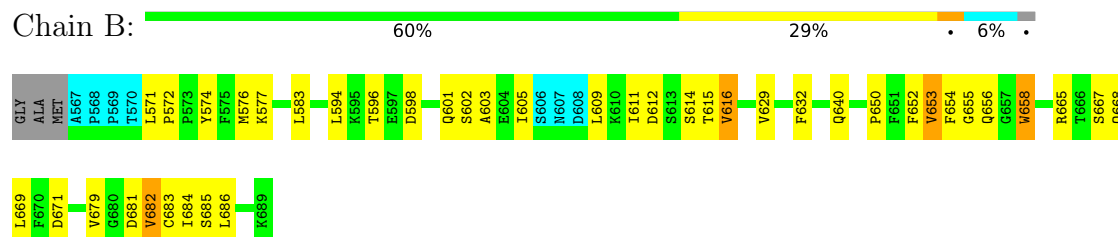


4.2.3 Score per residue for model 3

- Molecule 1: Protein capicua homolog

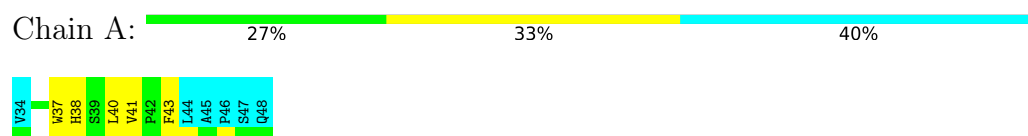


- Molecule 2: Ataxin-1

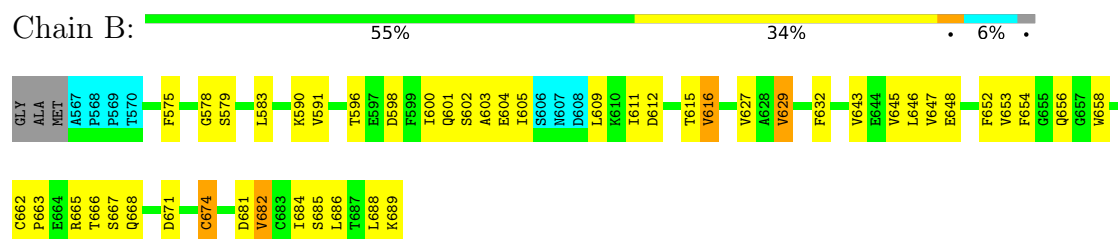


4.2.4 Score per residue for model 4

- Molecule 1: Protein capicua homolog



- Molecule 2: Ataxin-1

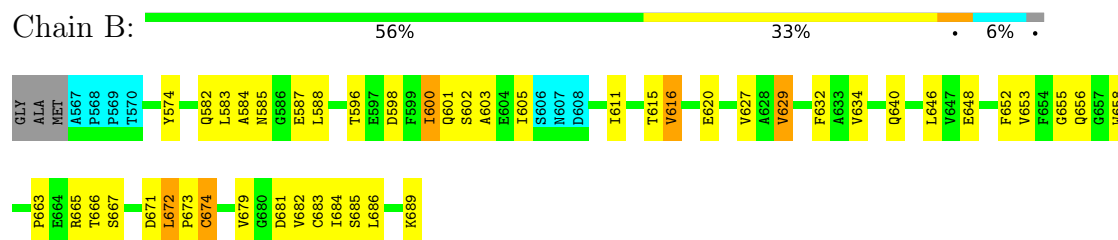


4.2.5 Score per residue for model 5

- Molecule 1: Protein capicua homolog

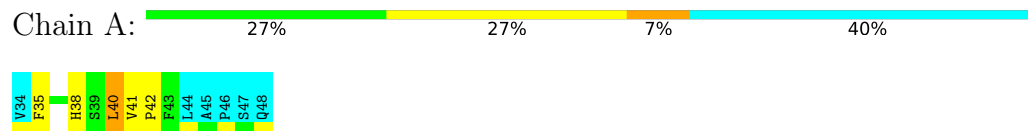


- Molecule 2: Ataxin-1

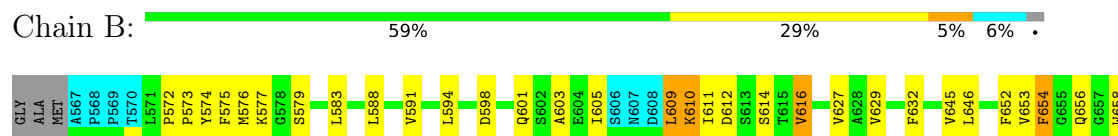


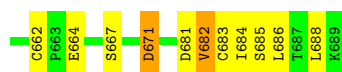
4.2.6 Score per residue for model 6

- Molecule 1: Protein capicua homolog



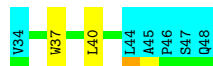
- Molecule 2: Ataxin-1



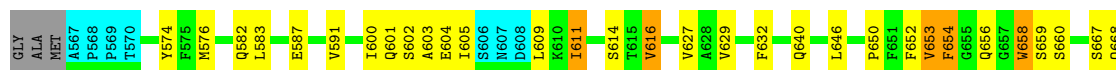


4.2.7 Score per residue for model 7

- Molecule 1: Protein capicua homolog

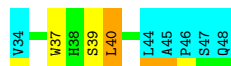


- Molecule 2: Ataxin-1

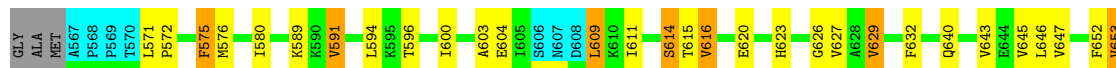


4.2.8 Score per residue for model 8

- Molecule 1: Protein capicua homolog



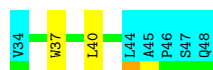
- Molecule 2: Ataxin-1



4.2.9 Score per residue for model 9

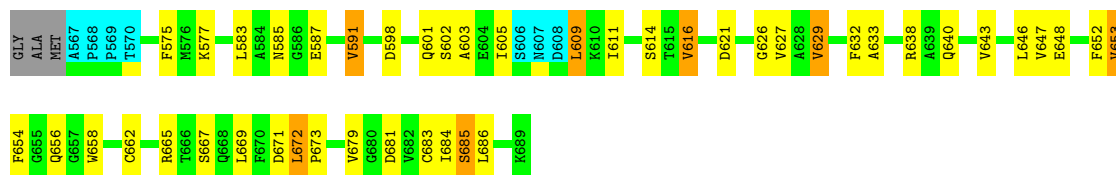
- Molecule 1: Protein capicua homolog





• Molecule 2: Ataxin-1

Chain B: 56% 30% 6% 6%



4.2.10 Score per residue for model 10

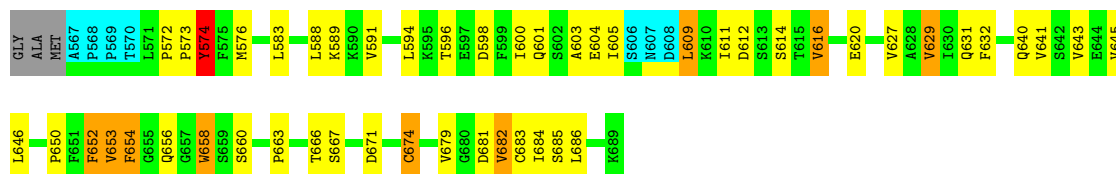
• Molecule 1: Protein capicua homolog

Chain A: 33% 27% 40%



• Molecule 2: Ataxin-1

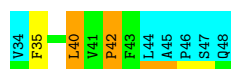
Chain B: 52% 32% 7% 6%



4.2.11 Score per residue for model 11

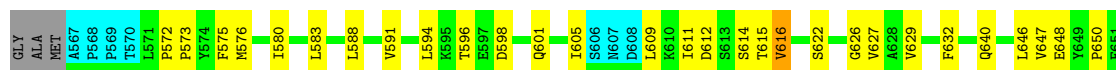
• Molecule 1: Protein capicua homolog

Chain A: 40% 7% 13% 40%



• Molecule 2: Ataxin-1

Chain B: 53% 36% 6%





4.2.12 Score per residue for model 12

- Molecule 1: Protein capicua homolog



- Molecule 2: Ataxin-1



4.2.13 Score per residue for model 13

- Molecule 1: Protein capicua homolog



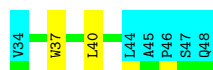
- Molecule 2: Ataxin-1



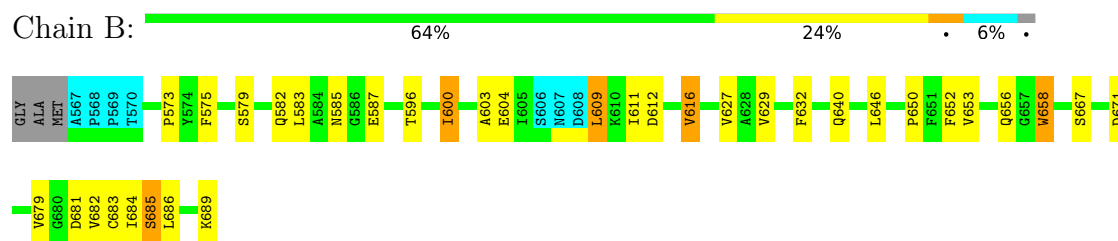
4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: Protein capicua homolog



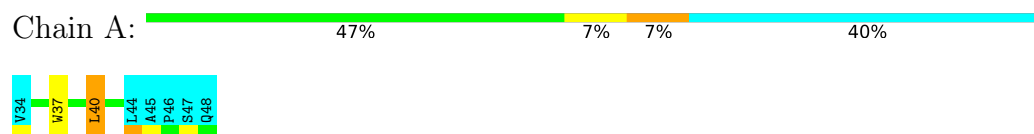


• Molecule 2: Ataxin-1

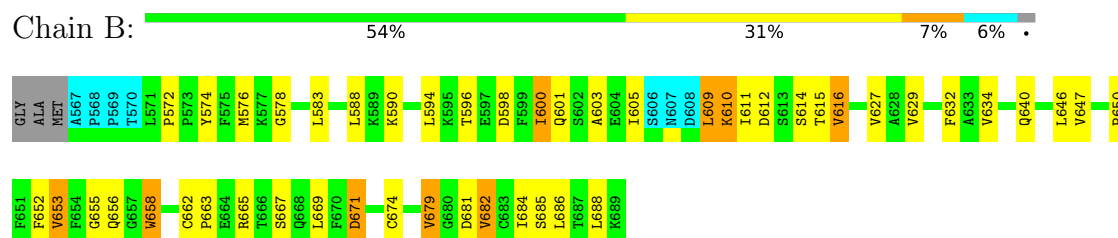


4.2.15 Score per residue for model 15

• Molecule 1: Protein capicua homolog



• Molecule 2: Ataxin-1



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
ARIA	structure solution	2.3
ARIA	refinement	2.3

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1420
Number of shifts mapped to atoms	1420
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.44±0.03	0±0/88 (0.0± 0.0%)	0.80±0.08	0±0/123 (0.0± 0.0%)
2	B	0.48±0.02	0±0/919 (0.0± 0.0%)	0.76±0.02	0±0/1243 (0.0± 0.0%)
All	All	0.48	0/15105 (0.0%)	0.77	3/20490 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	591	VAL	CB-CA-C	-5.40	104.97	111.88	8	3

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	81	75	74	3±1
2	B	901	902	900	30±4
All	All	14730	14655	14610	459

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:653:VAL:HG12	2:B:656:GLN:HE21	0.88	1.25	13	14
2:B:653:VAL:HG12	2:B:656:GLN:NE2	0.87	1.85	12	15
2:B:653:VAL:HG11	2:B:681:ASP:HB3	0.82	1.50	10	14
2:B:653:VAL:HG11	2:B:681:ASP:HB2	0.78	1.56	7	1
2:B:672:LEU:HD22	2:B:673:PRO:HD2	0.76	1.54	8	2
2:B:666:THR:HB	2:B:674:CYS:SG	0.74	2.22	8	5
2:B:663:PRO:HA	2:B:674:CYS:SG	0.68	2.28	4	5
2:B:632:PHE:O	2:B:640:GLN:HA	0.68	1.89	13	12
2:B:596:THR:O	2:B:600:ILE:HD13	0.67	1.89	14	3
2:B:656:GLN:NE2	2:B:682:VAL:HG13	0.67	2.04	4	6
2:B:616:VAL:HG12	2:B:681:ASP:O	0.67	1.90	6	15
2:B:653:VAL:CG1	2:B:656:GLN:HB2	0.63	2.22	5	8
2:B:600:ILE:O	2:B:604:GLU:HG3	0.62	1.94	14	5
2:B:627:VAL:HG22	2:B:646:LEU:CD2	0.62	2.25	7	14
2:B:650:PRO:HB2	2:B:658:TRP:CH2	0.60	2.31	10	9
2:B:662:CYS:SG	2:B:665:ARG:HB3	0.60	2.36	4	1
2:B:603:ALA:HB3	2:B:611:ILE:HG12	0.60	1.72	13	12
2:B:656:GLN:NE2	2:B:682:VAL:HB	0.60	2.11	5	2
2:B:667:SER:O	2:B:671:ASP:HA	0.60	1.96	11	13
2:B:647:VAL:HB	2:B:662:CYS:SG	0.60	2.37	15	5
1:A:37:TRP:CZ2	2:B:609:LEU:HG	0.59	2.32	9	5
2:B:654:PHE:HB3	2:B:682:VAL:HG13	0.59	1.74	3	5
2:B:672:LEU:HD23	2:B:673:PRO:HD2	0.59	1.74	9	1
2:B:653:VAL:CG1	2:B:681:ASP:HB2	0.59	2.28	7	1
2:B:632:PHE:HE1	2:B:683:CYS:SG	0.58	2.22	3	5
2:B:614:SER:N	2:B:682:VAL:HG23	0.56	2.15	10	9
2:B:601:GLN:O	2:B:605:ILE:HG13	0.56	2.01	13	13
1:A:37:TRP:CZ2	2:B:609:LEU:HD13	0.56	2.36	12	5
2:B:603:ALA:CB	2:B:611:ILE:HG12	0.55	2.31	7	11
2:B:655:GLY:H	2:B:656:GLN:NE2	0.54	2.00	3	2
2:B:665:ARG:O	2:B:669:LEU:HG	0.54	2.02	9	5
2:B:620:GLU:HB2	2:B:629:VAL:HG13	0.54	1.78	5	3
2:B:582:GLN:HA	2:B:587:GLU:O	0.53	2.03	7	6
2:B:653:VAL:CG1	2:B:681:ASP:HB3	0.53	2.33	12	3
2:B:583:LEU:HB3	2:B:602:SER:OG	0.53	2.03	1	7
2:B:572:PRO:HD2	2:B:576:MET:SD	0.53	2.42	6	3
2:B:583:LEU:HD13	2:B:598:ASP:HB3	0.53	1.79	6	3
2:B:583:LEU:HB2	2:B:587:GLU:OE2	0.53	2.03	9	1
2:B:572:PRO:O	2:B:576:MET:HB2	0.52	2.05	10	6
2:B:647:VAL:HG23	2:B:662:CYS:SG	0.52	2.46	4	1
1:A:35:PHE:CD2	2:B:574:TYR:HA	0.51	2.40	10	1
2:B:632:PHE:HE1	2:B:683:CYS:HG	0.51	1.49	14	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:664:GLU:CD	2:B:664:GLU:H	0.50	2.15	6	1
2:B:656:GLN:HE22	2:B:682:VAL:HG13	0.50	1.65	6	6
2:B:572:PRO:HB2	2:B:576:MET:SD	0.50	2.46	10	2
2:B:654:PHE:N	2:B:684:ILE:HG13	0.50	2.20	6	6
2:B:653:VAL:HG12	2:B:656:GLN:CD	0.50	2.31	12	1
2:B:596:THR:OG1	2:B:684:ILE:HD11	0.50	2.07	4	9
2:B:577:LYS:HB2	2:B:671:ASP:O	0.49	2.07	9	1
2:B:573:PRO:O	2:B:579:SER:HB2	0.49	2.07	13	1
2:B:583:LEU:CD1	2:B:598:ASP:HB3	0.49	2.38	6	7
2:B:603:ALA:HB1	2:B:610:LYS:HA	0.49	1.84	13	1
2:B:653:VAL:HB	2:B:656:GLN:HB2	0.49	1.84	3	3
2:B:631:GLN:HA	2:B:641:VAL:O	0.49	2.07	10	3
2:B:577:LYS:HD2	2:B:671:ASP:O	0.49	2.08	6	1
2:B:612:ASP:HB3	2:B:685:SER:HB3	0.48	1.85	4	9
2:B:583:LEU:HD11	2:B:598:ASP:HB3	0.48	1.85	9	3
2:B:648:GLU:HB3	2:B:665:ARG:CD	0.48	2.38	5	1
2:B:612:ASP:HB3	2:B:685:SER:CB	0.48	2.38	14	1
2:B:645:VAL:HG12	2:B:646:LEU:N	0.48	2.23	4	4
2:B:591:VAL:HB	2:B:672:LEU:HD21	0.48	1.85	8	1
2:B:583:LEU:CD1	2:B:598:ASP:HB2	0.48	2.38	10	1
2:B:571:LEU:HD21	2:B:577:LYS:O	0.48	2.09	3	1
2:B:596:THR:HG21	2:B:655:GLY:HA2	0.48	1.86	15	3
2:B:571:LEU:HD11	2:B:577:LYS:O	0.47	2.09	1	1
1:A:37:TRP:CD1	1:A:37:TRP:H	0.47	2.27	8	5
2:B:575:PHE:O	2:B:672:LEU:HG	0.47	2.10	8	1
2:B:615:THR:HA	2:B:682:VAL:HA	0.47	1.87	15	7
1:A:40:LEU:HD11	2:B:594:LEU:CD1	0.47	2.40	2	9
2:B:653:VAL:HG12	2:B:656:GLN:HB2	0.47	1.87	5	3
1:A:38:HIS:HA	1:A:41:VAL:HG12	0.47	1.86	4	1
2:B:672:LEU:HD22	2:B:673:PRO:CD	0.46	2.35	8	1
2:B:583:LEU:HD12	2:B:587:GLU:HB2	0.46	1.87	5	1
2:B:630:ILE:HB	2:B:632:PHE:CE2	0.46	2.45	1	1
1:A:42:PRO:HD3	2:B:650:PRO:O	0.46	2.11	10	1
2:B:668:GLN:OE1	2:B:668:GLN:HA	0.46	2.11	3	3
2:B:596:THR:HA	2:B:652:PHE:CE1	0.45	2.47	10	2
1:A:37:TRP:CZ2	2:B:609:LEU:HD22	0.45	2.47	15	1
2:B:629:VAL:HA	2:B:643:VAL:O	0.45	2.11	4	6
2:B:614:SER:HB2	2:B:683:CYS:SG	0.45	2.51	9	2
2:B:626:GLY:O	2:B:646:LEU:HA	0.45	2.12	8	4
2:B:584:ALA:HB3	2:B:602:SER:HA	0.45	1.87	5	1
2:B:576:MET:SD	2:B:576:MET:N	0.45	2.89	10	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:589:LYS:NZ	2:B:594:LEU:HA	0.45	2.25	10	1
1:A:42:PRO:HG3	2:B:650:PRO:O	0.45	2.11	11	1
2:B:653:VAL:CG1	2:B:656:GLN:HE21	0.45	2.20	3	3
1:A:37:TRP:HA	2:B:581:ILE:CG2	0.45	2.42	1	1
2:B:677:LEU:HD21	2:B:683:CYS:SG	0.45	2.52	7	3
2:B:633:ALA:HB1	2:B:638:ARG:HB3	0.45	1.88	9	1
2:B:654:PHE:HA	2:B:684:ILE:CG1	0.44	2.42	8	2
2:B:632:PHE:CE1	2:B:683:CYS:SG	0.44	3.10	10	1
2:B:612:ASP:CB	2:B:685:SER:HB3	0.44	2.41	12	2
2:B:578:GLY:HA2	2:B:590:LYS:CE	0.44	2.43	13	1
2:B:616:VAL:HG22	2:B:679:VAL:HA	0.44	1.90	11	6
2:B:667:SER:OG	2:B:673:PRO:HA	0.44	2.13	7	1
2:B:662:CYS:SG	2:B:662:CYS:O	0.44	2.76	4	1
2:B:583:LEU:HD11	2:B:598:ASP:HB2	0.44	1.90	10	1
2:B:688:LEU:HD22	2:B:688:LEU:N	0.44	2.28	7	2
1:A:39:SER:C	1:A:40:LEU:HD23	0.44	2.37	8	1
2:B:610:LYS:NZ	2:B:610:LYS:HB3	0.43	2.27	6	2
1:A:38:HIS:CG	2:B:688:LEU:HD11	0.43	2.47	4	1
2:B:585:ASN:ND2	2:B:587:GLU:HG3	0.43	2.28	12	1
2:B:609:LEU:CD1	2:B:688:LEU:HA	0.43	2.43	11	1
1:A:37:TRP:HZ2	2:B:609:LEU:HD13	0.43	1.73	12	1
2:B:583:LEU:HB2	2:B:585:ASN:OD1	0.43	2.14	5	3
2:B:600:ILE:HD11	2:B:654:PHE:O	0.43	2.13	4	1
2:B:612:ASP:HB2	2:B:685:SER:HB3	0.43	1.89	6	1
2:B:573:PRO:HA	2:B:579:SER:OG	0.43	2.13	6	1
1:A:35:PHE:CZ	2:B:573:PRO:HG2	0.42	2.49	10	3
2:B:676:LYS:HG3	2:B:678:SER:OG	0.42	2.14	11	1
2:B:609:LEU:HD11	2:B:688:LEU:HD13	0.42	1.91	6	1
2:B:576:MET:O	2:B:591:VAL:HG21	0.42	2.15	7	1
2:B:663:PRO:HB3	2:B:674:CYS:O	0.42	2.13	8	2
2:B:615:THR:OG1	2:B:682:VAL:HG22	0.42	2.14	1	2
2:B:578:GLY:N	2:B:590:LYS:HE3	0.42	2.29	4	1
2:B:575:PHE:O	2:B:591:VAL:HG11	0.42	2.14	8	4
1:A:40:LEU:HD13	2:B:591:VAL:HG13	0.42	1.92	1	2
2:B:578:GLY:HA2	2:B:590:LYS:HE3	0.42	1.92	15	1
2:B:632:PHE:CE1	2:B:683:CYS:HB3	0.42	2.49	6	1
2:B:579:SER:HB2	2:B:591:VAL:CG2	0.42	2.44	4	1
1:A:38:HIS:HA	1:A:41:VAL:CG1	0.42	2.45	6	1
2:B:610:LYS:HB2	2:B:687:THR:OG1	0.41	2.15	2	1
2:B:672:LEU:CD2	2:B:673:PRO:HD2	0.41	2.45	5	1
2:B:579:SER:HB3	2:B:591:VAL:CG2	0.41	2.45	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:662:CYS:SG	2:B:664:GLU:HB2	0.41	2.56	6	1
2:B:656:GLN:OE1	2:B:682:VAL:HG12	0.41	2.15	12	1
2:B:581:ILE:HG13	2:B:594:LEU:HD11	0.41	1.92	13	2
2:B:650:PRO:HA	2:B:660:SER:CB	0.41	2.46	7	1
2:B:577:LYS:HG3	2:B:592:GLU:OE2	0.41	2.15	12	1
2:B:590:LYS:O	2:B:594:LEU:HG	0.41	2.15	15	1
2:B:580:ILE:CG2	2:B:588:LEU:HB3	0.41	2.46	11	1
2:B:600:ILE:O	2:B:604:GLU:HG2	0.41	2.16	8	1
2:B:612:ASP:HB3	2:B:685:SER:HB2	0.41	1.92	14	1
2:B:587:GLU:H	2:B:587:GLU:CD	0.41	2.24	9	1
2:B:659:SER:OG	2:B:675:SER:HB2	0.40	2.16	7	1
2:B:672:LEU:HD12	2:B:673:PRO:HD2	0.40	1.92	11	1
2:B:585:ASN:HB3	2:B:587:GLU:OE2	0.40	2.16	9	1
2:B:650:PRO:HA	2:B:660:SER:OG	0.40	2.15	10	1
2:B:611:ILE:HG23	2:B:684:ILE:HG23	0.40	1.94	11	1
2:B:573:PRO:O	2:B:579:SER:HB3	0.40	2.16	14	1

6.3 Torsion angles ⓘ

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	9/15 (60%)	7±1 (77±10%)	2±1 (21±10%)	0±0 (1±4%)	11	57
2	B	115/126 (91%)	110±1 (95±1%)	4±2 (4±1%)	1±1 (1±1%)	15	65
All	All	1860/2115 (88%)	1748 (94%)	93 (5%)	19 (1%)	15	65

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

Mol	Chain	Res	Type	Models (Total)
2	B	574	TYR	9
2	B	654	PHE	6
1	A	42	PRO	2
2	B	571	LEU	1
2	B	575	PHE	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	9/14 (64%)	8±0 (89±0%)	1±0 (11±0%)	8 51
2	B	104/111 (94%)	94±2 (90±2%)	10±2 (10±2%)	10 54
All	All	1695/1875 (90%)	1526 (90%)	169 (10%)	9 54

All 31 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	40	LEU	15
2	B	616	VAL	15
2	B	629	VAL	15
2	B	652	PHE	15
2	B	658	TRP	15
2	B	686	LEU	15
2	B	679	VAL	10
2	B	682	VAL	10
2	B	653	VAL	9
2	B	609	LEU	8
2	B	674	CYS	5
2	B	575	PHE	4
2	B	671	ASP	4
2	B	648	GLU	3
2	B	600	ILE	3
2	B	672	LEU	3
2	B	688	LEU	3
2	B	689	LYS	2
2	B	610	LYS	2
2	B	685	SER	2
2	B	571	LEU	1
2	B	668	GLN	1
2	B	611	ILE	1
2	B	589	LYS	1
2	B	614	SER	1
2	B	623	HIS	1
2	B	591	VAL	1
2	B	621	ASP	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
2	B	574	TYR	1
2	B	622	SER	1
2	B	656	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 79% for the well-defined parts and 77% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

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

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	90	-0.20 ± 0.19	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	119	0.16 ± 0.29	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	115	-0.34 ± 0.56	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

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

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

Continued on next page...

Continued from previous page...

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

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

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

7.1.4 Statistically unusual chemical shifts ⓘ

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

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

Continued on next page...

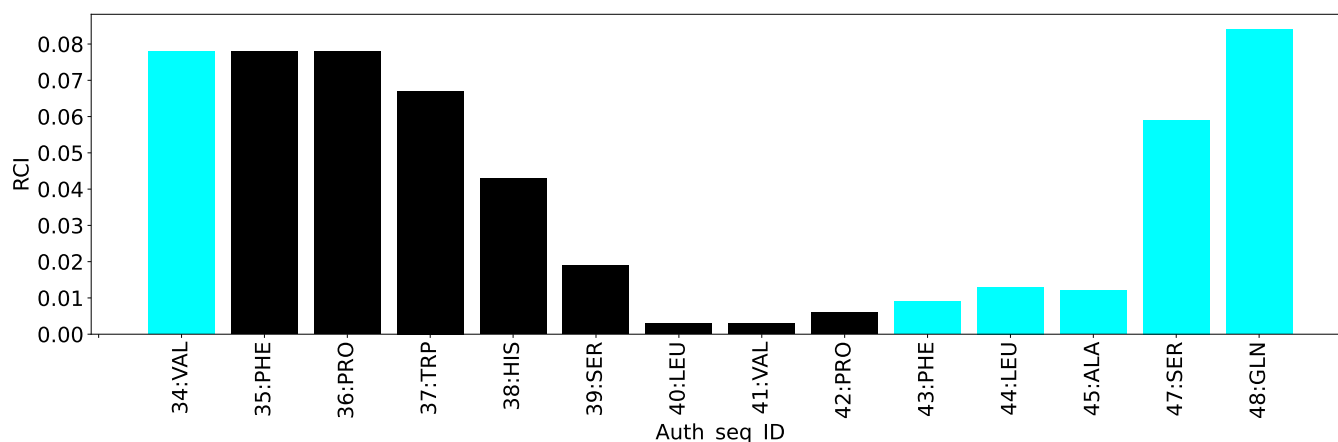
Continued from previous page...

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

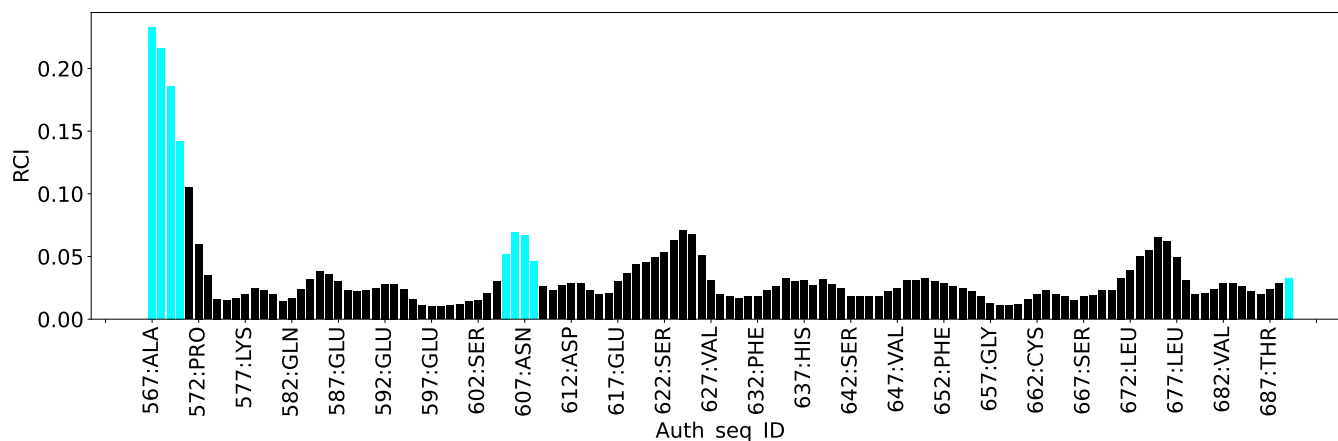
7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

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

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	28.5	0.2
0.2-0.5 (Medium)	62.3	0.5
>0.5 (Large)	109.0	32.27

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

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

9 Distance violation analysis ⓘ

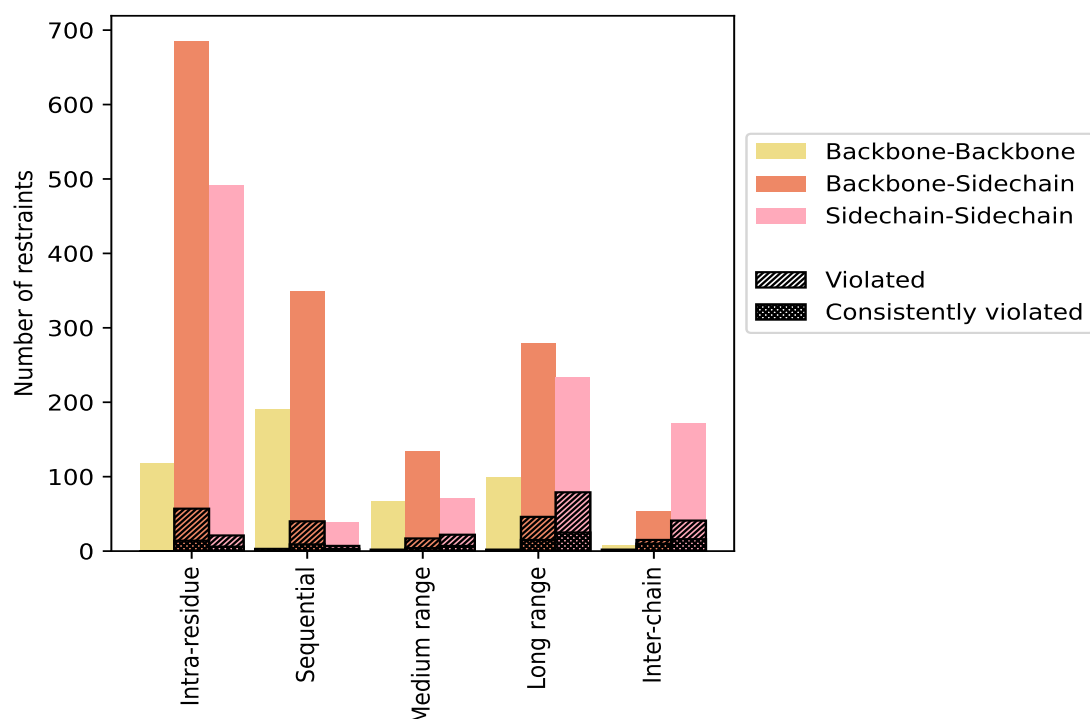
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	1294	43.3	78	6.0	2.6	20	1.5	0.7
Backbone-Backbone	118	4.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	685	22.9	57	8.3	1.9	14	2.0	0.5
Sidechain-Sidechain	491	16.4	21	4.3	0.7	6	1.2	0.2
Sequential ($i-j =1$)	578	19.4	50	8.7	1.7	12	2.1	0.4
Backbone-Backbone	191	6.4	3	1.6	0.1	0	0.0	0.0
Backbone-Sidechain	349	11.7	40	11.5	1.3	9	2.6	0.3
Sidechain-Sidechain	38	1.3	7	18.4	0.2	3	7.9	0.1
Medium range ($i-j >1$ & $i-j <5$)	272	9.1	41	15.1	1.4	11	4.0	0.4
Backbone-Backbone	67	2.2	2	3.0	0.1	0	0.0	0.0
Backbone-Sidechain	134	4.5	17	12.7	0.6	4	3.0	0.1
Sidechain-Sidechain	71	2.4	22	31.0	0.7	7	9.9	0.2
Long range ($i-j \geq 5$)	611	20.5	127	20.8	4.3	41	6.7	1.4
Backbone-Backbone	99	3.3	2	2.0	0.1	1	1.0	0.0
Backbone-Sidechain	279	9.3	46	16.5	1.5	15	5.4	0.5
Sidechain-Sidechain	233	7.8	79	33.9	2.6	25	10.7	0.8
Inter-chain	231	7.7	58	25.1	1.9	26	11.3	0.9
Backbone-Backbone	7	0.2	2	28.6	0.1	0	0.0	0.0
Backbone-Sidechain	53	1.8	15	28.3	0.5	10	18.9	0.3
Sidechain-Sidechain	171	5.7	41	24.0	1.4	16	9.4	0.5
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2986	100.0	354	11.9	11.9	110	3.7	3.7
Backbone-Backbone	482	16.1	9	1.9	0.3	1	0.2	0.0
Backbone-Sidechain	1500	50.2	175	11.7	5.9	52	3.5	1.7
Sidechain-Sidechain	1004	33.6	170	16.9	5.7	57	5.7	1.9

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

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



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and 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	47	32	19	79	33	210	0.97	26.24	1.98	0.55
2	42	25	21	77	33	198	1.02	30.25	2.3	0.51
3	45	27	22	71	27	192	1.02	25.23	2.05	0.55
4	41	35	24	74	36	210	1.11	26.18	2.04	0.64
5	37	27	19	86	35	204	1.05	30.31	2.27	0.6
6	36	28	22	74	32	192	1.04	32.27	2.46	0.54
7	45	28	18	73	32	196	1.0	30.02	2.32	0.53
8	39	31	18	84	31	203	1.02	26.23	1.98	0.6
9	45	28	23	78	33	207	1.04	31.64	2.33	0.57
10	46	29	22	72	32	201	0.99	24.39	1.94	0.49

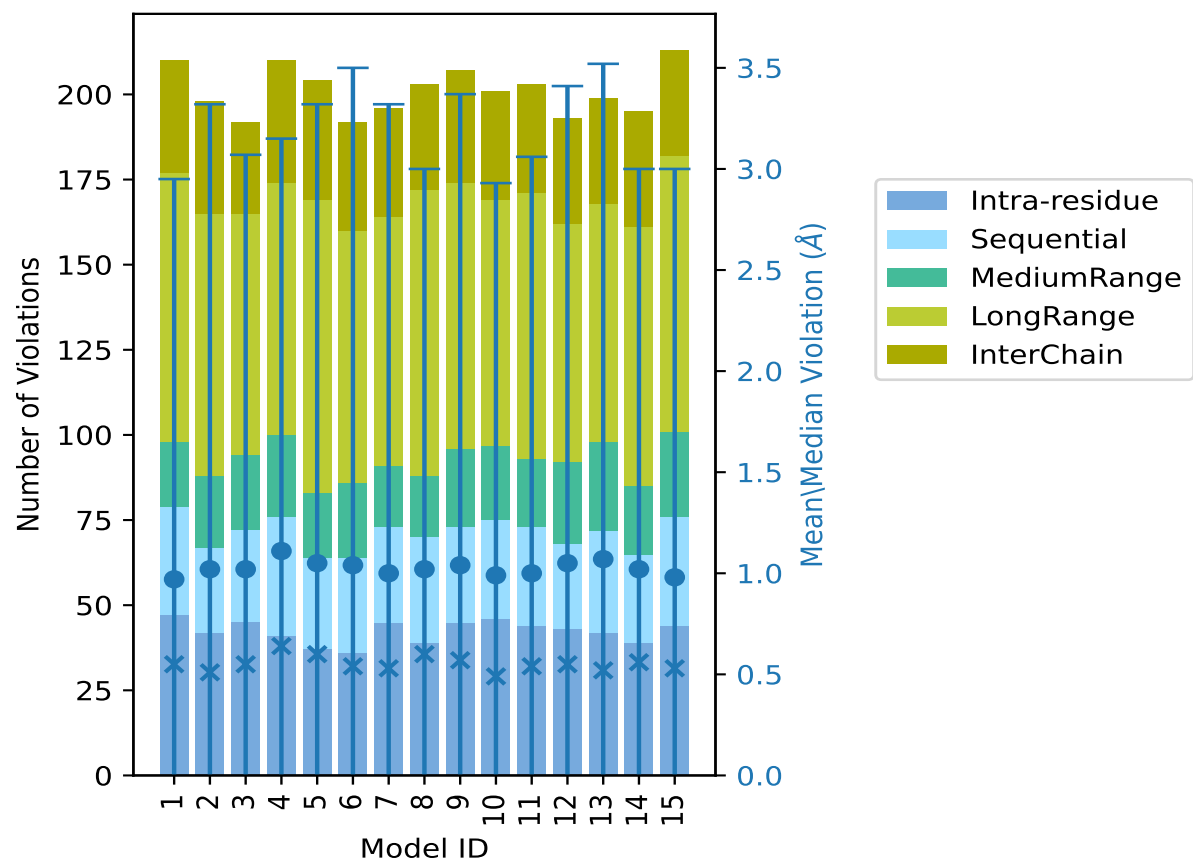
Continued on next page...

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	44	29	20	78	32	203	1.0	26.44	2.06	0.54
12	43	25	24	70	31	193	1.05	30.39	2.36	0.55
13	42	30	26	70	31	199	1.07	31.63	2.45	0.52
14	39	26	20	76	34	195	1.02	24.51	1.98	0.56
15	44	32	25	81	31	213	0.98	26.59	2.02	0.53

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

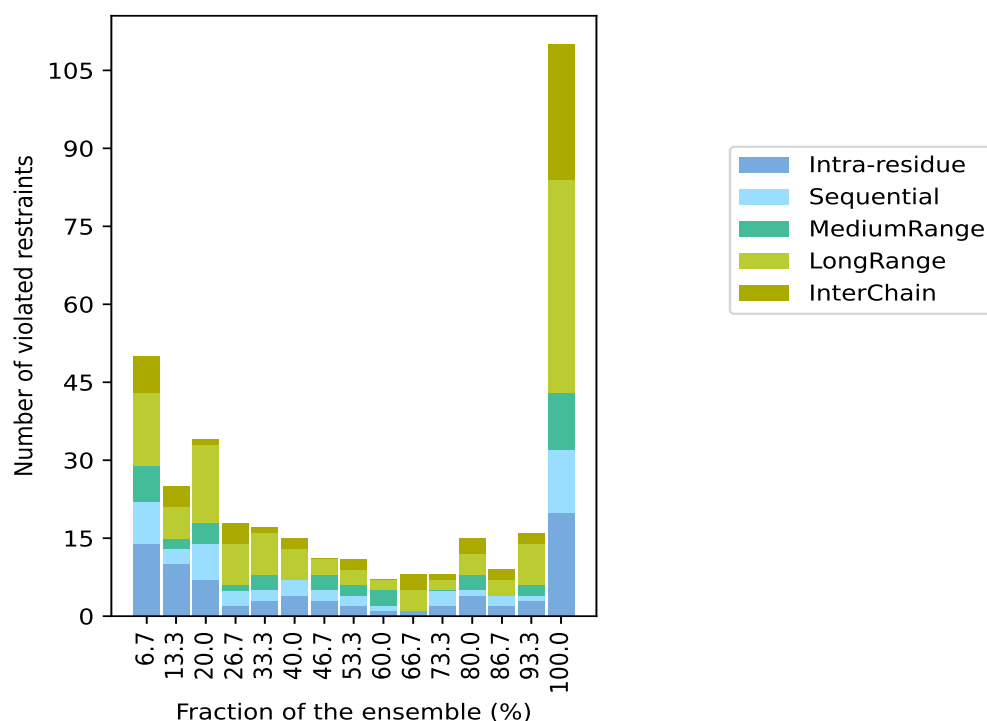
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2632(IR:1216, SQ:528, MR:231, LR:484, IC:173) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
14	8	7	14	7	50	1	6.7
10	3	2	6	4	25	2	13.3
7	7	4	15	1	34	3	20.0
2	3	1	8	4	18	4	26.7
3	2	3	8	1	17	5	33.3
4	3	0	6	2	15	6	40.0
3	2	3	3	0	11	7	46.7
2	2	2	3	2	11	8	53.3
1	1	3	2	0	7	9	60.0
1	0	0	4	3	8	10	66.7
2	3	0	2	1	8	11	73.3
4	1	3	4	3	15	12	80.0
2	2	0	3	2	9	13	86.7
3	1	2	8	2	16	14	93.3
20	12	11	41	26	110	15	100.0

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

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

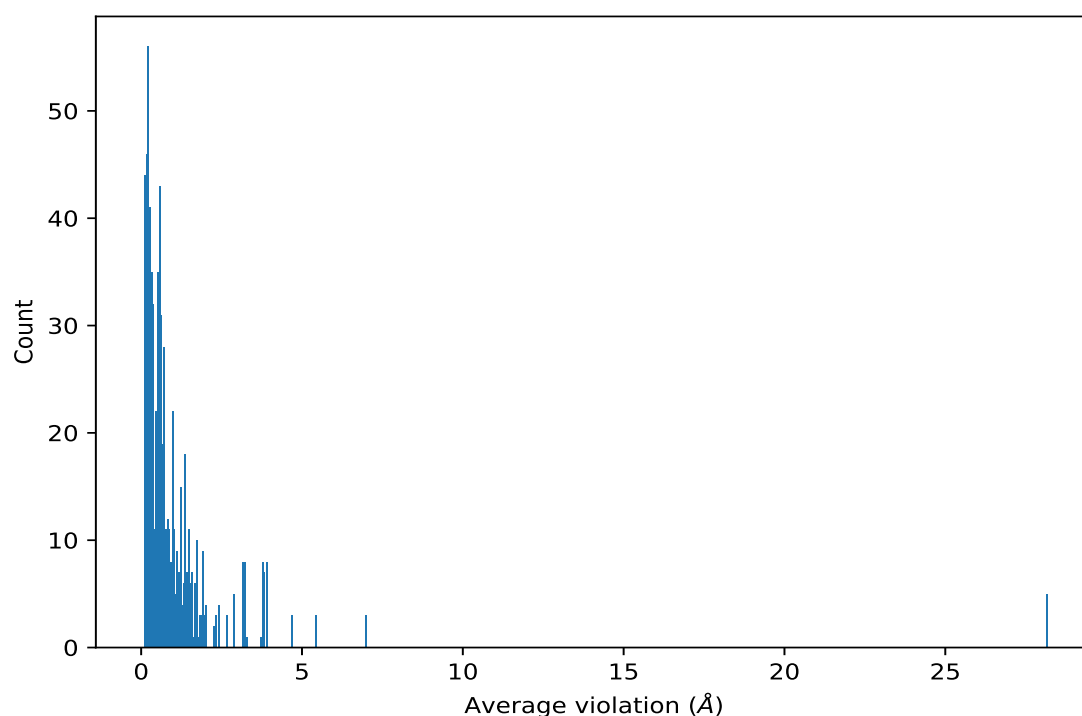
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2303)	2:567:B:ALA:HB1	1:45:A:ALA:H	15	28.15	2.72	26.59
(1,2303)	2:567:B:ALA:HB3	1:45:A:ALA:H	15	28.15	2.72	26.59
(1,2303)	2:567:B:ALA:HB2	1:45:A:ALA:H	15	28.15	2.72	26.59
(1,2303)	2:567:B:ALA:HB3	2:644:B:GLU:H	15	28.15	2.72	26.59
(1,2303)	2:567:B:ALA:HB2	2:644:B:GLU:H	15	28.15	2.72	26.59
(1,1363)	1:40:A:LEU:HA	1:34:A:VAL:HG13	15	6.97	0.88	7.07
(1,1363)	1:40:A:LEU:HA	1:34:A:VAL:HG11	15	6.97	0.88	7.07
(1,1363)	1:40:A:LEU:HA	1:34:A:VAL:HG12	15	6.97	0.88	7.07
(1,1350)	1:40:A:LEU:HG	1:34:A:VAL:HG13	15	5.44	0.95	5.4
(1,1350)	1:40:A:LEU:HG	1:34:A:VAL:HG11	15	5.44	0.95	5.4
(1,1350)	1:40:A:LEU:HG	1:34:A:VAL:HG12	15	5.44	0.95	5.4
(1,243)	2:616:B:VAL:HG11	2:631:B:GLN:HE22	15	4.66	1.07	4.56
(1,243)	2:616:B:VAL:HG13	2:631:B:GLN:HE22	15	4.66	1.07	4.56
(1,243)	2:616:B:VAL:HG12	2:631:B:GLN:HE22	15	4.66	1.07	4.56
(1,564)	2:688:B:LEU:HD22	2:583:B:LEU:HD23	15	3.9	1.01	3.31
(1,564)	2:688:B:LEU:HD21	2:583:B:LEU:HD23	15	3.9	1.01	3.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,564)	2:688:B:LEU:HD22	2:583:B:LEU:HD21	15	3.9	1.01	3.31
(1,564)	2:688:B:LEU:HD23	2:583:B:LEU:HD21	15	3.9	1.01	3.31
(1,564)	2:688:B:LEU:HD22	2:583:B:LEU:HD22	15	3.9	1.01	3.31
(1,564)	2:688:B:LEU:HD21	2:583:B:LEU:HD22	15	3.9	1.01	3.31
(1,564)	2:688:B:LEU:HD23	2:583:B:LEU:HD23	15	3.9	1.01	3.31
(1,564)	2:688:B:LEU:HD21	2:583:B:LEU:HD21	15	3.9	1.01	3.31
(1,563)	2:688:B:LEU:HD11	2:583:B:LEU:HD23	15	3.83	0.28	3.81
(1,563)	2:688:B:LEU:HD11	2:583:B:LEU:HD21	15	3.83	0.28	3.81
(1,563)	2:688:B:LEU:HD12	2:583:B:LEU:HD21	15	3.83	0.28	3.81
(1,563)	2:688:B:LEU:HD12	2:583:B:LEU:HD23	15	3.83	0.28	3.81
(1,563)	2:688:B:LEU:HD12	2:583:B:LEU:HD22	15	3.83	0.28	3.81
(1,563)	2:688:B:LEU:HD13	2:583:B:LEU:HD21	15	3.83	0.28	3.81
(1,563)	2:688:B:LEU:HD13	2:583:B:LEU:HD22	15	3.83	0.28	3.81
(1,2422)	2:643:B:VAL:HG12	1:48:A:GLN:HE21	15	3.76	0.99	4.15
(1,2422)	2:643:B:VAL:HG11	1:48:A:GLN:HE21	15	3.76	0.99	4.15
(1,2422)	2:682:B:VAL:HG12	2:652:B:PHE:HE1	15	3.76	0.99	4.15
(1,2422)	2:643:B:VAL:HG12	2:640:B:GLN:HE22	15	3.76	0.99	4.15
(1,2422)	2:682:B:VAL:HG13	2:652:B:PHE:HE1	15	3.76	0.99	4.15
(1,2422)	2:682:B:VAL:HG11	2:652:B:PHE:HE1	15	3.76	0.99	4.15
(1,2422)	2:643:B:VAL:HG11	2:640:B:GLN:HE22	15	3.76	0.99	4.15
(1,2422)	2:643:B:VAL:HG13	2:640:B:GLN:HE22	15	3.76	0.99	4.15
(1,2952)	2:573:B:PRO:HB2	1:40:A:LEU:HB2	15	3.7	0.25	3.73
(2,12)	2:683:B:CYS:HB2	2:656:B:GLN:HB3	15	3.26	0.26	3.27
(1,562)	2:688:B:LEU:HD12	2:686:B:LEU:HD21	15	3.23	1.1	3.85
(1,562)	2:688:B:LEU:HD11	2:686:B:LEU:HD21	15	3.23	1.1	3.85
(1,562)	2:688:B:LEU:HD12	2:686:B:LEU:HD23	15	3.23	1.1	3.85
(1,562)	2:688:B:LEU:HD13	2:686:B:LEU:HD22	15	3.23	1.1	3.85
(1,562)	2:688:B:LEU:HD12	2:686:B:LEU:HD22	15	3.23	1.1	3.85
(1,562)	2:688:B:LEU:HD13	2:686:B:LEU:HD23	15	3.23	1.1	3.85
(1,562)	2:688:B:LEU:HD13	2:686:B:LEU:HD21	15	3.23	1.1	3.85
(1,562)	2:688:B:LEU:HD11	2:686:B:LEU:HD22	15	3.23	1.1	3.85
(1,893)	2:630:B:ILE:HD11	2:645:B:VAL:HG13	15	3.18	0.77	3.24
(1,893)	2:630:B:ILE:HD11	2:645:B:VAL:HG12	15	3.18	0.77	3.24
(1,893)	2:630:B:ILE:HD13	2:645:B:VAL:HG12	15	3.18	0.77	3.24
(1,893)	2:630:B:ILE:HD11	2:645:B:VAL:HG11	15	3.18	0.77	3.24
(1,893)	2:630:B:ILE:HD13	2:645:B:VAL:HG13	15	3.18	0.77	3.24
(1,893)	2:630:B:ILE:HD12	2:645:B:VAL:HG13	15	3.18	0.77	3.24
(1,893)	2:630:B:ILE:HD12	2:645:B:VAL:HG12	15	3.18	0.77	3.24
(1,893)	2:630:B:ILE:HD13	2:645:B:VAL:HG11	15	3.18	0.77	3.24
(1,2674)	2:571:B:LEU:HD11	2:568:B:PRO:HG2	15	2.88	1.57	3.18
(1,2674)	2:571:B:LEU:HD12	2:569:B:PRO:HB3	15	2.88	1.57	3.18
(1,2674)	2:571:B:LEU:HD13	2:568:B:PRO:HG2	15	2.88	1.57	3.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2674)	2:571:B:LEU:HD12	2:568:B:PRO:HG2	15	2.88	1.57	3.18
(1,2674)	2:571:B:LEU:HD11	2:569:B:PRO:HB3	15	2.88	1.57	3.18
(1,2549)	2:647:B:VAL:HG11	2:649:B:TYR:HA	15	2.67	0.06	2.68
(1,2549)	2:647:B:VAL:HG12	2:649:B:TYR:HA	15	2.67	0.06	2.68
(1,2549)	2:647:B:VAL:HG13	2:649:B:TYR:HA	15	2.67	0.06	2.68
(1,799)	2:660:B:SER:HB3	1:40:A:LEU:HA	15	2.44	0.81	2.38
(1,1351)	1:37:A:TRP:HA	1:41:A:VAL:HG21	15	2.43	0.43	2.54
(1,1351)	1:37:A:TRP:HA	1:41:A:VAL:HG22	15	2.43	0.43	2.54
(1,1351)	1:37:A:TRP:HA	1:41:A:VAL:HG23	15	2.43	0.43	2.54
(1,2204)	2:616:B:VAL:HG12	1:44:A:LEU:HB2	15	2.34	0.24	2.47
(1,2204)	2:616:B:VAL:HG11	1:44:A:LEU:HB2	15	2.34	0.24	2.47
(1,2204)	2:616:B:VAL:HG13	1:44:A:LEU:HB2	15	2.34	0.24	2.47
(1,598)	2:582:B:GLN:HB3	2:580:B:ILE:HG22	15	1.98	0.21	1.95
(1,598)	2:582:B:GLN:HB3	2:580:B:ILE:HG21	15	1.98	0.21	1.95
(1,598)	2:582:B:GLN:HB3	2:580:B:ILE:HG23	15	1.98	0.21	1.95
(1,2523)	2:611:B:ILE:HD11	1:43:A:PHE:HD1	15	1.92	0.23	2.03
(1,2523)	2:611:B:ILE:HD13	2:584:B:ALA:H	15	1.92	0.23	2.03
(1,2523)	2:611:B:ILE:HD11	2:584:B:ALA:H	15	1.92	0.23	2.03
(1,2523)	2:611:B:ILE:HD12	2:584:B:ALA:H	15	1.92	0.23	2.03
(1,2523)	2:611:B:ILE:HD12	1:43:A:PHE:HD1	15	1.92	0.23	2.03
(1,2523)	2:611:B:ILE:HD13	1:43:A:PHE:HD1	15	1.92	0.23	2.03
(1,976)	2:574:B:TYR:HB2	2:581:B:ILE:HD11	15	1.91	0.15	1.99
(1,976)	2:574:B:TYR:HB2	2:581:B:ILE:HD13	15	1.91	0.15	1.99
(1,976)	2:574:B:TYR:HB2	2:581:B:ILE:HD12	15	1.91	0.15	1.99
(1,2286)	2:659:B:SER:HA	1:40:A:LEU:HB2	15	1.79	0.11	1.76
(1,489)	2:674:B:CYS:HB3	2:663:B:PRO:HB2	15	1.74	0.5	1.84
(1,2218)	2:666:B:THR:HG22	1:39:A:SER:HG	15	1.69	0.46	1.9
(1,2218)	2:666:B:THR:HG21	1:39:A:SER:HG	15	1.69	0.46	1.9
(1,2218)	2:666:B:THR:HG23	1:39:A:SER:HG	15	1.69	0.46	1.9
(1,2357)	2:616:B:VAL:HG13	2:630:B:ILE:HB	15	1.67	0.1	1.67
(1,2357)	2:616:B:VAL:HG12	2:630:B:ILE:HB	15	1.67	0.1	1.67
(1,2357)	2:616:B:VAL:HG11	2:630:B:ILE:HB	15	1.67	0.1	1.67
(1,2607)	2:659:B:SER:HA	2:673:B:PRO:HB2	15	1.6	0.14	1.65
(1,2207)	2:674:B:CYS:HB2	1:40:A:LEU:HB2	15	1.55	0.19	1.57
(1,763)	2:611:B:ILE:HD12	2:652:B:PHE:HE1	15	1.52	0.09	1.56
(1,763)	2:611:B:ILE:HD13	2:652:B:PHE:HE1	15	1.52	0.09	1.56
(1,763)	2:611:B:ILE:HD11	2:652:B:PHE:HE1	15	1.52	0.09	1.56
(1,322)	2:629:B:VAL:HG23	1:44:A:LEU:HD22	15	1.46	0.97	1.08
(1,322)	2:629:B:VAL:HG23	1:44:A:LEU:HD23	15	1.46	0.97	1.08
(1,322)	2:629:B:VAL:HG21	1:44:A:LEU:HD21	15	1.46	0.97	1.08
(1,322)	2:629:B:VAL:HG22	1:44:A:LEU:HD21	15	1.46	0.97	1.08
(1,322)	2:629:B:VAL:HG22	1:44:A:LEU:HD23	15	1.46	0.97	1.08

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,322)	2:629:B:VAL:HG21	1:44:A:LEU:HD22	15	1.46	0.97	1.08
(1,322)	2:629:B:VAL:HG23	1:44:A:LEU:HD21	15	1.46	0.97	1.08
(1,322)	2:629:B:VAL:HG21	1:44:A:LEU:HD23	15	1.46	0.97	1.08
(1,637)	2:658:B:TRP:HB2	2:672:B:LEU:HD22	15	1.45	0.29	1.37
(1,637)	2:658:B:TRP:HB2	2:672:B:LEU:HD23	15	1.45	0.29	1.37
(1,637)	2:658:B:TRP:HB2	2:672:B:LEU:HD21	15	1.45	0.29	1.37
(1,1067)	2:582:B:GLN:HG2	2:580:B:ILE:HG22	15	1.43	0.15	1.44
(1,1067)	2:582:B:GLN:HG2	2:580:B:ILE:HG21	15	1.43	0.15	1.44
(1,1067)	2:582:B:GLN:HG2	2:580:B:ILE:HG23	15	1.43	0.15	1.44
(1,1309)	2:579:B:SER:HB3	1:39:A:SER:HG	15	1.41	0.41	1.5
(1,1308)	2:579:B:SER:HB2	1:39:A:SER:HG	15	1.37	0.37	1.39
(1,1256)	2:592:B:GLU:HA	2:591:B:VAL:HG21	15	1.37	0.15	1.4
(1,1256)	2:592:B:GLU:HA	2:591:B:VAL:HG23	15	1.37	0.15	1.4
(1,1256)	2:592:B:GLU:HA	2:591:B:VAL:HG22	15	1.37	0.15	1.4
(1,1251)	2:594:B:LEU:HD12	2:658:B:TRP:HZ2	15	1.36	0.18	1.39
(1,1251)	2:594:B:LEU:HD11	2:658:B:TRP:HZ2	15	1.36	0.18	1.39
(1,1251)	2:594:B:LEU:HD13	2:658:B:TRP:HZ2	15	1.36	0.18	1.39
(1,2431)	2:646:B:LEU:HD13	2:625:B:PRO:HA	15	1.31	0.34	1.23
(1,2431)	2:646:B:LEU:HD12	2:625:B:PRO:HA	15	1.31	0.34	1.23
(1,2431)	2:646:B:LEU:HD11	2:625:B:PRO:HA	15	1.31	0.34	1.23
(1,642)	2:683:B:CYS:HB2	2:651:B:PHE:HB2	15	1.31	0.51	1.38
(1,639)	2:658:B:TRP:HB3	2:593:B:ASP:HA	15	1.28	0.05	1.29
(1,2457)	2:674:B:CYS:HB3	2:666:B:THR:HA	15	1.23	0.48	1.37
(1,2457)	2:674:B:CYS:HB3	2:667:B:SER:HA	15	1.23	0.48	1.37
(1,2380)	2:620:B:GLU:HB3	2:629:B:VAL:HG21	15	1.22	0.42	1.39
(1,2380)	2:620:B:GLU:HB3	2:629:B:VAL:HG22	15	1.22	0.42	1.39
(1,2380)	2:620:B:GLU:HB3	2:629:B:VAL:HG23	15	1.22	0.42	1.39
(1,2380)	2:620:B:GLU:HB3	2:619:B:ILE:HG23	15	1.22	0.42	1.39
(1,2577)	2:630:B:ILE:HD13	2:681:B:ASP:HB2	15	1.21	0.26	1.16
(1,2577)	2:630:B:ILE:HD12	2:681:B:ASP:HB2	15	1.21	0.26	1.16
(1,2577)	2:630:B:ILE:HD13	2:683:B:CYS:HB3	15	1.21	0.26	1.16
(1,2577)	2:630:B:ILE:HD12	2:683:B:CYS:HB3	15	1.21	0.26	1.16
(1,2577)	2:630:B:ILE:HD11	2:681:B:ASP:HB2	15	1.21	0.26	1.16
(1,1403)	1:41:A:VAL:HG21	1:39:A:SER:H	15	1.16	0.39	1.3
(1,1403)	1:41:A:VAL:HG22	1:39:A:SER:H	15	1.16	0.39	1.3
(1,1403)	1:41:A:VAL:HG23	1:39:A:SER:H	15	1.16	0.39	1.3
(1,2525)	2:611:B:ILE:HG21	1:37:A:TRP:HZ3	15	1.15	0.16	1.19
(1,2525)	2:611:B:ILE:HG22	1:37:A:TRP:HZ3	15	1.15	0.16	1.19
(1,2525)	2:611:B:ILE:HG23	1:37:A:TRP:HZ3	15	1.15	0.16	1.19
(1,2358)	2:616:B:VAL:HG11	2:617:B:GLU:HB3	15	1.13	0.07	1.14
(1,2358)	2:616:B:VAL:HG13	2:617:B:GLU:HB3	15	1.13	0.07	1.14
(1,2358)	2:616:B:VAL:HG12	2:617:B:GLU:HB3	15	1.13	0.07	1.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2397)	2:629:B:VAL:HG23	2:641:B:VAL:HA	15	1.1	0.09	1.11
(1,2397)	2:629:B:VAL:HG21	2:641:B:VAL:HA	15	1.1	0.09	1.11
(1,2397)	2:629:B:VAL:HG22	2:641:B:VAL:HA	15	1.1	0.09	1.11
(1,2666)	2:591:B:VAL:HG13	2:658:B:TRP:HE3	15	1.03	0.2	1.06
(1,2666)	2:591:B:VAL:HG11	2:658:B:TRP:HE3	15	1.03	0.2	1.06
(1,2666)	2:591:B:VAL:HG12	2:658:B:TRP:HE3	15	1.03	0.2	1.06
(1,797)	2:660:B:SER:HB2	1:40:A:LEU:HA	15	1.03	0.66	0.83
(1,977)	2:574:B:TYR:HB2	1:40:A:LEU:HD22	15	0.96	0.07	0.96
(1,977)	2:574:B:TYR:HB2	1:40:A:LEU:HD23	15	0.96	0.07	0.96
(1,977)	2:574:B:TYR:HB2	1:40:A:LEU:HD21	15	0.96	0.07	0.96
(1,8)	2:568:B:PRO:HB3	2:569:B:PRO:HD3	15	0.96	0.16	0.98
(1,1429)	2:576:B:MET:H	2:575:B:PHE:HZ	15	0.95	0.05	0.98
(1,2930)	2:576:B:MET:HB3	1:39:A:SER:HG	15	0.88	0.27	0.87
(1,2930)	2:573:B:PRO:HB3	1:39:A:SER:HG	15	0.88	0.27	0.87
(1,1583)	2:596:B:THR:H	2:652:B:PHE:HZ	15	0.87	0.12	0.88
(1,2942)	2:688:B:LEU:HG	1:40:A:LEU:HB2	15	0.86	0.16	0.9
(1,2942)	2:663:B:PRO:HG3	1:40:A:LEU:HB2	15	0.86	0.16	0.9
(1,801)	2:680:B:GLY:HA3	2:615:B:THR:HG23	15	0.84	0.08	0.84
(1,801)	2:680:B:GLY:HA3	2:615:B:THR:HG21	15	0.84	0.08	0.84
(1,801)	2:680:B:GLY:HA3	2:615:B:THR:HG22	15	0.84	0.08	0.84
(1,404)	2:648:B:GLU:HG3	2:669:B:LEU:HD11	15	0.84	0.48	0.72
(1,404)	2:648:B:GLU:HG3	2:669:B:LEU:HD13	15	0.84	0.48	0.72
(1,404)	2:648:B:GLU:HG3	2:669:B:LEU:HD12	15	0.84	0.48	0.72
(1,1468)	2:580:B:ILE:H	2:580:B:ILE:HG13	15	0.84	0.09	0.83
(1,1774)	2:621:B:ASP:H	2:620:B:GLU:HB2	15	0.81	0.09	0.84
(1,2082)	2:670:B:PHE:H	2:575:B:PHE:HZ	15	0.77	0.08	0.76
(1,1605)	2:598:B:ASP:H	2:597:B:GLU:HG2	15	0.74	0.07	0.73
(1,996)	2:647:B:VAL:HG23	2:625:B:PRO:HA	15	0.73	0.05	0.73
(1,996)	2:647:B:VAL:HG22	2:625:B:PRO:HA	15	0.73	0.05	0.73
(1,996)	2:647:B:VAL:HG21	2:625:B:PRO:HA	15	0.73	0.05	0.73
(1,1288)	2:581:B:ILE:HG23	1:34:A:VAL:HA	15	0.73	0.18	0.76
(1,1288)	2:581:B:ILE:HG22	1:34:A:VAL:HA	15	0.73	0.18	0.76
(1,1288)	2:581:B:ILE:HG21	1:34:A:VAL:HA	15	0.73	0.18	0.76
(1,1113)	2:674:B:CYS:HA	2:663:B:PRO:HB2	15	0.72	0.16	0.73
(1,2272)	2:641:B:VAL:HG11	1:44:A:LEU:HB3	15	0.71	0.23	0.68
(1,2272)	2:641:B:VAL:HG13	1:44:A:LEU:HB3	15	0.71	0.23	0.68
(1,2272)	2:641:B:VAL:HG12	1:44:A:LEU:HB3	15	0.71	0.23	0.68
(1,515)	2:679:B:VAL:HG13	2:618:B:ARG:HA	15	0.68	0.11	0.69
(1,515)	2:679:B:VAL:HG12	2:618:B:ARG:HA	15	0.68	0.11	0.69
(1,515)	2:679:B:VAL:HG11	2:618:B:ARG:HA	15	0.68	0.11	0.69
(1,1543)	2:590:B:LYS:H	2:590:B:LYS:HB3	15	0.68	0.06	0.71
(1,2388)	2:628:B:ALA:HB1	2:629:B:VAL:HA	15	0.68	0.04	0.67

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2388)	2:628:B:ALA:HB2	2:629:B:VAL:HA	15	0.68	0.04	0.67
(1,2388)	2:628:B:ALA:HB3	2:629:B:VAL:HA	15	0.68	0.04	0.67
(1,98)	2:672:B:LEU:HD13	2:591:B:VAL:HG23	15	0.64	0.51	0.43
(1,98)	2:672:B:LEU:HD11	2:591:B:VAL:HG23	15	0.64	0.51	0.43
(1,98)	2:672:B:LEU:HD13	2:591:B:VAL:HG22	15	0.64	0.51	0.43
(1,98)	2:672:B:LEU:HD12	2:591:B:VAL:HG22	15	0.64	0.51	0.43
(1,98)	2:672:B:LEU:HD13	2:591:B:VAL:HG21	15	0.64	0.51	0.43
(1,98)	2:672:B:LEU:HD12	2:591:B:VAL:HG21	15	0.64	0.51	0.43
(1,98)	2:672:B:LEU:HD11	2:591:B:VAL:HG22	15	0.64	0.51	0.43
(1,98)	2:672:B:LEU:HD12	2:591:B:VAL:HG23	15	0.64	0.51	0.43
(1,98)	2:672:B:LEU:HD11	2:591:B:VAL:HG21	15	0.64	0.51	0.43
(1,2675)	2:571:B:LEU:HD21	2:572:B:PRO:HG2	15	0.63	0.53	0.46
(1,2675)	2:571:B:LEU:HD23	2:569:B:PRO:HB3	15	0.63	0.53	0.46
(1,2675)	2:571:B:LEU:HD22	2:568:B:PRO:HG2	15	0.63	0.53	0.46
(1,2675)	2:571:B:LEU:HD22	2:572:B:PRO:HG2	15	0.63	0.53	0.46
(1,2675)	2:571:B:LEU:HD23	2:572:B:PRO:HG2	15	0.63	0.53	0.46
(1,1559)	2:592:B:GLU:H	2:591:B:VAL:HG21	15	0.62	0.12	0.64
(1,1559)	2:592:B:GLU:H	2:591:B:VAL:HG23	15	0.62	0.12	0.64
(1,1559)	2:592:B:GLU:H	2:591:B:VAL:HG22	15	0.62	0.12	0.64
(1,2738)	2:679:B:VAL:H	2:619:B:ILE:HG12	15	0.62	0.17	0.6
(1,552)	2:686:B:LEU:HD13	2:611:B:ILE:HA	15	0.61	0.23	0.57
(1,552)	2:686:B:LEU:HD11	2:611:B:ILE:HA	15	0.61	0.23	0.57
(1,552)	2:686:B:LEU:HD12	2:611:B:ILE:HA	15	0.61	0.23	0.57
(1,2320)	2:617:B:GLU:HG3	2:679:B:VAL:HG22	15	0.6	0.35	0.37
(1,2320)	2:617:B:GLU:HG3	2:679:B:VAL:HG21	15	0.6	0.35	0.37
(1,2320)	2:617:B:GLU:HG3	2:679:B:VAL:HG13	15	0.6	0.35	0.37
(1,2320)	2:617:B:GLU:HG3	2:679:B:VAL:HG23	15	0.6	0.35	0.37
(1,1628)	2:600:B:ILE:H	2:600:B:ILE:HG12	15	0.59	0.13	0.63
(1,1988)	2:656:B:GLN:H	2:656:B:GLN:HB3	15	0.59	0.06	0.61
(1,2209)	2:576:B:MET:HB2	1:39:A:SER:HG	15	0.58	0.15	0.54
(1,85)	2:588:B:LEU:HD23	2:582:B:GLN:HB3	15	0.58	0.08	0.58
(1,85)	2:588:B:LEU:HD21	2:582:B:GLN:HB3	15	0.58	0.08	0.58
(1,85)	2:588:B:LEU:HD22	2:582:B:GLN:HB3	15	0.58	0.08	0.58
(1,1070)	2:581:B:ILE:HD13	2:594:B:LEU:HD13	15	0.58	0.06	0.58
(1,1070)	2:581:B:ILE:HD13	2:594:B:LEU:HD12	15	0.58	0.06	0.58
(1,1070)	2:581:B:ILE:HD13	2:594:B:LEU:HD11	15	0.58	0.06	0.58
(1,1070)	2:581:B:ILE:HD11	2:594:B:LEU:HD11	15	0.58	0.06	0.58
(1,1070)	2:581:B:ILE:HD12	2:594:B:LEU:HD12	15	0.58	0.06	0.58
(1,1070)	2:581:B:ILE:HD12	2:594:B:LEU:HD11	15	0.58	0.06	0.58
(1,1070)	2:581:B:ILE:HD12	2:594:B:LEU:HD13	15	0.58	0.06	0.58
(1,1070)	2:581:B:ILE:HD11	2:594:B:LEU:HD13	15	0.58	0.06	0.58
(1,1070)	2:581:B:ILE:HD11	2:594:B:LEU:HD12	15	0.58	0.06	0.58

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,638)	2:658:B:TRP:HB2	2:593:B:ASP:HA	15	0.52	0.03	0.51
(1,1399)	1:41:A:VAL:HG23	1:41:A:VAL:H	15	0.51	0.05	0.52
(1,1399)	1:41:A:VAL:HG21	1:41:A:VAL:H	15	0.51	0.05	0.52
(1,1399)	1:41:A:VAL:HG22	1:41:A:VAL:H	15	0.51	0.05	0.52
(1,1763)	2:620:B:GLU:H	2:620:B:GLU:HB3	15	0.51	0.05	0.53
(1,2630)	2:673:B:PRO:HD3	2:577:B:LYS:HG2	15	0.51	0.16	0.52
(1,2630)	2:672:B:LEU:HB3	2:673:B:PRO:HD3	15	0.51	0.16	0.52
(1,1250)	2:619:B:ILE:HG12	2:618:B:ARG:H	15	0.51	0.03	0.5
(1,2517)	2:605:B:ILE:HG21	2:604:B:GLU:HB3	15	0.5	0.11	0.52
(1,2517)	2:605:B:ILE:HG22	2:604:B:GLU:HB3	15	0.5	0.11	0.52
(1,2517)	2:605:B:ILE:HG23	2:604:B:GLU:HB3	15	0.5	0.11	0.52
(1,245)	2:616:B:VAL:HG13	2:630:B:ILE:HG22	15	0.5	0.09	0.48
(1,245)	2:616:B:VAL:HG12	2:630:B:ILE:HG21	15	0.5	0.09	0.48
(1,245)	2:616:B:VAL:HG11	2:630:B:ILE:HG22	15	0.5	0.09	0.48
(1,245)	2:616:B:VAL:HG11	2:630:B:ILE:HG23	15	0.5	0.09	0.48
(1,245)	2:616:B:VAL:HG11	2:630:B:ILE:HG21	15	0.5	0.09	0.48
(1,245)	2:616:B:VAL:HG13	2:630:B:ILE:HG23	15	0.5	0.09	0.48
(1,2499)	2:619:B:ILE:H	2:619:B:ILE:HG12	15	0.49	0.06	0.48
(1,534)	2:684:B:ILE:HG23	2:611:B:ILE:HB	15	0.47	0.04	0.48
(1,534)	2:684:B:ILE:HG21	2:611:B:ILE:HB	15	0.47	0.04	0.48
(1,534)	2:684:B:ILE:HG22	2:611:B:ILE:HB	15	0.47	0.04	0.48
(1,128)	2:591:B:VAL:HG12	2:591:B:VAL:H	15	0.47	0.05	0.48
(1,128)	2:591:B:VAL:HG13	2:591:B:VAL:H	15	0.47	0.05	0.48
(1,128)	2:591:B:VAL:HG11	2:591:B:VAL:H	15	0.47	0.05	0.48
(1,2654)	2:674:B:CYS:HB2	2:676:B:LYS:HD3	15	0.46	0.2	0.44
(1,1222)	2:601:B:GLN:HG3	2:605:B:ILE:HD12	15	0.41	0.09	0.39
(1,1222)	2:601:B:GLN:HG3	2:605:B:ILE:HD13	15	0.41	0.09	0.39
(1,1222)	2:601:B:GLN:HG3	2:605:B:ILE:HD11	15	0.41	0.09	0.39
(1,1753)	2:619:B:ILE:H	2:619:B:ILE:HG12	15	0.39	0.06	0.38
(1,1389)	1:37:A:TRP:HB3	1:37:A:TRP:HE3	15	0.39	0.03	0.4
(1,1205)	2:569:B:PRO:HA	2:568:B:PRO:HG2	15	0.38	0.12	0.34
(1,2001)	2:658:B:TRP:HE1	2:594:B:LEU:HB2	15	0.38	0.12	0.37
(1,2608)	2:660:B:SER:HA	2:662:B:CYS:HA	15	0.37	0.07	0.37
(1,2709)	2:580:B:ILE:H	2:580:B:ILE:HG22	15	0.37	0.04	0.38
(1,2709)	2:580:B:ILE:H	2:580:B:ILE:HG21	15	0.37	0.04	0.38
(1,2709)	2:580:B:ILE:H	2:580:B:ILE:HG23	15	0.37	0.04	0.38
(1,1730)	2:617:B:GLU:H	2:617:B:GLU:HB3	15	0.37	0.05	0.37
(1,149)	2:596:B:THR:H	2:595:B:LYS:HB2	15	0.36	0.12	0.36
(1,2217)	2:583:B:LEU:HD23	1:38:A:HIS:HA	15	0.36	0.05	0.36
(1,2217)	2:583:B:LEU:HD21	1:38:A:HIS:HA	15	0.36	0.05	0.36
(1,2217)	2:583:B:LEU:HD22	1:38:A:HIS:HA	15	0.36	0.05	0.36
(1,375)	2:644:B:GLU:H	2:643:B:VAL:HB	15	0.32	0.03	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2935)	2:583:B:LEU:HD23	1:39:A:SER:HB3	15	0.32	0.09	0.35
(1,2935)	2:583:B:LEU:HD21	1:39:A:SER:HB3	15	0.32	0.09	0.35
(1,2935)	2:583:B:LEU:HD22	1:39:A:SER:HB3	15	0.32	0.09	0.35
(1,1211)	2:630:B:ILE:HA	2:619:B:ILE:HG13	15	0.32	0.11	0.31
(1,2019)	2:660:B:SER:H	2:663:B:PRO:HB2	15	0.28	0.06	0.29
(1,124)	2:596:B:THR:HG22	2:684:B:ILE:HD12	15	0.28	0.09	0.27
(1,124)	2:596:B:THR:HG22	2:684:B:ILE:HD13	15	0.28	0.09	0.27
(1,124)	2:596:B:THR:HG22	2:684:B:ILE:HD11	15	0.28	0.09	0.27
(1,124)	2:596:B:THR:HG23	2:684:B:ILE:HD12	15	0.28	0.09	0.27
(1,124)	2:596:B:THR:HG21	2:684:B:ILE:HD12	15	0.28	0.09	0.27
(1,124)	2:596:B:THR:HG21	2:684:B:ILE:HD11	15	0.28	0.09	0.27
(1,124)	2:596:B:THR:HG23	2:684:B:ILE:HD13	15	0.28	0.09	0.27
(1,124)	2:596:B:THR:HG21	2:684:B:ILE:HD13	15	0.28	0.09	0.27
(1,1789)	2:624:B:SER:H	2:624:B:SER:HB3	15	0.26	0.15	0.17
(1,2176)	2:684:B:ILE:H	2:684:B:ILE:HG12	15	0.26	0.03	0.26
(1,671)	2:596:B:THR:HG23	2:596:B:THR:HA	15	0.25	0.03	0.26
(1,671)	2:596:B:THR:HG21	2:596:B:THR:HA	15	0.25	0.03	0.26
(1,671)	2:596:B:THR:HG22	2:596:B:THR:HA	15	0.25	0.03	0.26
(1,1130)	2:580:B:ILE:HG23	2:580:B:ILE:HG12	15	0.23	0.02	0.24
(1,1130)	2:580:B:ILE:HG22	2:580:B:ILE:HG12	15	0.23	0.02	0.24
(1,1130)	2:580:B:ILE:HG21	2:580:B:ILE:HG12	15	0.23	0.02	0.24
(1,2678)	1:34:A:VAL:HB	1:34:A:VAL:HG13	15	0.22	0.02	0.22
(1,2678)	1:34:A:VAL:HB	1:34:A:VAL:HG11	15	0.22	0.02	0.22
(1,2678)	1:34:A:VAL:HB	1:34:A:VAL:HG21	15	0.22	0.02	0.22
(1,2678)	1:34:A:VAL:HB	1:34:A:VAL:HG23	15	0.22	0.02	0.22
(1,2678)	1:34:A:VAL:HB	1:34:A:VAL:HG12	15	0.22	0.02	0.22
(1,83)	2:588:B:LEU:HD13	2:588:B:LEU:HD22	15	0.19	0.04	0.19
(1,83)	2:588:B:LEU:HD13	2:588:B:LEU:HD23	15	0.19	0.04	0.19
(1,83)	2:588:B:LEU:HD12	2:588:B:LEU:HD21	15	0.19	0.04	0.19
(1,83)	2:588:B:LEU:HD11	2:588:B:LEU:HD23	15	0.19	0.04	0.19
(1,83)	2:588:B:LEU:HD11	2:588:B:LEU:HD22	15	0.19	0.04	0.19
(1,83)	2:588:B:LEU:HD11	2:588:B:LEU:HD21	15	0.19	0.04	0.19
(1,83)	2:588:B:LEU:HD12	2:588:B:LEU:HD22	15	0.19	0.04	0.19
(1,83)	2:588:B:LEU:HD12	2:588:B:LEU:HD23	15	0.19	0.04	0.19
(1,83)	2:588:B:LEU:HD13	2:588:B:LEU:HD21	15	0.19	0.04	0.19
(1,1725)	2:616:B:VAL:H	2:616:B:VAL:HG22	15	0.17	0.02	0.16
(1,1725)	2:616:B:VAL:H	2:616:B:VAL:HG21	15	0.17	0.02	0.16
(1,1725)	2:616:B:VAL:H	2:616:B:VAL:HG23	15	0.17	0.02	0.16
(1,1337)	1:40:A:LEU:HD13	1:40:A:LEU:HD21	15	0.14	0.02	0.14
(1,1337)	1:40:A:LEU:HD11	1:40:A:LEU:HD22	15	0.14	0.02	0.14
(1,1337)	1:40:A:LEU:HD12	1:40:A:LEU:HD22	15	0.14	0.02	0.14
(1,1337)	1:40:A:LEU:HD13	1:40:A:LEU:HD23	15	0.14	0.02	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1337)	1:40:A:LEU:HD11	1:40:A:LEU:HD21	15	0.14	0.02	0.14
(1,1337)	1:40:A:LEU:HD12	1:40:A:LEU:HD21	15	0.14	0.02	0.14
(1,1337)	1:40:A:LEU:HD12	1:40:A:LEU:HD23	15	0.14	0.02	0.14
(1,1337)	1:40:A:LEU:HD13	1:40:A:LEU:HD22	15	0.14	0.02	0.14
(1,2637)	2:679:B:VAL:HG12	2:679:B:VAL:HB	15	0.14	0.02	0.13
(1,2637)	2:679:B:VAL:HG11	2:679:B:VAL:HB	15	0.14	0.02	0.13
(1,2637)	2:679:B:VAL:HG21	2:679:B:VAL:HB	15	0.14	0.02	0.13
(1,2637)	2:679:B:VAL:HG13	2:679:B:VAL:HB	15	0.14	0.02	0.13
(1,2267)	2:643:B:VAL:HG21	1:44:A:LEU:HD12	14	1.71	0.54	1.89
(1,2267)	2:643:B:VAL:HG22	1:44:A:LEU:HD12	14	1.71	0.54	1.89
(1,2267)	2:643:B:VAL:HG23	1:44:A:LEU:HD12	14	1.71	0.54	1.89
(1,2267)	2:643:B:VAL:HG23	1:44:A:LEU:HD13	14	1.71	0.54	1.89
(1,2267)	2:643:B:VAL:HG21	1:44:A:LEU:HD13	14	1.71	0.54	1.89
(1,2267)	2:643:B:VAL:HG22	1:44:A:LEU:HD13	14	1.71	0.54	1.89
(1,2267)	2:643:B:VAL:HG22	1:44:A:LEU:HD11	14	1.71	0.54	1.89
(1,152)	2:595:B:LYS:HG2	2:658:B:TRP:HB3	14	1.18	0.29	1.29
(1,1086)	2:609:B:LEU:HD22	1:37:A:TRP:HZ3	14	1.09	0.39	1.28
(1,1086)	2:609:B:LEU:HD23	1:37:A:TRP:HZ3	14	1.09	0.39	1.28
(1,1086)	2:609:B:LEU:HD21	1:37:A:TRP:HZ3	14	1.09	0.39	1.28
(1,1353)	1:44:A:LEU:HA	1:44:A:LEU:HD12	14	0.79	0.1	0.77
(1,1353)	1:44:A:LEU:HA	1:44:A:LEU:HD13	14	0.79	0.1	0.77
(1,1353)	1:44:A:LEU:HA	1:44:A:LEU:HD11	14	0.79	0.1	0.77
(1,1109)	2:672:B:LEU:HG	2:673:B:PRO:HD3	14	0.79	0.4	0.57
(1,2596)	2:574:B:TYR:HB3	2:581:B:ILE:HD11	14	0.7	0.36	0.59
(1,2596)	2:574:B:TYR:HB3	2:581:B:ILE:HD13	14	0.7	0.36	0.59
(1,2596)	2:574:B:TYR:HB3	2:581:B:ILE:HD12	14	0.7	0.36	0.59
(1,513)	2:679:B:VAL:HG12	2:616:B:VAL:HG22	14	0.66	0.06	0.66
(1,513)	2:679:B:VAL:HG12	2:616:B:VAL:HG21	14	0.66	0.06	0.66
(1,513)	2:679:B:VAL:HG12	2:616:B:VAL:HG23	14	0.66	0.06	0.66
(1,513)	2:679:B:VAL:HG11	2:616:B:VAL:HG21	14	0.66	0.06	0.66
(1,513)	2:679:B:VAL:HG13	2:616:B:VAL:HG21	14	0.66	0.06	0.66
(1,513)	2:679:B:VAL:HG13	2:616:B:VAL:HG23	14	0.66	0.06	0.66
(1,513)	2:679:B:VAL:HG13	2:616:B:VAL:HG22	14	0.66	0.06	0.66
(1,513)	2:679:B:VAL:HG11	2:616:B:VAL:HG22	14	0.66	0.06	0.66
(1,2804)	2:619:B:ILE:H	2:679:B:VAL:HG13	14	0.56	0.12	0.54
(1,2804)	2:619:B:ILE:H	2:679:B:VAL:HG21	14	0.56	0.12	0.54
(1,2804)	2:619:B:ILE:H	2:679:B:VAL:HG11	14	0.56	0.12	0.54
(1,2804)	2:619:B:ILE:H	2:679:B:VAL:HG22	14	0.56	0.12	0.54
(1,2804)	2:619:B:ILE:H	2:679:B:VAL:HG12	14	0.56	0.12	0.54
(1,931)	2:639:B:ALA:HB3	2:634:B:VAL:HG23	14	0.52	0.23	0.52
(1,931)	2:639:B:ALA:HB1	2:634:B:VAL:HG22	14	0.52	0.23	0.52
(1,931)	2:639:B:ALA:HB2	2:634:B:VAL:HG21	14	0.52	0.23	0.52

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,931)	2:639:B:ALA:HB2	2:634:B:VAL:HG23	14	0.52	0.23	0.52
(1,931)	2:639:B:ALA:HB1	2:634:B:VAL:HG21	14	0.52	0.23	0.52
(1,931)	2:639:B:ALA:HB2	2:634:B:VAL:HG22	14	0.52	0.23	0.52
(1,2898)	2:675:B:SER:H	2:673:B:PRO:HB2	14	0.42	0.08	0.42
(1,2665)	2:591:B:VAL:HG13	2:594:B:LEU:H	14	0.34	0.11	0.38
(1,2665)	2:591:B:VAL:HG11	2:658:B:TRP:HH2	14	0.34	0.11	0.38
(1,2665)	2:591:B:VAL:HG12	2:594:B:LEU:H	14	0.34	0.11	0.38
(1,2665)	2:591:B:VAL:HG12	2:658:B:TRP:HH2	14	0.34	0.11	0.38
(1,2665)	2:591:B:VAL:HG13	2:658:B:TRP:HH2	14	0.34	0.11	0.38
(1,276)	2:619:B:ILE:HG21	2:628:B:ALA:HB1	14	0.33	0.05	0.36
(1,276)	2:619:B:ILE:HG23	2:628:B:ALA:HB2	14	0.33	0.05	0.36
(1,276)	2:619:B:ILE:HG23	2:628:B:ALA:HB1	14	0.33	0.05	0.36
(1,276)	2:619:B:ILE:HG23	2:628:B:ALA:HB3	14	0.33	0.05	0.36
(1,276)	2:619:B:ILE:HG22	2:628:B:ALA:HB3	14	0.33	0.05	0.36
(1,276)	2:619:B:ILE:HG21	2:628:B:ALA:HB2	14	0.33	0.05	0.36
(1,276)	2:619:B:ILE:HG22	2:628:B:ALA:HB2	14	0.33	0.05	0.36
(1,1194)	2:689:B:LYS:HA	2:610:B:LYS:HE2	14	0.3	0.07	0.3
(1,1194)	2:689:B:LYS:HA	2:610:B:LYS:HE3	14	0.3	0.07	0.3
(1,1533)	2:589:B:LYS:H	2:589:B:LYS:HB3	14	0.25	0.03	0.26
(1,1835)	2:627:B:VAL:H	2:646:B:LEU:HA	14	0.25	0.04	0.25
(1,351)	2:679:B:VAL:HG12	2:679:B:VAL:HA	14	0.14	0.02	0.15
(1,351)	2:679:B:VAL:HG11	2:679:B:VAL:HA	14	0.14	0.02	0.15
(1,351)	2:679:B:VAL:HG13	2:679:B:VAL:HA	14	0.14	0.02	0.15
(1,2222)	2:686:B:LEU:HD21	1:38:A:HIS:HB2	13	1.35	0.43	1.43
(1,2222)	2:686:B:LEU:HD23	1:38:A:HIS:HB2	13	1.35	0.43	1.43
(1,2222)	2:686:B:LEU:HD22	1:38:A:HIS:HB2	13	1.35	0.43	1.43
(1,641)	2:683:B:CYS:HB3	2:651:B:PHE:HB2	13	1.02	0.7	0.79
(1,2926)	2:682:B:VAL:HG11	1:44:A:LEU:HB2	13	0.98	0.36	1.0
(1,2926)	2:653:B:VAL:HG13	1:44:A:LEU:HB2	13	0.98	0.36	1.0
(1,2926)	2:653:B:VAL:HG12	1:44:A:LEU:HB2	13	0.98	0.36	1.0
(1,2926)	2:682:B:VAL:HG13	1:44:A:LEU:HB2	13	0.98	0.36	1.0
(1,2926)	2:653:B:VAL:HG11	1:44:A:LEU:HB2	13	0.98	0.36	1.0
(1,2926)	2:682:B:VAL:HG12	1:44:A:LEU:HB2	13	0.98	0.36	1.0
(1,1541)	2:590:B:LYS:H	2:589:B:LYS:HE2	13	0.73	0.4	0.67
(1,1117)	2:589:B:LYS:HB2	2:589:B:LYS:HE2	13	0.45	0.05	0.46
(1,1931)	2:679:B:VAL:H	2:678:B:SER:HB2	13	0.34	0.14	0.34
(1,887)	2:630:B:ILE:HG21	2:643:B:VAL:HG11	13	0.32	0.14	0.29
(1,887)	2:630:B:ILE:HG23	2:643:B:VAL:HG11	13	0.32	0.14	0.29
(1,887)	2:630:B:ILE:HG23	2:643:B:VAL:HG13	13	0.32	0.14	0.29
(1,887)	2:630:B:ILE:HG21	2:643:B:VAL:HG12	13	0.32	0.14	0.29
(1,887)	2:630:B:ILE:HG22	2:643:B:VAL:HG13	13	0.32	0.14	0.29
(1,887)	2:630:B:ILE:HG22	2:643:B:VAL:HG12	13	0.32	0.14	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,887)	2:630:B:ILE:HG22	2:643:B:VAL:HG11	13	0.32	0.14	0.29
(1,132)	2:591:B:VAL:HG23	2:577:B:LYS:HA	13	0.26	0.07	0.24
(1,132)	2:591:B:VAL:HG22	2:577:B:LYS:HA	13	0.26	0.07	0.24
(1,132)	2:591:B:VAL:HG21	2:577:B:LYS:HA	13	0.26	0.07	0.24
(1,2107)	2:674:B:CYS:H	2:674:B:CYS:HB3	13	0.22	0.07	0.22
(1,2270)	2:641:B:VAL:HG11	1:44:A:LEU:HD12	12	0.97	0.46	1.14
(1,2270)	2:641:B:VAL:HG13	1:44:A:LEU:HD11	12	0.97	0.46	1.14
(1,2270)	2:641:B:VAL:HG11	1:44:A:LEU:HD13	12	0.97	0.46	1.14
(1,2270)	2:641:B:VAL:HG13	1:44:A:LEU:HD12	12	0.97	0.46	1.14
(1,2270)	2:641:B:VAL:HG13	1:44:A:LEU:HD13	12	0.97	0.46	1.14
(1,2270)	2:641:B:VAL:HG12	1:44:A:LEU:HD13	12	0.97	0.46	1.14
(1,2270)	2:641:B:VAL:HG12	1:44:A:LEU:HD11	12	0.97	0.46	1.14
(1,2270)	2:641:B:VAL:HG11	1:44:A:LEU:HD11	12	0.97	0.46	1.14
(2,6)	2:590:B:LYS:HD2	2:589:B:LYS:HA	12	0.76	0.21	0.84
(1,2490)	2:656:B:GLN:HB2	2:682:B:VAL:HA	12	0.55	0.16	0.55
(1,2490)	2:625:B:PRO:HB3	2:623:B:HIS:HA	12	0.55	0.16	0.55
(1,99)	2:672:B:LEU:HD11	2:672:B:LEU:HB3	12	0.54	0.02	0.55
(1,99)	2:672:B:LEU:HD13	2:672:B:LEU:HB3	12	0.54	0.02	0.55
(1,99)	2:672:B:LEU:HD12	2:672:B:LEU:HB3	12	0.54	0.02	0.55
(1,2511)	2:600:B:ILE:HA	2:600:B:ILE:HD12	12	0.5	0.01	0.5
(1,2511)	2:600:B:ILE:HA	2:600:B:ILE:HD13	12	0.5	0.01	0.5
(1,2511)	2:600:B:ILE:HA	2:600:B:ILE:HD11	12	0.5	0.01	0.5
(1,416)	2:653:B:VAL:HB	2:656:B:GLN:HB3	12	0.45	0.21	0.44
(1,116)	2:578:B:GLY:HA3	2:590:B:LYS:HD3	12	0.43	0.07	0.41
(1,105)	2:672:B:LEU:HD21	2:591:B:VAL:HB	12	0.43	0.08	0.42
(1,105)	2:672:B:LEU:HD22	2:591:B:VAL:HB	12	0.43	0.08	0.42
(1,105)	2:672:B:LEU:HD23	2:591:B:VAL:HB	12	0.43	0.08	0.42
(1,686)	2:600:B:ILE:HG13	2:600:B:ILE:HG21	12	0.29	0.02	0.29
(1,686)	2:600:B:ILE:HG13	2:600:B:ILE:HG22	12	0.29	0.02	0.29
(1,686)	2:600:B:ILE:HG13	2:600:B:ILE:HG23	12	0.29	0.02	0.29
(1,1006)	2:652:B:PHE:HA	1:41:A:VAL:HA	12	0.24	0.13	0.2
(1,503)	2:677:B:LEU:HB2	2:677:B:LEU:HD11	12	0.22	0.02	0.21
(1,503)	2:677:B:LEU:HB2	2:677:B:LEU:HD12	12	0.22	0.02	0.21
(1,503)	2:677:B:LEU:HB2	2:677:B:LEU:HD13	12	0.22	0.02	0.21
(1,1060)	2:666:B:THR:HG22	1:40:A:LEU:HA	12	0.2	0.06	0.21
(1,1060)	2:666:B:THR:HG21	1:40:A:LEU:HA	12	0.2	0.06	0.21
(1,1060)	2:666:B:THR:HG23	1:40:A:LEU:HA	12	0.2	0.06	0.21
(1,1953)	2:649:B:TYR:H	2:649:B:TYR:HB3	12	0.19	0.03	0.18
(1,2860)	2:659:B:SER:H	2:675:B:SER:HA	12	0.17	0.05	0.15
(2,7)	2:578:B:GLY:HA3	2:590:B:LYS:HG3	12	0.16	0.02	0.16
(1,62)	2:586:B:GLY:HA3	2:587:B:GLU:HG3	11	1.35	0.58	1.58
(1,510)	2:682:B:VAL:HG21	2:613:B:SER:HB2	11	0.97	0.55	0.8

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,510)	2:682:B:VAL:HG22	2:613:B:SER:HB2	11	0.97	0.55	0.8
(1,510)	2:682:B:VAL:HG23	2:613:B:SER:HB2	11	0.97	0.55	0.8
(1,1928)	2:645:B:VAL:H	2:645:B:VAL:HG12	11	0.54	0.18	0.47
(1,1928)	2:645:B:VAL:H	2:645:B:VAL:HG11	11	0.54	0.18	0.47
(1,1928)	2:645:B:VAL:H	2:645:B:VAL:HG13	11	0.54	0.18	0.47
(1,1312)	2:654:B:PHE:HB3	2:684:B:ILE:HG12	11	0.38	0.14	0.41
(1,2132)	2:678:B:SER:H	2:678:B:SER:HB3	11	0.33	0.05	0.34
(1,950)	2:572:B:PRO:HB2	2:573:B:PRO:HD3	11	0.23	0.05	0.23
(1,2465)	2:677:B:LEU:HD12	2:651:B:PHE:HD2	11	0.2	0.08	0.2
(1,2465)	2:677:B:LEU:HD11	2:651:B:PHE:HD1	11	0.2	0.08	0.2
(1,2465)	2:686:B:LEU:HD23	1:37:A:TRP:HE3	11	0.2	0.08	0.2
(1,2465)	2:686:B:LEU:HD22	1:37:A:TRP:HE3	11	0.2	0.08	0.2
(1,2465)	2:686:B:LEU:HD21	1:37:A:TRP:HE3	11	0.2	0.08	0.2
(1,2465)	2:677:B:LEU:HD13	2:651:B:PHE:HD1	11	0.2	0.08	0.2
(1,2698)	2:576:B:MET:H	2:575:B:PHE:HB2	11	0.16	0.03	0.17
(1,2698)	2:576:B:MET:H	2:576:B:MET:HE1	11	0.16	0.03	0.17
(1,2698)	2:576:B:MET:H	2:576:B:MET:HE3	11	0.16	0.03	0.17
(1,2454)	2:674:B:CYS:HB2	2:666:B:THR:HA	10	0.79	0.18	0.74
(1,2454)	2:674:B:CYS:HB2	2:677:B:LEU:HA	10	0.79	0.18	0.74
(1,2454)	2:674:B:CYS:HB2	2:667:B:SER:HA	10	0.79	0.18	0.74
(1,420)	2:654:B:PHE:HB2	2:682:B:VAL:HB	10	0.64	0.25	0.58
(1,2866)	2:661:B:CYS:H	2:674:B:CYS:HB2	10	0.56	0.19	0.52
(1,2866)	2:651:B:PHE:H	2:674:B:CYS:HB2	10	0.56	0.19	0.52
(2,2)	2:595:B:LYS:HD2	2:658:B:TRP:HB3	10	0.42	0.19	0.4
(1,2263)	2:614:B:SER:HB2	1:47:A:SER:HB3	10	0.41	0.1	0.42
(1,2263)	2:614:B:SER:HB2	1:47:A:SER:HB2	10	0.41	0.1	0.42
(1,2455)	2:674:B:CYS:HB3	2:673:B:PRO:HB2	10	0.38	0.06	0.39
(1,2289)	2:575:B:PHE:HE2	1:39:A:SER:HB3	10	0.34	0.07	0.34
(1,2289)	2:575:B:PHE:HE1	1:39:A:SER:HB3	10	0.34	0.07	0.34
(1,393)	2:646:B:LEU:HB2	2:646:B:LEU:HD23	10	0.13	0.02	0.14
(1,393)	2:646:B:LEU:HB2	2:646:B:LEU:HD22	10	0.13	0.02	0.14
(1,393)	2:646:B:LEU:HB2	2:646:B:LEU:HD21	10	0.13	0.02	0.14
(1,2622)	2:587:B:GLU:HB2	2:583:B:LEU:HD12	9	0.92	0.16	0.95
(1,2622)	2:587:B:GLU:HB2	2:583:B:LEU:HD11	9	0.92	0.16	0.95
(1,2622)	2:648:B:GLU:HG3	2:669:B:LEU:HD13	9	0.92	0.16	0.95
(1,2622)	2:587:B:GLU:HB2	2:583:B:LEU:HD13	9	0.92	0.16	0.95
(1,2622)	2:648:B:GLU:HG3	2:669:B:LEU:HD12	9	0.92	0.16	0.95
(1,1518)	2:587:B:GLU:H	2:587:B:GLU:HB2	9	0.9	0.05	0.93
(1,1057)	2:650:B:PRO:HG2	2:666:B:THR:HG23	9	0.73	0.52	0.67
(1,1057)	2:650:B:PRO:HG2	2:666:B:THR:HG21	9	0.73	0.52	0.67
(1,64)	2:587:B:GLU:HB2	2:583:B:LEU:HD12	9	0.73	0.14	0.73
(1,64)	2:587:B:GLU:HB2	2:583:B:LEU:HD11	9	0.73	0.14	0.73

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,64)	2:587:B:GLU:HB2	2:583:B:LEU:HD13	9	0.73	0.14	0.73
(1,2846)	2:649:B:TYR:H	2:645:B:VAL:HB	9	0.59	0.15	0.66
(1,2317)	2:587:B:GLU:HB3	2:589:B:LYS:HG3	9	0.56	0.18	0.51
(1,1295)	2:589:B:LYS:HB2	2:590:B:LYS:H	9	0.19	0.09	0.15
(1,896)	2:630:B:ILE:HD11	2:651:B:PHE:HE1	8	0.64	0.3	0.59
(1,896)	2:630:B:ILE:HD13	2:651:B:PHE:HE1	8	0.64	0.3	0.59
(1,896)	2:630:B:ILE:HD12	2:651:B:PHE:HE1	8	0.64	0.3	0.59
(1,2679)	1:34:A:VAL:HA	1:34:A:VAL:HG22	8	0.56	0.01	0.56
(1,2679)	1:34:A:VAL:HA	1:34:A:VAL:HG21	8	0.56	0.01	0.56
(1,2679)	1:34:A:VAL:HA	1:34:A:VAL:HG23	8	0.56	0.01	0.56
(1,1188)	2:687:B:THR:H	2:687:B:THR:HG22	8	0.35	0.03	0.34
(1,1188)	2:687:B:THR:H	2:687:B:THR:HG21	8	0.35	0.03	0.34
(1,1188)	2:687:B:THR:H	2:687:B:THR:HG23	8	0.35	0.03	0.34
(1,2210)	2:579:B:SER:HA	1:39:A:SER:HG	8	0.34	0.17	0.34
(1,2203)	2:609:B:LEU:HD11	1:37:A:TRP:HZ3	8	0.29	0.2	0.18
(1,2203)	2:609:B:LEU:HD12	1:37:A:TRP:HZ3	8	0.29	0.2	0.18
(1,2203)	2:609:B:LEU:HD13	1:37:A:TRP:HZ3	8	0.29	0.2	0.18
(1,232)	2:611:B:ILE:HG22	2:684:B:ILE:HD12	8	0.24	0.13	0.19
(1,232)	2:611:B:ILE:HG23	2:684:B:ILE:HD11	8	0.24	0.13	0.19
(1,232)	2:611:B:ILE:HG21	2:684:B:ILE:HD12	8	0.24	0.13	0.19
(1,232)	2:611:B:ILE:HG21	2:684:B:ILE:HD11	8	0.24	0.13	0.19
(1,232)	2:611:B:ILE:HG23	2:684:B:ILE:HD13	8	0.24	0.13	0.19
(1,1525)	2:588:B:LEU:H	2:587:B:GLU:HB3	8	0.22	0.04	0.24
(1,1980)	2:655:B:GLY:H	2:654:B:PHE:HB2	8	0.21	0.02	0.22
(1,2488)	2:590:B:LYS:HB3	2:592:B:GLU:HA	8	0.2	0.06	0.2
(1,427)	2:654:B:PHE:HB2	2:656:B:GLN:HE22	8	0.17	0.04	0.17
(1,1527)	2:588:B:LEU:H	2:588:B:LEU:HD12	8	0.14	0.02	0.14
(1,1527)	2:588:B:LEU:H	2:588:B:LEU:HD13	8	0.14	0.02	0.14
(1,1527)	2:588:B:LEU:H	2:588:B:LEU:HD11	8	0.14	0.02	0.14
(1,257)	2:617:B:GLU:HG3	2:615:B:THR:HG22	7	0.56	0.16	0.49
(1,257)	2:617:B:GLU:HG3	2:615:B:THR:HG23	7	0.56	0.16	0.49
(1,257)	2:617:B:GLU:HG3	2:615:B:THR:HG21	7	0.56	0.16	0.49
(1,2646)	2:687:B:THR:HB	2:610:B:LYS:HA	7	0.5	0.1	0.47
(1,2646)	2:687:B:THR:HB	2:611:B:ILE:HA	7	0.5	0.1	0.47
(1,259)	2:617:B:GLU:HG3	2:617:B:GLU:HA	7	0.38	0.01	0.38
(1,1979)	2:655:B:GLY:H	2:654:B:PHE:HA	7	0.33	0.04	0.34
(1,1557)	2:592:B:GLU:H	2:590:B:LYS:HB2	7	0.28	0.21	0.16
(1,2647)	2:687:B:THR:HG22	2:689:B:LYS:HB2	7	0.23	0.14	0.18
(1,2647)	2:687:B:THR:HG22	2:610:B:LYS:HB3	7	0.23	0.14	0.18
(1,2647)	2:687:B:THR:HG22	2:610:B:LYS:HD3	7	0.23	0.14	0.18
(1,2647)	2:687:B:THR:HG23	2:689:B:LYS:HB2	7	0.23	0.14	0.18
(1,2647)	2:687:B:THR:HG23	2:610:B:LYS:HD3	7	0.23	0.14	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1638)	2:601:B:GLN:H	2:601:B:GLN:HG2	7	0.18	0.07	0.17
(1,2535)	2:660:B:SER:HB2	2:662:B:CYS:HA	7	0.17	0.05	0.15
(1,2702)	2:578:B:GLY:H	2:577:B:LYS:HD2	7	0.16	0.03	0.18
(1,2702)	2:578:B:GLY:H	2:590:B:LYS:HB2	7	0.16	0.03	0.18
(1,1335)	1:44:A:LEU:HD11	1:44:A:LEU:HD21	7	0.14	0.03	0.13
(1,1335)	1:44:A:LEU:HD11	1:44:A:LEU:HD22	7	0.14	0.03	0.13
(1,1335)	1:44:A:LEU:HD11	1:44:A:LEU:HD23	7	0.14	0.03	0.13
(1,1335)	1:44:A:LEU:HD13	1:44:A:LEU:HD22	7	0.14	0.03	0.13
(1,1335)	1:44:A:LEU:HD12	1:44:A:LEU:HD21	7	0.14	0.03	0.13
(1,1335)	1:44:A:LEU:HD12	1:44:A:LEU:HD22	7	0.14	0.03	0.13
(1,1090)	2:670:B:PHE:HB2	2:575:B:PHE:HZ	7	0.11	0.01	0.11
(1,204)	2:609:B:LEU:HD12	2:688:B:LEU:HA	6	1.59	0.54	1.66
(1,204)	2:609:B:LEU:HD13	2:688:B:LEU:HA	6	1.59	0.54	1.66
(1,204)	2:609:B:LEU:HD11	2:688:B:LEU:HA	6	1.59	0.54	1.66
(1,203)	2:609:B:LEU:HD12	2:609:B:LEU:HA	6	1.26	0.06	1.29
(1,203)	2:609:B:LEU:HD13	2:609:B:LEU:HA	6	1.26	0.06	1.29
(1,203)	2:609:B:LEU:HD11	2:609:B:LEU:HA	6	1.26	0.06	1.29
(1,1352)	1:47:A:SER:HA	1:48:A:GLN:HG2	6	1.21	0.51	1.45
(1,1352)	1:47:A:SER:HA	1:48:A:GLN:HG3	6	1.21	0.51	1.45
(1,2200)	2:689:B:LYS:H	2:609:B:LEU:HD11	6	0.68	0.29	0.6
(1,2200)	2:689:B:LYS:H	2:609:B:LEU:HD12	6	0.68	0.29	0.6
(1,2200)	2:689:B:LYS:H	2:609:B:LEU:HD13	6	0.68	0.29	0.6
(1,1698)	2:610:B:LYS:H	2:609:B:LEU:HD12	6	0.57	0.28	0.6
(1,1698)	2:610:B:LYS:H	2:609:B:LEU:HD13	6	0.57	0.28	0.6
(1,1698)	2:610:B:LYS:H	2:609:B:LEU:HD11	6	0.57	0.28	0.6
(1,2208)	2:674:B:CYS:HB3	1:40:A:LEU:HB2	6	0.47	0.15	0.52
(1,2451)	2:674:B:CYS:HB2	2:673:B:PRO:HB2	6	0.39	0.13	0.4
(1,576)	2:577:B:LYS:HD2	2:671:B:ASP:HB2	6	0.38	0.13	0.38
(1,591)	2:580:B:ILE:HD12	2:590:B:LYS:HE3	6	0.36	0.21	0.34
(1,591)	2:580:B:ILE:HD13	2:590:B:LYS:HE3	6	0.36	0.21	0.34
(1,591)	2:580:B:ILE:HD11	2:590:B:LYS:HE3	6	0.36	0.21	0.34
(1,591)	2:580:B:ILE:HD12	2:590:B:LYS:HE2	6	0.36	0.21	0.34
(1,1649)	2:602:B:SER:H	2:602:B:SER:HB2	6	0.32	0.02	0.32
(1,578)	2:577:B:LYS:HD3	2:671:B:ASP:HB2	6	0.26	0.09	0.28
(1,1697)	2:610:B:LYS:H	2:610:B:LYS:HG2	6	0.25	0.09	0.22
(1,383)	2:646:B:LEU:H	2:645:B:VAL:HB	6	0.24	0.08	0.22
(1,2313)	2:583:B:LEU:HD11	2:589:B:LYS:HE2	6	0.19	0.08	0.16
(1,2313)	2:583:B:LEU:HD12	2:589:B:LYS:HE2	6	0.19	0.08	0.16
(1,2313)	2:583:B:LEU:HD13	2:589:B:LYS:HE2	6	0.19	0.08	0.16
(1,1437)	2:576:B:MET:H	2:576:B:MET:HG3	6	0.15	0.03	0.15
(1,2161)	2:682:B:VAL:H	2:682:B:VAL:HG12	5	1.5	0.03	1.52
(1,2161)	2:682:B:VAL:H	2:682:B:VAL:HG11	5	1.5	0.03	1.52

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2161)	2:682:B:VAL:H	2:682:B:VAL:HG13	5	1.5	0.03	1.52
(1,423)	2:654:B:PHE:HB2	2:682:B:VAL:HG21	5	1.41	0.29	1.56
(1,423)	2:654:B:PHE:HB2	2:682:B:VAL:HG23	5	1.41	0.29	1.56
(1,423)	2:654:B:PHE:HB2	2:682:B:VAL:HG22	5	1.41	0.29	1.56
(1,2519)	2:608:B:ASP:HB3	2:688:B:LEU:HD21	5	1.36	0.31	1.34
(1,2519)	2:608:B:ASP:HB2	2:688:B:LEU:HD11	5	1.36	0.31	1.34
(1,2519)	2:608:B:ASP:HB2	2:688:B:LEU:HD13	5	1.36	0.31	1.34
(1,1709)	2:614:B:SER:H	2:682:B:VAL:HG23	5	0.86	0.08	0.89
(1,1709)	2:614:B:SER:H	2:682:B:VAL:HG22	5	0.86	0.08	0.89
(1,1709)	2:614:B:SER:H	2:682:B:VAL:HG21	5	0.86	0.08	0.89
(1,2530)	2:642:B:SER:HB3	2:629:B:VAL:HG12	5	0.85	0.5	0.51
(1,2530)	2:682:B:VAL:HG21	2:613:B:SER:HB3	5	0.85	0.5	0.51
(1,2530)	2:642:B:SER:HB3	2:629:B:VAL:HG13	5	0.85	0.5	0.51
(1,487)	2:674:B:CYS:HB2	2:659:B:SER:HA	5	0.77	0.09	0.77
(1,2171)	2:683:B:CYS:H	2:682:B:VAL:HG23	5	0.7	0.02	0.69
(1,2171)	2:683:B:CYS:H	2:682:B:VAL:HG22	5	0.7	0.02	0.69
(1,2171)	2:683:B:CYS:H	2:682:B:VAL:HG21	5	0.7	0.02	0.69
(1,425)	2:654:B:PHE:HB3	2:682:B:VAL:HG21	5	0.59	0.19	0.5
(1,425)	2:654:B:PHE:HB3	2:682:B:VAL:HG23	5	0.59	0.19	0.5
(1,425)	2:654:B:PHE:HB3	2:682:B:VAL:HG22	5	0.59	0.19	0.5
(1,2065)	2:667:B:SER:H	2:667:B:SER:HB3	5	0.45	0.0	0.45
(1,2070)	2:668:B:GLN:H	2:668:B:GLN:HG2	5	0.37	0.05	0.35
(1,1449)	2:577:B:LYS:H	2:672:B:LEU:HB3	5	0.27	0.11	0.24
(1,1967)	2:653:B:VAL:H	1:41:A:VAL:HA	5	0.26	0.11	0.2
(1,1430)	2:575:B:PHE:H	2:576:B:MET:H	5	0.25	0.02	0.25
(1,712)	2:603:B:ALA:HA	2:606:B:SER:HA	5	0.23	0.08	0.19
(1,426)	2:654:B:PHE:HB3	2:656:B:GLN:HE22	5	0.22	0.06	0.25
(1,2903)	2:678:B:SER:H	2:676:B:LYS:HG3	5	0.19	0.1	0.15
(1,2018)	2:660:B:SER:H	2:674:B:CYS:HB2	5	0.15	0.06	0.12
(1,910)	2:672:B:LEU:HD12	2:592:B:GLU:HB2	4	1.56	0.98	1.58
(1,910)	2:672:B:LEU:HD13	2:592:B:GLU:HB2	4	1.56	0.98	1.58
(1,910)	2:672:B:LEU:HD11	2:592:B:GLU:HB2	4	1.56	0.98	1.58
(1,2269)	2:629:B:VAL:HG23	1:44:A:LEU:HB2	4	1.0	0.15	1.02
(1,2269)	2:629:B:VAL:HG21	1:44:A:LEU:HB2	4	1.0	0.15	1.02
(1,566)	2:688:B:LEU:HD23	1:38:A:HIS:H	4	0.63	0.04	0.61
(1,566)	2:688:B:LEU:HD22	1:38:A:HIS:H	4	0.63	0.04	0.61
(1,978)	2:574:B:TYR:HB3	1:40:A:LEU:HD22	4	0.57	0.04	0.56
(1,978)	2:574:B:TYR:HB3	1:40:A:LEU:HD21	4	0.57	0.04	0.56
(1,978)	2:574:B:TYR:HB3	1:40:A:LEU:HD23	4	0.57	0.04	0.56
(1,2353)	2:609:B:LEU:HD11	1:38:A:HIS:H	4	0.45	0.24	0.34
(1,2353)	2:609:B:LEU:HD12	1:38:A:HIS:H	4	0.45	0.24	0.34
(1,2353)	2:609:B:LEU:HD13	1:38:A:HIS:H	4	0.45	0.24	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1402)	1:40:A:LEU:HD12	1:39:A:SER:H	4	0.31	0.11	0.33
(1,1402)	1:40:A:LEU:HD13	1:39:A:SER:H	4	0.31	0.11	0.33
(1,1982)	2:655:B:GLY:H	2:596:B:THR:HG21	4	0.27	0.05	0.26
(1,1982)	2:655:B:GLY:H	2:596:B:THR:HG22	4	0.27	0.05	0.26
(1,365)	2:665:B:ARG:HD3	2:647:B:VAL:HG22	4	0.26	0.14	0.18
(1,365)	2:665:B:ARG:HD3	2:647:B:VAL:HG23	4	0.26	0.14	0.18
(1,365)	2:665:B:ARG:HD3	2:647:B:VAL:HG21	4	0.26	0.14	0.18
(1,1540)	2:590:B:LYS:H	2:590:B:LYS:HE3	4	0.25	0.07	0.24
(1,1540)	2:590:B:LYS:H	2:590:B:LYS:HE2	4	0.25	0.07	0.24
(1,27)	2:577:B:LYS:HE3	2:577:B:LYS:HG3	4	0.21	0.05	0.2
(1,2529)	2:613:B:SER:HB2	2:682:B:VAL:HG13	4	0.21	0.03	0.2
(1,2529)	2:613:B:SER:HB2	2:682:B:VAL:HG12	4	0.21	0.03	0.2
(1,2529)	2:613:B:SER:HB2	2:682:B:VAL:HG11	4	0.21	0.03	0.2
(1,574)	2:576:B:MET:HB2	2:575:B:PHE:HD1	4	0.2	0.14	0.13
(1,574)	2:576:B:MET:HB2	2:575:B:PHE:HD2	4	0.2	0.14	0.13
(1,1465)	2:580:B:ILE:H	2:579:B:SER:HB3	4	0.2	0.04	0.18
(1,1298)	2:615:B:THR:HA	2:682:B:VAL:HB	4	0.17	0.01	0.16
(1,2407)	2:618:B:ARG:HB3	2:631:B:GLN:HG2	4	0.16	0.05	0.16
(1,2463)	2:678:B:SER:H	2:677:B:LEU:HG	4	0.16	0.03	0.15
(1,1240)	2:600:B:ILE:HG12	2:597:B:GLU:HA	4	0.14	0.03	0.15
(1,2155)	2:681:B:ASP:H	2:616:B:VAL:HG23	4	0.13	0.01	0.13
(1,2155)	2:681:B:ASP:H	2:616:B:VAL:HG22	4	0.13	0.01	0.13
(1,1102)	2:672:B:LEU:HD23	2:666:B:THR:HA	3	2.04	0.31	2.21
(1,1102)	2:672:B:LEU:HD22	2:666:B:THR:HA	3	2.04	0.31	2.21
(1,1056)	2:666:B:THR:HG22	2:672:B:LEU:HD23	3	1.85	0.46	1.98
(1,1056)	2:666:B:THR:HG23	2:672:B:LEU:HD22	3	1.85	0.46	1.98
(1,1056)	2:666:B:THR:HG22	2:672:B:LEU:HD22	3	1.85	0.46	1.98
(1,102)	2:672:B:LEU:HD12	2:673:B:PRO:HD3	3	1.73	1.02	2.08
(1,102)	2:672:B:LEU:HD11	2:673:B:PRO:HD3	3	1.73	1.02	2.08
(1,1220)	2:677:B:LEU:HA	2:677:B:LEU:HD23	3	1.39	0.02	1.4
(1,1220)	2:677:B:LEU:HA	2:677:B:LEU:HD21	3	1.39	0.02	1.4
(1,1215)	2:681:B:ASP:HB3	2:677:B:LEU:HD21	3	1.35	0.05	1.38
(1,1215)	2:681:B:ASP:HB3	2:677:B:LEU:HD22	3	1.35	0.05	1.38
(1,2138)	2:678:B:SER:H	2:677:B:LEU:HD21	3	1.33	0.04	1.34
(1,2138)	2:678:B:SER:H	2:677:B:LEU:HD22	3	1.33	0.04	1.34
(1,501)	2:677:B:LEU:HD13	2:630:B:ILE:HG22	3	1.13	0.07	1.09
(1,501)	2:677:B:LEU:HD11	2:630:B:ILE:HG23	3	1.13	0.07	1.09
(1,501)	2:677:B:LEU:HD13	2:630:B:ILE:HG23	3	1.13	0.07	1.09
(1,1255)	2:672:B:LEU:HD12	2:592:B:GLU:HA	3	1.05	0.62	1.04
(1,1255)	2:672:B:LEU:HD13	2:592:B:GLU:HA	3	1.05	0.62	1.04
(1,1269)	2:672:B:LEU:HD22	2:575:B:PHE:HB2	3	1.02	0.45	0.71
(1,1269)	2:672:B:LEU:HD23	2:575:B:PHE:HB2	3	1.02	0.45	0.71

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1560)	2:592:B:GLU:H	2:672:B:LEU:HD12	3	0.74	0.21	0.64
(1,1560)	2:592:B:GLU:H	2:672:B:LEU:HD13	3	0.74	0.21	0.64
(1,1216)	2:681:B:ASP:HB2	2:677:B:LEU:HD21	3	0.74	0.1	0.71
(1,1216)	2:681:B:ASP:HB2	2:677:B:LEU:HD22	3	0.74	0.1	0.71
(1,22)	2:571:B:LEU:HD23	2:571:B:LEU:HA	3	0.65	0.3	0.72
(1,101)	2:672:B:LEU:HD11	2:591:B:VAL:HB	3	0.48	0.04	0.47
(1,101)	2:672:B:LEU:HD13	2:591:B:VAL:HB	3	0.48	0.04	0.47
(1,2069)	2:668:B:GLN:H	2:667:B:SER:HB3	3	0.47	0.02	0.46
(1,1219)	2:659:B:SER:HB2	2:677:B:LEU:HD23	3	0.46	0.12	0.47
(1,1219)	2:659:B:SER:HB2	2:677:B:LEU:HD21	3	0.46	0.12	0.47
(1,1076)	2:581:B:ILE:HD12	1:35:A:PHE:HD1	3	0.39	0.09	0.43
(1,1076)	2:581:B:ILE:HD13	1:35:A:PHE:HD1	3	0.39	0.09	0.43
(1,1977)	2:654:B:PHE:H	2:682:B:VAL:HG22	3	0.28	0.14	0.3
(1,1424)	2:571:B:LEU:H	2:570:B:THR:HA	3	0.27	0.07	0.28
(1,2108)	2:674:B:CYS:H	2:673:B:PRO:HB2	3	0.26	0.12	0.31
(1,2318)	2:665:B:ARG:HB2	2:669:B:LEU:HD11	3	0.23	0.06	0.25
(1,2318)	2:665:B:ARG:HB2	2:669:B:LEU:HD12	3	0.23	0.06	0.25
(1,2318)	2:587:B:GLU:HB3	2:583:B:LEU:HD12	3	0.23	0.06	0.25
(1,1425)	2:571:B:LEU:H	2:571:B:LEU:HB2	3	0.23	0.09	0.23
(1,2599)	2:645:B:VAL:HG12	2:629:B:VAL:HA	3	0.21	0.07	0.21
(1,2599)	2:645:B:VAL:HG13	2:629:B:VAL:HA	3	0.21	0.07	0.21
(1,2599)	2:645:B:VAL:HG11	2:629:B:VAL:HA	3	0.21	0.07	0.21
(1,2411)	2:679:B:VAL:H	2:679:B:VAL:HG23	3	0.18	0.05	0.17
(1,2411)	2:646:B:LEU:H	2:645:B:VAL:HG23	3	0.18	0.05	0.17
(1,2411)	2:646:B:LEU:H	2:645:B:VAL:HG21	3	0.18	0.05	0.17
(1,253)	2:617:B:GLU:HG2	2:633:B:ALA:HB2	3	0.18	0.05	0.16
(1,253)	2:617:B:GLU:HG2	2:633:B:ALA:HB3	3	0.18	0.05	0.16
(1,2029)	2:662:B:CYS:H	2:660:B:SER:HB2	3	0.16	0.06	0.14
(1,211)	2:611:B:ILE:H	2:610:B:LYS:HB2	3	0.15	0.05	0.12
(1,1723)	2:616:B:VAL:H	2:615:B:THR:HG21	3	0.14	0.01	0.13
(1,1723)	2:616:B:VAL:H	2:615:B:THR:HG22	3	0.14	0.01	0.13
(1,663)	2:589:B:LYS:HB3	2:594:B:LEU:HD21	3	0.13	0.01	0.13
(1,1422)	2:570:B:THR:H	2:570:B:THR:HG21	3	0.13	0.03	0.12
(1,1422)	2:570:B:THR:H	2:570:B:THR:HG23	3	0.13	0.03	0.12
(1,2656)	2:619:B:ILE:HG21	2:630:B:ILE:HA	3	0.13	0.04	0.11
(1,2656)	2:619:B:ILE:HG22	2:630:B:ILE:HA	3	0.13	0.04	0.11
(1,1901)	2:640:B:GLN:H	2:640:B:GLN:HG2	3	0.12	0.02	0.11
(1,66)	2:587:B:GLU:HG2	2:587:B:GLU:HA	3	0.11	0.01	0.11
(1,441)	2:594:B:LEU:HG	2:589:B:LYS:HA	3	0.11	0.01	0.12
(1,608)	2:589:B:LYS:HE2	2:589:B:LYS:HG3	3	0.11	0.0	0.11
(1,2472)	2:686:B:LEU:HD13	2:610:B:LYS:HB2	2	2.26	0.1	2.26
(1,2472)	2:686:B:LEU:HD12	2:688:B:LEU:HB2	2	2.26	0.1	2.26

Continued on next page...

Continued from previous page...

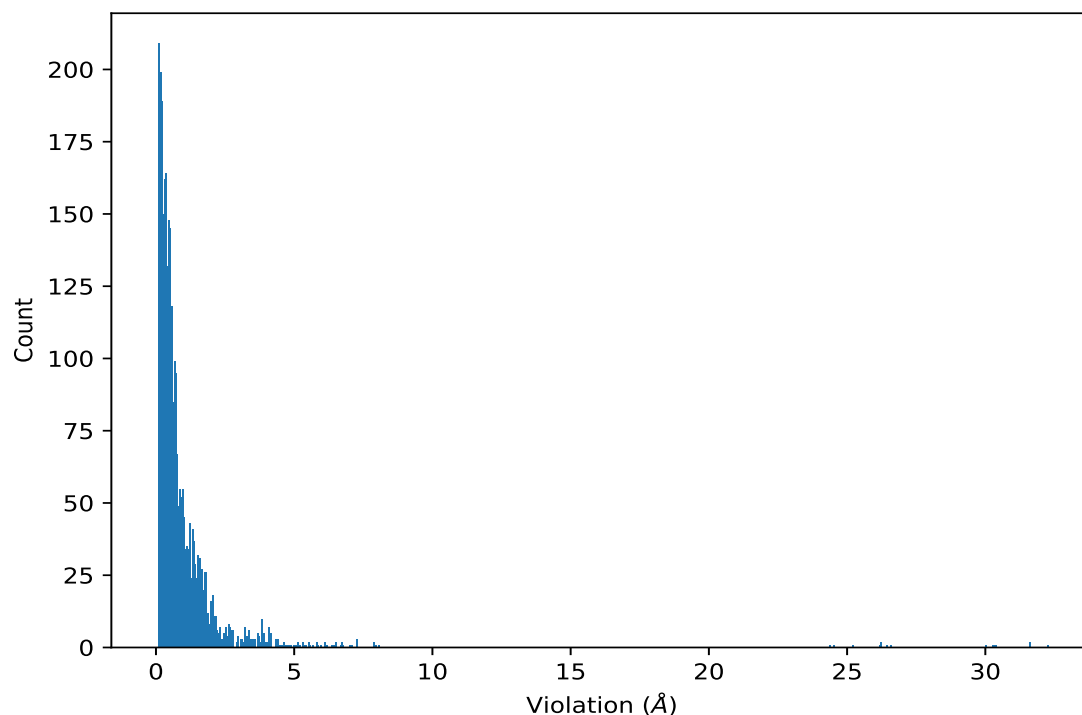
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2268)	2:643:B:VAL:HG22	1:44:A:LEU:HD21	2	2.0	0.04	2.0
(1,2268)	2:643:B:VAL:HG21	1:44:A:LEU:HD21	2	2.0	0.04	2.0
(1,556)	2:687:B:THR:H	2:686:B:LEU:HD11	2	1.81	0.04	1.81
(1,775)	2:612:B:ASP:HB2	1:44:A:LEU:HD11	2	1.8	0.67	1.8
(1,775)	2:612:B:ASP:HB2	1:44:A:LEU:HD13	2	1.8	0.67	1.8
(1,1168)	2:686:B:LEU:HD13	2:609:B:LEU:HB2	2	1.23	0.3	1.23
(1,1168)	2:686:B:LEU:HD11	2:609:B:LEU:HB2	2	1.23	0.3	1.23
(1,2928)	2:645:B:VAL:HG23	1:44:A:LEU:HD13	2	1.01	0.68	1.01
(1,2928)	2:682:B:VAL:HG23	1:44:A:LEU:HD13	2	1.01	0.68	1.01
(1,2045)	2:664:B:GLU:H	2:664:B:GLU:HG3	2	0.9	0.01	0.9
(1,2045)	2:664:B:GLU:H	2:664:B:GLU:HG2	2	0.9	0.01	0.9
(1,2277)	2:639:B:ALA:HB1	1:48:A:GLN:HB3	2	0.84	0.4	0.84
(1,2277)	2:639:B:ALA:HB2	1:48:A:GLN:HB3	2	0.84	0.4	0.84
(1,553)	2:686:B:LEU:HD12	2:686:B:LEU:HA	2	0.82	0.03	0.82
(1,553)	2:686:B:LEU:HD13	2:686:B:LEU:HA	2	0.82	0.03	0.82
(1,103)	2:672:B:LEU:HD11	2:672:B:LEU:HA	2	0.77	0.2	0.77
(1,1073)	2:579:B:SER:HB3	2:581:B:ILE:HD12	2	0.72	0.03	0.72
(1,133)	2:591:B:VAL:HG21	2:579:B:SER:HB2	2	0.56	0.08	0.56
(1,133)	2:591:B:VAL:HG23	2:579:B:SER:HB2	2	0.56	0.08	0.56
(1,1454)	2:579:B:SER:H	2:579:B:SER:HB2	2	0.5	0.01	0.5
(1,1773)	2:621:B:ASP:H	2:621:B:ASP:HB3	2	0.46	0.01	0.46
(1,1544)	2:590:B:LYS:H	2:590:B:LYS:HG2	2	0.46	0.32	0.46
(1,422)	2:654:B:PHE:HB2	2:682:B:VAL:HG13	2	0.38	0.16	0.38
(1,422)	2:654:B:PHE:HB2	2:682:B:VAL:HG11	2	0.38	0.16	0.38
(1,1171)	2:677:B:LEU:HD12	2:678:B:SER:HA	2	0.35	0.02	0.35
(1,1902)	2:640:B:GLN:H	2:640:B:GLN:HG3	2	0.35	0.01	0.35
(1,1870)	2:636:B:GLU:H	2:636:B:GLU:HG2	2	0.24	0.04	0.24
(1,1870)	2:636:B:GLU:H	2:636:B:GLU:HG3	2	0.24	0.04	0.24
(1,2609)	2:660:B:SER:HA	2:677:B:LEU:HB3	2	0.2	0.06	0.2
(1,1370)	1:44:A:LEU:HA	1:44:A:LEU:HD21	2	0.18	0.07	0.18
(1,1370)	1:44:A:LEU:HA	1:44:A:LEU:HD23	2	0.18	0.07	0.18
(1,2681)	1:34:A:VAL:HG13	1:35:A:PHE:H	2	0.17	0.0	0.17
(1,2681)	1:34:A:VAL:HG11	1:35:A:PHE:H	2	0.17	0.0	0.17
(1,1218)	2:659:B:SER:HB3	2:677:B:LEU:HD23	2	0.16	0.02	0.16
(1,1218)	2:659:B:SER:HB3	2:677:B:LEU:HD21	2	0.16	0.02	0.16
(1,21)	2:571:B:LEU:HD21	2:571:B:LEU:HB2	2	0.12	0.01	0.12
(1,303)	2:627:B:VAL:HB	2:624:B:SER:HB3	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2303)	2:567:B:ALA:HB3	2:644:B:GLU:H	6	32.27
(1,2303)	2:567:B:ALA:HB3	1:45:A:ALA:H	9	31.64
(1,2303)	2:567:B:ALA:HB3	1:45:A:ALA:H	13	31.63
(1,2303)	2:567:B:ALA:HB3	1:45:A:ALA:H	12	30.39
(1,2303)	2:567:B:ALA:HB2	1:45:A:ALA:H	5	30.31
(1,2303)	2:567:B:ALA:HB3	1:45:A:ALA:H	2	30.25
(1,2303)	2:567:B:ALA:HB3	1:45:A:ALA:H	7	30.02
(1,2303)	2:567:B:ALA:HB3	2:644:B:GLU:H	15	26.59
(1,2303)	2:567:B:ALA:HB2	1:45:A:ALA:H	11	26.44
(1,2303)	2:567:B:ALA:HB1	1:45:A:ALA:H	1	26.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2303)	2:567:B:ALA:HB3	1:45:A:ALA:H	8	26.23
(1,2303)	2:567:B:ALA:HB3	1:45:A:ALA:H	4	26.18
(1,2303)	2:567:B:ALA:HB2	1:45:A:ALA:H	3	25.23
(1,2303)	2:567:B:ALA:HB2	2:644:B:GLU:H	14	24.51
(1,2303)	2:567:B:ALA:HB3	2:644:B:GLU:H	10	24.39
(1,1363)	1:40:A:LEU:HA	1:34:A:VAL:HG11	13	8.05
(1,1363)	1:40:A:LEU:HA	1:34:A:VAL:HG11	4	7.96
(1,1363)	1:40:A:LEU:HA	1:34:A:VAL:HG11	7	7.88
(1,1363)	1:40:A:LEU:HA	1:34:A:VAL:HG11	3	7.87
(1,1363)	1:40:A:LEU:HA	1:34:A:VAL:HG13	1	7.29
(1,1363)	1:40:A:LEU:HA	1:34:A:VAL:HG12	11	7.28
(1,1363)	1:40:A:LEU:HA	1:34:A:VAL:HG11	14	7.27
(1,1363)	1:40:A:LEU:HA	1:34:A:VAL:HG11	12	7.07
(1,1363)	1:40:A:LEU:HA	1:34:A:VAL:HG11	5	7.02
(1,1363)	1:40:A:LEU:HA	1:34:A:VAL:HG13	6	6.79
(1,1363)	1:40:A:LEU:HA	1:34:A:VAL:HG11	2	6.73
(1,1350)	1:40:A:LEU:HG	1:34:A:VAL:HG11	13	6.7
(1,1363)	1:40:A:LEU:HA	1:34:A:VAL:HG13	15	6.65
(1,1350)	1:40:A:LEU:HG	1:34:A:VAL:HG11	3	6.52
(1,1363)	1:40:A:LEU:HA	1:34:A:VAL:HG13	10	6.51
(1,1350)	1:40:A:LEU:HG	1:34:A:VAL:HG11	7	6.42
(1,1350)	1:40:A:LEU:HG	1:34:A:VAL:HG11	4	6.35
(1,243)	2:616:B:VAL:HG12	2:631:B:GLN:HE22	13	6.18
(1,1350)	1:40:A:LEU:HG	1:34:A:VAL:HG12	11	6.14
(1,2674)	2:571:B:LEU:HD12	2:568:B:PRO:HG2	9	6.11
(1,1350)	1:40:A:LEU:HG	1:34:A:VAL:HG11	14	5.99
(1,243)	2:616:B:VAL:HG13	2:631:B:GLN:HE22	14	5.88
(1,243)	2:616:B:VAL:HG12	2:631:B:GLN:HE22	4	5.84
(1,243)	2:616:B:VAL:HG12	2:631:B:GLN:HE22	15	5.81
(1,564)	2:688:B:LEU:HD22	2:583:B:LEU:HD22	12	5.66
(1,564)	2:688:B:LEU:HD23	2:583:B:LEU:HD23	11	5.57
(1,564)	2:688:B:LEU:HD23	2:583:B:LEU:HD21	5	5.54
(1,1350)	1:40:A:LEU:HG	1:34:A:VAL:HG13	1	5.5
(1,1350)	1:40:A:LEU:HG	1:34:A:VAL:HG11	5	5.4
(1,564)	2:688:B:LEU:HD22	2:583:B:LEU:HD23	7	5.37
(1,1363)	1:40:A:LEU:HA	1:34:A:VAL:HG13	9	5.33
(1,1350)	1:40:A:LEU:HG	1:34:A:VAL:HG11	12	5.3
(1,243)	2:616:B:VAL:HG11	2:631:B:GLN:HE22	11	5.24
(1,1350)	1:40:A:LEU:HG	1:34:A:VAL:HG11	2	5.13
(1,1350)	1:40:A:LEU:HG	1:34:A:VAL:HG13	6	5.1
(1,1350)	1:40:A:LEU:HG	1:34:A:VAL:HG13	10	5.09
(1,1350)	1:40:A:LEU:HG	1:34:A:VAL:HG13	15	5.04

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,243)	2:616:B:VAL:HG12	2:631:B:GLN:HE22	12	4.96
(1,1363)	1:40:A:LEU:HA	1:34:A:VAL:HG13	8	4.89
(1,243)	2:616:B:VAL:HG12	2:631:B:GLN:HE22	8	4.82
(1,2422)	2:643:B:VAL:HG11	2:640:B:GLN:HE22	11	4.78
(1,2422)	2:643:B:VAL:HG12	1:48:A:GLN:HE21	8	4.73
(1,562)	2:688:B:LEU:HD13	2:686:B:LEU:HD21	13	4.65
(1,2422)	2:643:B:VAL:HG13	2:640:B:GLN:HE22	13	4.6
(1,2422)	2:643:B:VAL:HG13	2:640:B:GLN:HE22	15	4.6
(1,243)	2:616:B:VAL:HG12	2:631:B:GLN:HE22	7	4.56
(1,2422)	2:682:B:VAL:HG11	2:652:B:PHE:HE1	7	4.5
(1,2422)	2:682:B:VAL:HG13	2:652:B:PHE:HE1	6	4.46
(1,562)	2:688:B:LEU:HD13	2:686:B:LEU:HD23	9	4.41
(1,243)	2:616:B:VAL:HG12	2:631:B:GLN:HE22	5	4.41
(1,243)	2:616:B:VAL:HG12	2:631:B:GLN:HE22	6	4.4
(1,2422)	2:682:B:VAL:HG12	2:652:B:PHE:HE1	3	4.37
(1,562)	2:688:B:LEU:HD11	2:686:B:LEU:HD21	3	4.36
(1,563)	2:688:B:LEU:HD12	2:583:B:LEU:HD21	13	4.34
(1,562)	2:688:B:LEU:HD13	2:686:B:LEU:HD22	14	4.34
(1,2674)	2:571:B:LEU:HD12	2:568:B:PRO:HG2	15	4.31
(1,562)	2:688:B:LEU:HD11	2:686:B:LEU:HD21	2	4.19
(1,563)	2:688:B:LEU:HD11	2:583:B:LEU:HD23	1	4.16
(1,2422)	2:643:B:VAL:HG12	2:640:B:GLN:HE22	4	4.15
(1,563)	2:688:B:LEU:HD12	2:583:B:LEU:HD21	14	4.15
(1,243)	2:616:B:VAL:HG12	2:631:B:GLN:HE22	10	4.15
(1,893)	2:630:B:ILE:HD12	2:645:B:VAL:HG13	8	4.11
(1,243)	2:616:B:VAL:HG13	2:631:B:GLN:HE22	2	4.11
(1,563)	2:688:B:LEU:HD11	2:583:B:LEU:HD21	3	4.09
(1,562)	2:688:B:LEU:HD13	2:686:B:LEU:HD21	10	4.09
(1,322)	2:629:B:VAL:HG21	1:44:A:LEU:HD22	10	4.09
(1,2952)	2:573:B:PRO:HB2	1:40:A:LEU:HB2	5	4.08
(1,2674)	2:571:B:LEU:HD12	2:568:B:PRO:HG2	10	4.08
(1,893)	2:630:B:ILE:HD13	2:645:B:VAL:HG12	4	4.07
(1,2422)	2:682:B:VAL:HG12	2:652:B:PHE:HE1	10	4.05
(1,2952)	2:573:B:PRO:HB2	1:40:A:LEU:HB2	7	4.03
(1,562)	2:688:B:LEU:HD12	2:686:B:LEU:HD22	6	4.02
(1,2674)	2:571:B:LEU:HD12	2:569:B:PRO:HB3	4	3.97
(1,563)	2:688:B:LEU:HD11	2:583:B:LEU:HD23	2	3.97
(1,893)	2:630:B:ILE:HD12	2:645:B:VAL:HG13	11	3.94
(1,893)	2:630:B:ILE:HD12	2:645:B:VAL:HG13	10	3.93
(1,2952)	2:573:B:PRO:HB2	1:40:A:LEU:HB2	2	3.92
(1,563)	2:688:B:LEU:HD12	2:583:B:LEU:HD21	4	3.92
(1,2952)	2:573:B:PRO:HB2	1:40:A:LEU:HB2	14	3.91

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2952)	2:573:B:PRO:HB2	1:40:A:LEU:HB2	4	3.87
(1,2422)	2:643:B:VAL:HG12	2:640:B:GLN:HE22	12	3.87
(1,893)	2:630:B:ILE:HD11	2:645:B:VAL:HG12	2	3.86
(1,243)	2:616:B:VAL:HG11	2:631:B:GLN:HE22	1	3.86
(1,562)	2:688:B:LEU:HD12	2:686:B:LEU:HD23	4	3.85
(1,2674)	2:571:B:LEU:HD11	2:569:B:PRO:HB3	13	3.84
(1,2674)	2:571:B:LEU:HD12	2:568:B:PRO:HG2	6	3.83
(1,893)	2:630:B:ILE:HD13	2:645:B:VAL:HG11	15	3.83
(1,563)	2:688:B:LEU:HD12	2:583:B:LEU:HD21	6	3.83
(1,243)	2:616:B:VAL:HG12	2:631:B:GLN:HE22	9	3.83
(1,893)	2:630:B:ILE:HD13	2:645:B:VAL:HG12	3	3.82
(1,563)	2:688:B:LEU:HD13	2:583:B:LEU:HD21	9	3.81
(1,2674)	2:571:B:LEU:HD12	2:569:B:PRO:HB3	12	3.8
(1,564)	2:688:B:LEU:HD22	2:583:B:LEU:HD22	15	3.8
(1,563)	2:688:B:LEU:HD12	2:583:B:LEU:HD22	8	3.8
(1,2952)	2:573:B:PRO:HB2	1:40:A:LEU:HB2	13	3.76
(1,2952)	2:573:B:PRO:HB2	1:40:A:LEU:HB2	10	3.75
(2,12)	2:683:B:CYS:HB2	2:656:B:GLN:HB3	14	3.73
(1,2952)	2:573:B:PRO:HB2	1:40:A:LEU:HB2	3	3.73
(1,2952)	2:573:B:PRO:HB2	1:40:A:LEU:HB2	9	3.72
(1,563)	2:688:B:LEU:HD12	2:583:B:LEU:HD21	5	3.71
(1,2952)	2:573:B:PRO:HB2	1:40:A:LEU:HB2	1	3.69
(1,563)	2:688:B:LEU:HD12	2:583:B:LEU:HD22	12	3.69
(1,322)	2:629:B:VAL:HG22	1:44:A:LEU:HD21	4	3.69
(1,563)	2:688:B:LEU:HD11	2:583:B:LEU:HD21	11	3.66
(1,2952)	2:573:B:PRO:HB2	1:40:A:LEU:HB2	15	3.65
(1,564)	2:688:B:LEU:HD22	2:583:B:LEU:HD21	13	3.58
(1,1350)	1:40:A:LEU:HG	1:34:A:VAL:HG13	9	3.56
(2,12)	2:683:B:CYS:HB2	2:656:B:GLN:HB3	10	3.55
(1,564)	2:688:B:LEU:HD21	2:583:B:LEU:HD21	14	3.51
(1,563)	2:688:B:LEU:HD12	2:583:B:LEU:HD22	15	3.51
(2,12)	2:683:B:CYS:HB2	2:656:B:GLN:HB3	6	3.5
(2,12)	2:683:B:CYS:HB2	2:656:B:GLN:HB3	13	3.46
(2,12)	2:683:B:CYS:HB2	2:656:B:GLN:HB3	9	3.44
(1,2952)	2:573:B:PRO:HB2	1:40:A:LEU:HB2	8	3.44
(1,799)	2:660:B:SER:HB3	1:40:A:LEU:HA	14	3.44
(1,799)	2:660:B:SER:HB3	1:40:A:LEU:HA	1	3.39
(1,799)	2:660:B:SER:HB3	1:40:A:LEU:HA	3	3.39
(1,563)	2:688:B:LEU:HD12	2:583:B:LEU:HD23	7	3.39
(1,1350)	1:40:A:LEU:HG	1:34:A:VAL:HG11	8	3.37
(1,799)	2:660:B:SER:HB3	1:40:A:LEU:HA	12	3.36
(1,563)	2:688:B:LEU:HD13	2:583:B:LEU:HD22	10	3.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2952)	2:573:B:PRO:HB2	1:40:A:LEU:HB2	11	3.33
(1,2952)	2:573:B:PRO:HB2	1:40:A:LEU:HB2	6	3.32
(2,12)	2:683:B:CYS:HB2	2:656:B:GLN:HB3	3	3.31
(1,564)	2:688:B:LEU:HD21	2:583:B:LEU:HD23	2	3.31
(2,12)	2:683:B:CYS:HB2	2:656:B:GLN:HB3	8	3.29
(2,12)	2:683:B:CYS:HB2	2:656:B:GLN:HB3	5	3.27
(1,2952)	2:573:B:PRO:HB2	1:40:A:LEU:HB2	12	3.27
(1,564)	2:688:B:LEU:HD22	2:583:B:LEU:HD21	3	3.26
(1,893)	2:630:B:ILE:HD12	2:645:B:VAL:HG12	13	3.24
(1,564)	2:688:B:LEU:HD22	2:583:B:LEU:HD23	1	3.24
(2,12)	2:683:B:CYS:HB2	2:656:B:GLN:HB3	7	3.23
(1,1351)	1:37:A:TRP:HA	1:41:A:VAL:HG21	10	3.23
(1,564)	2:688:B:LEU:HD23	2:583:B:LEU:HD21	6	3.22
(2,12)	2:683:B:CYS:HB2	2:656:B:GLN:HB3	15	3.2
(1,799)	2:660:B:SER:HB3	1:40:A:LEU:HA	13	3.2
(2,12)	2:683:B:CYS:HB2	2:656:B:GLN:HB3	12	3.19
(1,2674)	2:571:B:LEU:HD12	2:569:B:PRO:HB3	5	3.18
(2,12)	2:683:B:CYS:HB2	2:656:B:GLN:HB3	2	3.13
(1,564)	2:688:B:LEU:HD22	2:583:B:LEU:HD21	4	3.11
(1,564)	2:688:B:LEU:HD22	2:583:B:LEU:HD22	8	3.1
(1,564)	2:688:B:LEU:HD21	2:583:B:LEU:HD22	9	3.09
(2,12)	2:683:B:CYS:HB2	2:656:B:GLN:HB3	1	3.07
(1,564)	2:688:B:LEU:HD21	2:583:B:LEU:HD22	10	3.07
(1,1351)	1:37:A:TRP:HA	1:41:A:VAL:HG21	1	2.99
(1,893)	2:630:B:ILE:HD11	2:645:B:VAL:HG11	6	2.97
(1,799)	2:660:B:SER:HB3	1:40:A:LEU:HA	6	2.97
(1,799)	2:660:B:SER:HB3	1:40:A:LEU:HA	9	2.97
(2,12)	2:683:B:CYS:HB2	2:656:B:GLN:HB3	4	2.93
(1,910)	2:672:B:LEU:HD13	2:592:B:GLU:HB2	9	2.9
(1,2422)	2:643:B:VAL:HG11	1:48:A:GLN:HE21	5	2.78
(1,1351)	1:37:A:TRP:HA	1:41:A:VAL:HG22	2	2.76
(1,893)	2:630:B:ILE:HD11	2:645:B:VAL:HG12	12	2.76
(1,102)	2:672:B:LEU:HD11	2:673:B:PRO:HD3	9	2.76
(1,2549)	2:647:B:VAL:HG12	2:649:B:TYR:HA	9	2.75
(1,1351)	1:37:A:TRP:HA	1:41:A:VAL:HG23	14	2.75
(1,2549)	2:647:B:VAL:HG11	2:649:B:TYR:HA	1	2.72
(1,2549)	2:647:B:VAL:HG11	2:649:B:TYR:HA	7	2.72
(1,2549)	2:647:B:VAL:HG12	2:649:B:TYR:HA	12	2.71
(1,2549)	2:647:B:VAL:HG12	2:649:B:TYR:HA	14	2.71
(1,2422)	2:643:B:VAL:HG11	1:48:A:GLN:HE21	14	2.71
(1,2549)	2:647:B:VAL:HG11	2:649:B:TYR:HA	10	2.7
(1,2204)	2:616:B:VAL:HG13	1:44:A:LEU:HB2	10	2.69

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2549)	2:647:B:VAL:HG12	2:649:B:TYR:HA	2	2.68
(1,2549)	2:647:B:VAL:HG13	2:649:B:TYR:HA	4	2.68
(1,2549)	2:647:B:VAL:HG11	2:649:B:TYR:HA	5	2.68
(1,2549)	2:647:B:VAL:HG13	2:649:B:TYR:HA	8	2.67
(1,1351)	1:37:A:TRP:HA	1:41:A:VAL:HG22	12	2.65
(1,1351)	1:37:A:TRP:HA	1:41:A:VAL:HG21	15	2.65
(1,2549)	2:647:B:VAL:HG11	2:649:B:TYR:HA	6	2.64
(1,2549)	2:647:B:VAL:HG13	2:649:B:TYR:HA	15	2.64
(1,2204)	2:616:B:VAL:HG11	1:44:A:LEU:HB2	3	2.64
(2,12)	2:683:B:CYS:HB2	2:656:B:GLN:HB3	11	2.63
(1,2549)	2:647:B:VAL:HG13	2:649:B:TYR:HA	13	2.63
(1,2422)	2:643:B:VAL:HG11	1:48:A:GLN:HE21	2	2.63
(1,2674)	2:571:B:LEU:HD13	2:568:B:PRO:HG2	8	2.62
(1,2549)	2:647:B:VAL:HG13	2:649:B:TYR:HA	11	2.62
(1,2431)	2:646:B:LEU:HD12	2:625:B:PRO:HA	3	2.59
(1,2422)	2:643:B:VAL:HG12	1:48:A:GLN:HE21	1	2.59
(1,2204)	2:616:B:VAL:HG13	1:44:A:LEU:HB2	13	2.56
(1,1351)	1:37:A:TRP:HA	1:41:A:VAL:HG23	13	2.55
(1,1351)	1:37:A:TRP:HA	1:41:A:VAL:HG23	5	2.54
(1,510)	2:682:B:VAL:HG21	2:613:B:SER:HB2	2	2.54
(1,2204)	2:616:B:VAL:HG13	1:44:A:LEU:HB2	15	2.53
(1,204)	2:609:B:LEU:HD12	2:688:B:LEU:HA	15	2.53
(1,641)	2:683:B:CYS:HB3	2:651:B:PHE:HB2	4	2.52
(1,2204)	2:616:B:VAL:HG11	1:44:A:LEU:HB2	14	2.51
(1,893)	2:630:B:ILE:HD11	2:645:B:VAL:HG13	1	2.5
(1,2549)	2:647:B:VAL:HG13	2:649:B:TYR:HA	3	2.49
(1,2204)	2:616:B:VAL:HG11	1:44:A:LEU:HB2	2	2.49
(1,2204)	2:616:B:VAL:HG13	1:44:A:LEU:HB2	6	2.48
(1,2204)	2:616:B:VAL:HG13	1:44:A:LEU:HB2	9	2.47
(1,775)	2:612:B:ASP:HB2	1:44:A:LEU:HD11	10	2.47
(1,2267)	2:643:B:VAL:HG22	1:44:A:LEU:HD12	2	2.44
(1,637)	2:658:B:TRP:HB2	2:672:B:LEU:HD21	8	2.41
(1,489)	2:674:B:CYS:HB3	2:663:B:PRO:HB2	10	2.4
(1,799)	2:660:B:SER:HB3	1:40:A:LEU:HA	10	2.38
(1,2472)	2:686:B:LEU:HD12	2:688:B:LEU:HB2	1	2.36
(1,797)	2:660:B:SER:HB2	1:40:A:LEU:HA	10	2.36
(1,1351)	1:37:A:TRP:HA	1:41:A:VAL:HG22	3	2.34
(1,1056)	2:666:B:THR:HG22	2:672:B:LEU:HD23	8	2.34
(1,598)	2:582:B:GLN:HB3	2:580:B:ILE:HG21	4	2.34
(1,893)	2:630:B:ILE:HD13	2:645:B:VAL:HG13	7	2.32
(1,598)	2:582:B:GLN:HB3	2:580:B:ILE:HG21	13	2.31
(1,489)	2:674:B:CYS:HB3	2:663:B:PRO:HB2	5	2.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1102)	2:672:B:LEU:HD22	2:666:B:THR:HA	5	2.3
(1,2204)	2:616:B:VAL:HG13	1:44:A:LEU:HB2	4	2.29
(1,489)	2:674:B:CYS:HB3	2:663:B:PRO:HB2	8	2.28
(1,1351)	1:37:A:TRP:HA	1:41:A:VAL:HG21	8	2.26
(1,2267)	2:643:B:VAL:HG22	1:44:A:LEU:HD12	13	2.25
(1,641)	2:683:B:CYS:HB3	2:651:B:PHE:HB2	11	2.25
(1,489)	2:674:B:CYS:HB3	2:663:B:PRO:HB2	4	2.24
(1,562)	2:688:B:LEU:HD11	2:686:B:LEU:HD22	15	2.22
(1,489)	2:674:B:CYS:HB3	2:663:B:PRO:HB2	2	2.22
(1,1102)	2:672:B:LEU:HD23	2:666:B:THR:HA	8	2.21
(1,893)	2:630:B:ILE:HD13	2:645:B:VAL:HG11	14	2.21
(1,2204)	2:616:B:VAL:HG13	1:44:A:LEU:HB2	12	2.2
(1,2218)	2:666:B:THR:HG21	1:39:A:SER:HG	2	2.19
(1,1351)	1:37:A:TRP:HA	1:41:A:VAL:HG21	9	2.18
(1,598)	2:582:B:GLN:HB3	2:580:B:ILE:HG22	3	2.18
(1,562)	2:688:B:LEU:HD13	2:686:B:LEU:HD23	12	2.18
(1,2675)	2:571:B:LEU:HD23	2:572:B:PRO:HG2	9	2.17
(1,893)	2:630:B:ILE:HD11	2:645:B:VAL:HG13	5	2.17
(1,598)	2:582:B:GLN:HB3	2:580:B:ILE:HG22	9	2.17
(1,2523)	2:611:B:ILE:HD12	2:584:B:ALA:H	11	2.16
(1,2523)	2:611:B:ILE:HD13	2:584:B:ALA:H	4	2.15
(1,2472)	2:686:B:LEU:HD13	2:610:B:LYS:HB2	8	2.15
(1,2218)	2:666:B:THR:HG21	1:39:A:SER:HG	15	2.15
(1,2204)	2:616:B:VAL:HG12	1:44:A:LEU:HB2	11	2.14
(1,2523)	2:611:B:ILE:HD13	2:584:B:ALA:H	2	2.13
(1,2523)	2:611:B:ILE:HD12	2:584:B:ALA:H	12	2.13
(1,2218)	2:666:B:THR:HG21	1:39:A:SER:HG	11	2.13
(1,598)	2:582:B:GLN:HB3	2:580:B:ILE:HG21	14	2.13
(1,598)	2:582:B:GLN:HB3	2:580:B:ILE:HG23	11	2.12
(1,562)	2:688:B:LEU:HD13	2:686:B:LEU:HD23	7	2.11
(1,2267)	2:643:B:VAL:HG22	1:44:A:LEU:HD12	14	2.1
(1,2218)	2:666:B:THR:HG22	1:39:A:SER:HG	7	2.1
(1,2204)	2:616:B:VAL:HG12	1:44:A:LEU:HB2	1	2.1
(1,799)	2:660:B:SER:HB3	1:40:A:LEU:HA	8	2.1
(1,2577)	2:630:B:ILE:HD12	2:683:B:CYS:HB3	7	2.09
(1,2523)	2:611:B:ILE:HD11	2:584:B:ALA:H	3	2.09
(1,2286)	2:659:B:SER:HA	1:40:A:LEU:HB2	10	2.09
(1,2267)	2:643:B:VAL:HG23	1:44:A:LEU:HD12	3	2.09
(1,562)	2:688:B:LEU:HD13	2:686:B:LEU:HD23	8	2.09
(1,1351)	1:37:A:TRP:HA	1:41:A:VAL:HG23	7	2.08
(1,976)	2:574:B:TYR:HB2	2:581:B:ILE:HD12	9	2.08
(1,102)	2:672:B:LEU:HD11	2:673:B:PRO:HD3	5	2.08

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2523)	2:611:B:ILE:HD11	2:584:B:ALA:H	15	2.07
(1,642)	2:683:B:CYS:HB2	2:651:B:PHE:HB2	5	2.07
(1,2674)	2:571:B:LEU:HD13	2:568:B:PRO:HG2	7	2.05
(1,2523)	2:611:B:ILE:HD12	2:584:B:ALA:H	7	2.05
(1,2268)	2:643:B:VAL:HG22	1:44:A:LEU:HD21	10	2.05
(1,2204)	2:616:B:VAL:HG13	1:44:A:LEU:HB2	7	2.05
(1,976)	2:574:B:TYR:HB2	2:581:B:ILE:HD11	2	2.05
(1,976)	2:574:B:TYR:HB2	2:581:B:ILE:HD11	3	2.05
(1,799)	2:660:B:SER:HB3	1:40:A:LEU:HA	4	2.05
(1,404)	2:648:B:GLU:HG3	2:669:B:LEU:HD13	4	2.05
(1,2218)	2:666:B:THR:HG23	1:39:A:SER:HG	3	2.04
(1,598)	2:582:B:GLN:HB3	2:580:B:ILE:HG23	7	2.04
(1,2674)	2:571:B:LEU:HD12	2:569:B:PRO:HB3	2	2.03
(1,2523)	2:611:B:ILE:HD13	1:43:A:PHE:HD1	10	2.03
(1,976)	2:574:B:TYR:HB2	2:581:B:ILE:HD12	15	2.02
(1,976)	2:574:B:TYR:HB2	2:581:B:ILE:HD13	6	2.01
(1,2218)	2:666:B:THR:HG22	1:39:A:SER:HG	10	2.0
(1,2204)	2:616:B:VAL:HG13	1:44:A:LEU:HB2	5	2.0
(1,2267)	2:643:B:VAL:HG22	1:44:A:LEU:HD13	12	1.99
(1,976)	2:574:B:TYR:HB2	2:581:B:ILE:HD12	11	1.99
(1,976)	2:574:B:TYR:HB2	2:581:B:ILE:HD11	12	1.99
(1,976)	2:574:B:TYR:HB2	2:581:B:ILE:HD12	13	1.99
(1,893)	2:630:B:ILE:HD11	2:645:B:VAL:HG11	9	1.99
(1,2523)	2:611:B:ILE:HD12	2:584:B:ALA:H	13	1.98
(1,1056)	2:666:B:THR:HG22	2:672:B:LEU:HD22	5	1.98
(1,1351)	1:37:A:TRP:HA	1:41:A:VAL:HG21	11	1.97
(1,562)	2:688:B:LEU:HD13	2:686:B:LEU:HD22	5	1.97
(1,2268)	2:643:B:VAL:HG21	1:44:A:LEU:HD21	4	1.96
(1,2218)	2:666:B:THR:HG23	1:39:A:SER:HG	12	1.96
(1,797)	2:660:B:SER:HB2	1:40:A:LEU:HA	8	1.96
(1,562)	2:688:B:LEU:HD12	2:686:B:LEU:HD21	1	1.96
(1,562)	2:688:B:LEU:HD12	2:686:B:LEU:HD23	11	1.96
(1,1351)	1:37:A:TRP:HA	1:41:A:VAL:HG21	6	1.95
(1,598)	2:582:B:GLN:HB3	2:580:B:ILE:HG21	12	1.95
(1,2286)	2:659:B:SER:HA	1:40:A:LEU:HB2	14	1.94
(1,2267)	2:643:B:VAL:HG23	1:44:A:LEU:HD13	9	1.94
(1,2267)	2:643:B:VAL:HG22	1:44:A:LEU:HD11	15	1.94
(1,642)	2:683:B:CYS:HB2	2:651:B:PHE:HB2	2	1.94
(1,2523)	2:611:B:ILE:HD11	2:584:B:ALA:H	6	1.93
(1,2204)	2:616:B:VAL:HG13	1:44:A:LEU:HB2	8	1.93
(1,2218)	2:666:B:THR:HG22	1:39:A:SER:HG	6	1.9
(1,976)	2:574:B:TYR:HB2	2:581:B:ILE:HD11	1	1.9

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2457)	2:674:B:CYS:HB3	2:666:B:THR:HA	14	1.89
(1,489)	2:674:B:CYS:HB3	2:663:B:PRO:HB2	7	1.89
(1,489)	2:674:B:CYS:HB3	2:663:B:PRO:HB2	14	1.89
(1,976)	2:574:B:TYR:HB2	2:581:B:ILE:HD11	10	1.88
(1,98)	2:672:B:LEU:HD13	2:591:B:VAL:HG21	5	1.88
(1,598)	2:582:B:GLN:HB3	2:580:B:ILE:HG22	6	1.87
(1,62)	2:586:B:GLY:HA3	2:587:B:GLU:HG3	9	1.87
(1,2218)	2:666:B:THR:HG21	1:39:A:SER:HG	13	1.86
(1,598)	2:582:B:GLN:HB3	2:580:B:ILE:HG22	1	1.86
(1,2357)	2:616:B:VAL:HG11	2:630:B:ILE:HB	4	1.85
(1,2286)	2:659:B:SER:HA	1:40:A:LEU:HB2	3	1.85
(1,556)	2:687:B:THR:H	2:686:B:LEU:HD11	8	1.85
(1,2267)	2:643:B:VAL:HG21	1:44:A:LEU:HD13	8	1.84
(1,489)	2:674:B:CYS:HB3	2:663:B:PRO:HB2	3	1.84
(1,2286)	2:659:B:SER:HA	1:40:A:LEU:HB2	9	1.83
(1,1309)	2:579:B:SER:HB3	1:39:A:SER:HG	15	1.83
(1,976)	2:574:B:TYR:HB2	2:581:B:ILE:HD12	8	1.83
(1,516)	2:679:B:VAL:HG13	2:678:B:SER:HA	4	1.83
(1,489)	2:674:B:CYS:HB3	2:663:B:PRO:HB2	13	1.83
(1,2286)	2:659:B:SER:HA	1:40:A:LEU:HB2	1	1.82
(1,2222)	2:686:B:LEU:HD22	1:38:A:HIS:HB2	13	1.82
(1,1309)	2:579:B:SER:HB3	1:39:A:SER:HG	8	1.82
(1,1309)	2:579:B:SER:HB3	1:39:A:SER:HG	9	1.82
(1,1309)	2:579:B:SER:HB3	1:39:A:SER:HG	14	1.82
(1,1308)	2:579:B:SER:HB2	1:39:A:SER:HG	1	1.82
(1,910)	2:672:B:LEU:HD11	2:592:B:GLU:HB2	5	1.82
(1,797)	2:660:B:SER:HB2	1:40:A:LEU:HA	4	1.82
(1,243)	2:616:B:VAL:HG13	2:631:B:GLN:HE22	3	1.82
(1,2457)	2:674:B:CYS:HB3	2:666:B:THR:HA	12	1.81
(1,2357)	2:616:B:VAL:HG12	2:630:B:ILE:HB	3	1.81
(1,2222)	2:686:B:LEU:HD23	1:38:A:HIS:HB2	4	1.81
(1,1255)	2:672:B:LEU:HD13	2:592:B:GLU:HA	9	1.81
(1,976)	2:574:B:TYR:HB2	2:581:B:ILE:HD13	7	1.81
(1,637)	2:658:B:TRP:HB2	2:672:B:LEU:HD23	5	1.81
(1,1109)	2:672:B:LEU:HG	2:673:B:PRO:HD3	5	1.8
(1,797)	2:660:B:SER:HB2	1:40:A:LEU:HA	2	1.8
(1,598)	2:582:B:GLN:HB3	2:580:B:ILE:HG21	15	1.8
(1,98)	2:672:B:LEU:HD11	2:591:B:VAL:HG22	8	1.8
(1,2286)	2:659:B:SER:HA	1:40:A:LEU:HB2	13	1.79
(1,2286)	2:659:B:SER:HA	1:40:A:LEU:HB2	15	1.79
(1,2222)	2:686:B:LEU:HD22	1:38:A:HIS:HB2	14	1.79
(1,1309)	2:579:B:SER:HB3	1:39:A:SER:HG	13	1.79

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,799)	2:660:B:SER:HB3	1:40:A:LEU:HA	2	1.79
(1,598)	2:582:B:GLN:HB3	2:580:B:ILE:HG21	2	1.79
(1,598)	2:582:B:GLN:HB3	2:580:B:ILE:HG21	8	1.79
(1,512)	2:679:B:VAL:HG13	2:619:B:ILE:HD12	4	1.79
(1,204)	2:609:B:LEU:HD13	2:688:B:LEU:HA	12	1.79
(1,2519)	2:608:B:ASP:HB2	2:688:B:LEU:HD13	11	1.78
(1,2222)	2:686:B:LEU:HD23	1:38:A:HIS:HB2	11	1.78
(1,1934)	2:679:B:VAL:H	2:679:B:VAL:HG11	4	1.78
(1,1309)	2:579:B:SER:HB3	1:39:A:SER:HG	11	1.78
(1,1308)	2:579:B:SER:HB2	1:39:A:SER:HG	8	1.78
(1,1308)	2:579:B:SER:HB2	1:39:A:SER:HG	9	1.78
(1,1308)	2:579:B:SER:HB2	1:39:A:SER:HG	14	1.78
(1,556)	2:687:B:THR:H	2:686:B:LEU:HD11	1	1.77
(1,2457)	2:674:B:CYS:HB3	2:666:B:THR:HA	13	1.76
(1,2357)	2:616:B:VAL:HG12	2:630:B:ILE:HB	14	1.76
(1,2286)	2:659:B:SER:HA	1:40:A:LEU:HB2	2	1.76
(1,2286)	2:659:B:SER:HA	1:40:A:LEU:HB2	4	1.76
(1,2286)	2:659:B:SER:HA	1:40:A:LEU:HB2	12	1.76
(1,642)	2:683:B:CYS:HB2	2:651:B:PHE:HB2	8	1.76
(1,642)	2:683:B:CYS:HB2	2:651:B:PHE:HB2	10	1.76
(1,2523)	2:611:B:ILE:HD11	1:43:A:PHE:HD1	1	1.75
(1,2218)	2:666:B:THR:HG21	1:39:A:SER:HG	5	1.75
(1,2286)	2:659:B:SER:HA	1:40:A:LEU:HB2	11	1.74
(1,2207)	2:674:B:CYS:HB2	1:40:A:LEU:HB2	3	1.74
(1,489)	2:674:B:CYS:HB3	2:663:B:PRO:HB2	12	1.74
(1,2607)	2:659:B:SER:HA	2:673:B:PRO:HB2	12	1.73
(1,2286)	2:659:B:SER:HA	1:40:A:LEU:HB2	8	1.73
(1,2207)	2:674:B:CYS:HB2	1:40:A:LEU:HB2	1	1.73
(1,641)	2:683:B:CYS:HB3	2:651:B:PHE:HB2	12	1.73
(1,2357)	2:616:B:VAL:HG11	2:630:B:ILE:HB	9	1.72
(1,2357)	2:616:B:VAL:HG11	2:630:B:ILE:HB	13	1.72
(1,2286)	2:659:B:SER:HA	1:40:A:LEU:HB2	6	1.72
(1,976)	2:574:B:TYR:HB2	2:581:B:ILE:HD13	4	1.72
(1,423)	2:654:B:PHE:HB2	2:682:B:VAL:HG21	2	1.72
(1,2607)	2:659:B:SER:HA	2:673:B:PRO:HB2	4	1.71
(1,598)	2:582:B:GLN:HB3	2:580:B:ILE:HG23	10	1.71
(1,2928)	2:682:B:VAL:HG23	1:44:A:LEU:HD13	2	1.7
(1,2523)	2:611:B:ILE:HD13	2:584:B:ALA:H	5	1.7
(1,2357)	2:616:B:VAL:HG11	2:630:B:ILE:HB	5	1.7
(1,2267)	2:643:B:VAL:HG23	1:44:A:LEU:HD12	6	1.7
(1,2207)	2:674:B:CYS:HB2	1:40:A:LEU:HB2	12	1.7
(1,204)	2:609:B:LEU:HD11	2:688:B:LEU:HA	13	1.7

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2207)	2:674:B:CYS:HB2	1:40:A:LEU:HB2	14	1.69
(1,1308)	2:579:B:SER:HB2	1:39:A:SER:HG	4	1.69
(1,976)	2:574:B:TYR:HB2	2:581:B:ILE:HD12	14	1.69
(1,2607)	2:659:B:SER:HA	2:673:B:PRO:HB2	7	1.68
(1,2607)	2:659:B:SER:HA	2:673:B:PRO:HB2	9	1.68
(1,2286)	2:659:B:SER:HA	1:40:A:LEU:HB2	7	1.68
(1,2267)	2:643:B:VAL:HG22	1:44:A:LEU:HD13	11	1.68
(1,2207)	2:674:B:CYS:HB2	1:40:A:LEU:HB2	11	1.68
(1,1067)	2:582:B:GLN:HG2	2:580:B:ILE:HG21	4	1.68
(1,2607)	2:659:B:SER:HA	2:673:B:PRO:HB2	10	1.67
(1,2357)	2:616:B:VAL:HG12	2:630:B:ILE:HB	2	1.67
(1,2357)	2:616:B:VAL:HG11	2:630:B:ILE:HB	10	1.67
(1,2357)	2:616:B:VAL:HG11	2:630:B:ILE:HB	15	1.67
(1,1308)	2:579:B:SER:HB2	1:39:A:SER:HG	11	1.67
(1,642)	2:683:B:CYS:HB2	2:651:B:PHE:HB2	13	1.67
(1,598)	2:582:B:GLN:HB3	2:580:B:ILE:HG21	5	1.67
(1,2607)	2:659:B:SER:HA	2:673:B:PRO:HB2	3	1.66
(1,2207)	2:674:B:CYS:HB2	1:40:A:LEU:HB2	9	1.66
(1,2674)	2:571:B:LEU:HD11	2:568:B:PRO:HG2	1	1.65
(1,2607)	2:659:B:SER:HA	2:673:B:PRO:HB2	2	1.65
(1,2607)	2:659:B:SER:HA	2:673:B:PRO:HB2	5	1.65
(1,2607)	2:659:B:SER:HA	2:673:B:PRO:HB2	14	1.65
(1,2457)	2:674:B:CYS:HB3	2:666:B:THR:HA	3	1.65
(1,2357)	2:616:B:VAL:HG13	2:630:B:ILE:HB	1	1.65
(1,1269)	2:672:B:LEU:HD23	2:575:B:PHE:HB2	9	1.65
(1,1067)	2:582:B:GLN:HG2	2:580:B:ILE:HG22	9	1.65
(1,763)	2:611:B:ILE:HD11	2:652:B:PHE:HE1	10	1.65
(1,1403)	1:41:A:VAL:HG23	1:39:A:SER:H	10	1.64
(1,763)	2:611:B:ILE:HD12	2:652:B:PHE:HE1	7	1.64
(1,62)	2:586:B:GLY:HA3	2:587:B:GLU:HG3	15	1.64
(1,763)	2:611:B:ILE:HD13	2:652:B:PHE:HE1	14	1.63
(1,204)	2:609:B:LEU:HD13	2:688:B:LEU:HA	7	1.63
(1,62)	2:586:B:GLY:HA3	2:587:B:GLU:HG3	3	1.63
(1,2357)	2:616:B:VAL:HG11	2:630:B:ILE:HB	6	1.62
(1,2357)	2:616:B:VAL:HG11	2:630:B:ILE:HB	12	1.62
(1,2207)	2:674:B:CYS:HB2	1:40:A:LEU:HB2	15	1.62
(1,2270)	2:641:B:VAL:HG13	1:44:A:LEU:HD13	11	1.61
(1,1403)	1:41:A:VAL:HG23	1:39:A:SER:H	14	1.61
(1,763)	2:611:B:ILE:HD12	2:652:B:PHE:HE1	1	1.61
(1,423)	2:654:B:PHE:HB2	2:682:B:VAL:HG23	5	1.61
(1,62)	2:586:B:GLY:HA3	2:587:B:GLU:HG3	6	1.61
(1,2926)	2:653:B:VAL:HG11	1:44:A:LEU:HB2	6	1.6

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2607)	2:659:B:SER:HA	2:673:B:PRO:HB2	11	1.6
(1,1541)	2:590:B:LYS:H	2:589:B:LYS:HE2	9	1.6
(1,1102)	2:672:B:LEU:HD22	2:666:B:THR:HA	9	1.6
(1,642)	2:683:B:CYS:HB2	2:651:B:PHE:HB2	15	1.6
(1,2607)	2:659:B:SER:HA	2:673:B:PRO:HB2	6	1.59
(1,2607)	2:659:B:SER:HA	2:673:B:PRO:HB2	13	1.59
(1,2523)	2:611:B:ILE:HD12	1:43:A:PHE:HD1	9	1.59
(1,2457)	2:674:B:CYS:HB3	2:666:B:THR:HA	7	1.59
(1,1067)	2:582:B:GLN:HG2	2:580:B:ILE:HG21	13	1.59
(1,799)	2:660:B:SER:HB3	1:40:A:LEU:HA	5	1.59
(1,763)	2:611:B:ILE:HD13	2:652:B:PHE:HE1	9	1.59
(1,62)	2:586:B:GLY:HA3	2:587:B:GLU:HG3	13	1.59
(1,2675)	2:571:B:LEU:HD21	2:572:B:PRO:HG2	1	1.58
(1,2530)	2:642:B:SER:HB3	2:629:B:VAL:HG13	9	1.58
(1,2380)	2:620:B:GLU:HB3	2:629:B:VAL:HG23	4	1.58
(1,2286)	2:659:B:SER:HA	1:40:A:LEU:HB2	5	1.58
(1,1352)	1:47:A:SER:HA	1:48:A:GLN:HG3	15	1.58
(1,976)	2:574:B:TYR:HB2	2:581:B:ILE:HD12	5	1.58
(1,62)	2:586:B:GLY:HA3	2:587:B:GLU:HG3	8	1.58
(1,2422)	2:643:B:VAL:HG11	1:48:A:GLN:HE21	9	1.57
(1,2207)	2:674:B:CYS:HB2	1:40:A:LEU:HB2	6	1.57
(1,1352)	1:47:A:SER:HA	1:48:A:GLN:HG3	12	1.57
(1,763)	2:611:B:ILE:HD11	2:652:B:PHE:HE1	12	1.57
(1,763)	2:611:B:ILE:HD13	2:652:B:PHE:HE1	15	1.57
(1,152)	2:595:B:LYS:HG2	2:658:B:TRP:HB3	7	1.57
(1,62)	2:586:B:GLY:HA3	2:587:B:GLU:HG3	11	1.57
(1,2519)	2:608:B:ASP:HB2	2:688:B:LEU:HD11	7	1.56
(1,2357)	2:616:B:VAL:HG11	2:630:B:ILE:HB	8	1.56
(1,1251)	2:594:B:LEU:HD13	2:658:B:TRP:HZ2	3	1.56
(1,763)	2:611:B:ILE:HD13	2:652:B:PHE:HE1	8	1.56
(1,423)	2:654:B:PHE:HB2	2:682:B:VAL:HG22	9	1.56
(1,2523)	2:611:B:ILE:HD12	1:43:A:PHE:HD1	14	1.55
(1,2222)	2:686:B:LEU:HD22	1:38:A:HIS:HB2	12	1.55
(1,1403)	1:41:A:VAL:HG22	1:39:A:SER:H	2	1.55
(1,62)	2:586:B:GLY:HA3	2:587:B:GLU:HG3	4	1.55
(1,2207)	2:674:B:CYS:HB2	1:40:A:LEU:HB2	7	1.54
(1,1309)	2:579:B:SER:HB3	1:39:A:SER:HG	6	1.54
(1,1256)	2:592:B:GLU:HA	2:591:B:VAL:HG23	12	1.54
(1,62)	2:586:B:GLY:HA3	2:587:B:GLU:HG3	10	1.54
(1,1351)	1:37:A:TRP:HA	1:41:A:VAL:HG22	4	1.53
(1,1308)	2:579:B:SER:HB2	1:39:A:SER:HG	6	1.53
(1,1168)	2:686:B:LEU:HD11	2:609:B:LEU:HB2	1	1.53

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1067)	2:582:B:GLN:HG2	2:580:B:ILE:HG21	14	1.53
(1,404)	2:648:B:GLU:HG3	2:669:B:LEU:HD11	3	1.53
(1,2607)	2:659:B:SER:HA	2:673:B:PRO:HB2	1	1.52
(1,2523)	2:611:B:ILE:HD12	1:43:A:PHE:HD1	8	1.52
(1,2380)	2:620:B:GLU:HB3	2:629:B:VAL:HG21	1	1.52
(1,2380)	2:620:B:GLU:HB3	2:629:B:VAL:HG21	2	1.52
(1,2161)	2:682:B:VAL:H	2:682:B:VAL:HG12	1	1.52
(1,2161)	2:682:B:VAL:H	2:682:B:VAL:HG11	5	1.52
(1,2161)	2:682:B:VAL:H	2:682:B:VAL:HG13	14	1.52
(1,1403)	1:41:A:VAL:HG23	1:39:A:SER:H	8	1.52
(1,2380)	2:620:B:GLU:HB3	2:629:B:VAL:HG21	14	1.51
(1,2207)	2:674:B:CYS:HB2	1:40:A:LEU:HB2	13	1.51
(1,1256)	2:592:B:GLU:HA	2:591:B:VAL:HG22	14	1.51
(1,1251)	2:594:B:LEU:HD12	2:658:B:TRP:HZ2	1	1.51
(1,1251)	2:594:B:LEU:HD13	2:658:B:TRP:HZ2	12	1.51
(1,1067)	2:582:B:GLN:HG2	2:580:B:ILE:HG21	12	1.51
(1,850)	2:679:B:VAL:HG21	2:617:B:GLU:HA	4	1.51
(1,763)	2:611:B:ILE:HD12	2:652:B:PHE:HE1	4	1.51
(1,2380)	2:620:B:GLU:HB3	2:629:B:VAL:HG22	13	1.5
(1,2357)	2:616:B:VAL:HG13	2:630:B:ILE:HB	11	1.5
(1,2207)	2:674:B:CYS:HB2	1:40:A:LEU:HB2	10	1.5
(1,2161)	2:682:B:VAL:H	2:682:B:VAL:HG12	2	1.5
(1,1309)	2:579:B:SER:HB3	1:39:A:SER:HG	12	1.5
(1,797)	2:660:B:SER:HB2	1:40:A:LEU:HA	5	1.5
(1,763)	2:611:B:ILE:HD11	2:652:B:PHE:HE1	13	1.5
(1,2380)	2:620:B:GLU:HB3	2:629:B:VAL:HG22	3	1.49
(1,2207)	2:674:B:CYS:HB2	1:40:A:LEU:HB2	2	1.49
(1,2357)	2:616:B:VAL:HG11	2:630:B:ILE:HB	7	1.48
(1,2270)	2:641:B:VAL:HG11	1:44:A:LEU:HD12	3	1.48
(1,1256)	2:592:B:GLU:HA	2:591:B:VAL:HG21	2	1.48
(1,1256)	2:592:B:GLU:HA	2:591:B:VAL:HG23	3	1.48
(1,2457)	2:674:B:CYS:HB3	2:666:B:THR:HA	6	1.47
(1,1256)	2:592:B:GLU:HA	2:591:B:VAL:HG22	5	1.47
(1,1256)	2:592:B:GLU:HA	2:591:B:VAL:HG21	11	1.47
(1,1251)	2:594:B:LEU:HD13	2:658:B:TRP:HZ2	8	1.47
(1,1067)	2:582:B:GLN:HG2	2:580:B:ILE:HG23	7	1.47
(1,642)	2:683:B:CYS:HB2	2:651:B:PHE:HB2	3	1.47
(1,637)	2:658:B:TRP:HB2	2:672:B:LEU:HD22	6	1.47
(1,637)	2:658:B:TRP:HB2	2:672:B:LEU:HD22	7	1.47
(1,2380)	2:620:B:GLU:HB3	2:619:B:ILE:HG23	7	1.46
(1,1403)	1:41:A:VAL:HG22	1:39:A:SER:H	5	1.46
(1,1352)	1:47:A:SER:HA	1:48:A:GLN:HG2	6	1.46

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1251)	2:594:B:LEU:HD11	2:658:B:TRP:HZ2	6	1.46
(1,1251)	2:594:B:LEU:HD12	2:658:B:TRP:HZ2	11	1.46
(1,1067)	2:582:B:GLN:HG2	2:580:B:ILE:HG22	3	1.46
(1,637)	2:658:B:TRP:HB2	2:672:B:LEU:HD22	14	1.46
(1,2926)	2:653:B:VAL:HG12	1:44:A:LEU:HB2	12	1.45
(1,1309)	2:579:B:SER:HB3	1:39:A:SER:HG	4	1.45
(1,152)	2:595:B:LYS:HG2	2:658:B:TRP:HB3	1	1.45
(1,2607)	2:659:B:SER:HA	2:673:B:PRO:HB2	15	1.44
(1,2267)	2:643:B:VAL:HG21	1:44:A:LEU:HD12	1	1.44
(1,2222)	2:686:B:LEU:HD23	1:38:A:HIS:HB2	5	1.44
(1,2161)	2:682:B:VAL:H	2:682:B:VAL:HG11	9	1.44
(1,1352)	1:47:A:SER:HA	1:48:A:GLN:HG3	8	1.44
(1,1256)	2:592:B:GLU:HA	2:591:B:VAL:HG21	6	1.44
(1,1251)	2:594:B:LEU:HD11	2:658:B:TRP:HZ2	15	1.44
(1,1067)	2:582:B:GLN:HG2	2:580:B:ILE:HG22	1	1.44
(1,1067)	2:582:B:GLN:HG2	2:580:B:ILE:HG21	15	1.44
(1,2222)	2:686:B:LEU:HD21	1:38:A:HIS:HB2	2	1.43
(1,1057)	2:650:B:PRO:HG2	2:666:B:THR:HG21	11	1.43
(1,2525)	2:611:B:ILE:HG21	1:37:A:TRP:HZ3	1	1.42
(1,763)	2:611:B:ILE:HD13	2:652:B:PHE:HE1	6	1.42
(1,763)	2:611:B:ILE:HD11	2:652:B:PHE:HE1	11	1.42
(1,152)	2:595:B:LYS:HG2	2:658:B:TRP:HB3	4	1.42
(1,2270)	2:641:B:VAL:HG13	1:44:A:LEU:HD13	9	1.41
(1,2207)	2:674:B:CYS:HB2	1:40:A:LEU:HB2	8	1.41
(1,1403)	1:41:A:VAL:HG21	1:39:A:SER:H	1	1.41
(1,1220)	2:677:B:LEU:HA	2:677:B:LEU:HD23	4	1.41
(1,1067)	2:582:B:GLN:HG2	2:580:B:ILE:HG22	6	1.41
(1,2457)	2:674:B:CYS:HB3	2:666:B:THR:HA	1	1.4
(1,2222)	2:686:B:LEU:HD21	1:38:A:HIS:HB2	15	1.4
(1,1256)	2:592:B:GLU:HA	2:591:B:VAL:HG21	1	1.4
(1,1256)	2:592:B:GLU:HA	2:591:B:VAL:HG22	15	1.4
(1,1220)	2:677:B:LEU:HA	2:677:B:LEU:HD21	15	1.4
(1,1215)	2:681:B:ASP:HB3	2:677:B:LEU:HD21	5	1.4
(1,763)	2:611:B:ILE:HD12	2:652:B:PHE:HE1	2	1.4
(1,763)	2:611:B:ILE:HD13	2:652:B:PHE:HE1	3	1.4
(1,322)	2:629:B:VAL:HG23	1:44:A:LEU:HD21	7	1.4
(1,2930)	2:576:B:MET:HB3	1:39:A:SER:HG	14	1.39
(1,2380)	2:620:B:GLU:HB3	2:629:B:VAL:HG22	9	1.39
(1,1309)	2:579:B:SER:HB3	1:39:A:SER:HG	1	1.39
(1,1308)	2:579:B:SER:HB2	1:39:A:SER:HG	2	1.39
(1,1251)	2:594:B:LEU:HD11	2:658:B:TRP:HZ2	14	1.39
(1,1109)	2:672:B:LEU:HG	2:673:B:PRO:HD3	8	1.39

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1086)	2:609:B:LEU:HD22	1:37:A:TRP:HZ3	11	1.39
(1,763)	2:611:B:ILE:HD12	2:652:B:PHE:HE1	5	1.39
(1,152)	2:595:B:LYS:HG2	2:658:B:TRP:HB3	8	1.39
(1,152)	2:595:B:LYS:HG2	2:658:B:TRP:HB3	11	1.39
(1,2666)	2:591:B:VAL:HG11	2:658:B:TRP:HE3	15	1.38
(1,2577)	2:630:B:ILE:HD13	2:681:B:ASP:HB2	12	1.38
(1,2207)	2:674:B:CYS:HB2	1:40:A:LEU:HB2	4	1.38
(1,1308)	2:579:B:SER:HB2	1:39:A:SER:HG	12	1.38
(1,1251)	2:594:B:LEU:HD11	2:658:B:TRP:HZ2	13	1.38
(1,1215)	2:681:B:ASP:HB3	2:677:B:LEU:HD22	15	1.38
(1,1109)	2:672:B:LEU:HG	2:673:B:PRO:HD3	9	1.38
(1,1086)	2:609:B:LEU:HD21	1:37:A:TRP:HZ3	4	1.38
(1,799)	2:660:B:SER:HB3	1:40:A:LEU:HA	15	1.38
(1,642)	2:683:B:CYS:HB2	2:651:B:PHE:HB2	1	1.38
(1,2525)	2:611:B:ILE:HG21	1:37:A:TRP:HZ3	10	1.37
(1,2457)	2:674:B:CYS:HB3	2:666:B:THR:HA	9	1.37
(1,2380)	2:620:B:GLU:HB3	2:629:B:VAL:HG22	6	1.37
(1,2138)	2:678:B:SER:H	2:677:B:LEU:HD21	4	1.37
(1,1067)	2:582:B:GLN:HG2	2:580:B:ILE:HG21	8	1.37
(1,637)	2:658:B:TRP:HB2	2:672:B:LEU:HD23	2	1.37
(1,637)	2:658:B:TRP:HB2	2:672:B:LEU:HD21	4	1.37
(1,637)	2:658:B:TRP:HB2	2:672:B:LEU:HD21	13	1.37
(1,1251)	2:594:B:LEU:HD13	2:658:B:TRP:HZ2	5	1.36
(1,1220)	2:677:B:LEU:HA	2:677:B:LEU:HD23	5	1.36
(1,1256)	2:592:B:GLU:HA	2:591:B:VAL:HG23	4	1.35
(1,1251)	2:594:B:LEU:HD12	2:658:B:TRP:HZ2	4	1.35
(1,1086)	2:609:B:LEU:HD22	1:37:A:TRP:HZ3	5	1.35
(1,896)	2:630:B:ILE:HD11	2:651:B:PHE:HE1	5	1.35
(1,639)	2:658:B:TRP:HB3	2:593:B:ASP:HA	4	1.35
(1,639)	2:658:B:TRP:HB3	2:593:B:ASP:HA	12	1.35
(1,637)	2:658:B:TRP:HB2	2:672:B:LEU:HD22	1	1.35
(1,2519)	2:608:B:ASP:HB2	2:688:B:LEU:HD11	5	1.34
(1,2222)	2:686:B:LEU:HD23	1:38:A:HIS:HB2	9	1.34
(1,2138)	2:678:B:SER:H	2:677:B:LEU:HD22	15	1.34
(1,1541)	2:590:B:LYS:H	2:589:B:LYS:HE2	4	1.34
(1,637)	2:658:B:TRP:HB2	2:672:B:LEU:HD21	11	1.34
(1,322)	2:629:B:VAL:HG23	1:44:A:LEU:HD22	1	1.34
(1,322)	2:629:B:VAL:HG22	1:44:A:LEU:HD23	5	1.34
(1,2930)	2:576:B:MET:HB3	1:39:A:SER:HG	4	1.33
(1,2577)	2:630:B:ILE:HD13	2:681:B:ASP:HB2	9	1.33
(1,1086)	2:609:B:LEU:HD21	1:37:A:TRP:HZ3	8	1.33
(1,1057)	2:650:B:PRO:HG2	2:666:B:THR:HG23	8	1.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,910)	2:672:B:LEU:HD12	2:592:B:GLU:HB2	8	1.33
(1,639)	2:658:B:TRP:HB3	2:593:B:ASP:HA	5	1.33
(1,639)	2:658:B:TRP:HB3	2:593:B:ASP:HA	13	1.33
(1,637)	2:658:B:TRP:HB2	2:672:B:LEU:HD22	3	1.33
(1,152)	2:595:B:LYS:HG2	2:658:B:TRP:HB3	2	1.33
(1,2530)	2:682:B:VAL:HG21	2:613:B:SER:HB3	14	1.32
(1,2380)	2:620:B:GLU:HB3	2:629:B:VAL:HG22	12	1.32
(1,1403)	1:41:A:VAL:HG21	1:39:A:SER:H	3	1.32
(1,1256)	2:592:B:GLU:HA	2:591:B:VAL:HG23	13	1.32
(1,799)	2:660:B:SER:HB3	1:40:A:LEU:HA	11	1.32
(1,637)	2:658:B:TRP:HB2	2:672:B:LEU:HD23	15	1.32
(1,152)	2:595:B:LYS:HG2	2:658:B:TRP:HB3	15	1.32
(1,2596)	2:574:B:TYR:HB3	2:581:B:ILE:HD11	1	1.31
(1,2222)	2:686:B:LEU:HD21	1:38:A:HIS:HB2	7	1.31
(1,2200)	2:689:B:LYS:H	2:609:B:LEU:HD11	15	1.31
(1,1086)	2:609:B:LEU:HD22	1:37:A:TRP:HZ3	1	1.31
(1,1086)	2:609:B:LEU:HD23	1:37:A:TRP:HZ3	2	1.31
(1,639)	2:658:B:TRP:HB3	2:593:B:ASP:HA	1	1.31
(1,639)	2:658:B:TRP:HB3	2:593:B:ASP:HA	6	1.31
(1,203)	2:609:B:LEU:HD12	2:609:B:LEU:HA	7	1.31
(1,203)	2:609:B:LEU:HD13	2:609:B:LEU:HA	13	1.31
(1,2525)	2:611:B:ILE:HG23	1:37:A:TRP:HZ3	14	1.3
(1,1403)	1:41:A:VAL:HG23	1:39:A:SER:H	9	1.3
(1,1256)	2:592:B:GLU:HA	2:591:B:VAL:HG22	7	1.3
(1,1086)	2:609:B:LEU:HD23	1:37:A:TRP:HZ3	6	1.3
(1,1067)	2:582:B:GLN:HG2	2:580:B:ILE:HG23	11	1.3
(1,1057)	2:650:B:PRO:HG2	2:666:B:THR:HG23	15	1.3
(1,799)	2:660:B:SER:HB3	1:40:A:LEU:HA	7	1.3
(1,639)	2:658:B:TRP:HB3	2:593:B:ASP:HA	2	1.3
(1,203)	2:609:B:LEU:HD11	2:609:B:LEU:HA	15	1.3
(1,2519)	2:608:B:ASP:HB2	2:688:B:LEU:HD11	12	1.29
(1,1251)	2:594:B:LEU:HD12	2:658:B:TRP:HZ2	9	1.29
(1,639)	2:658:B:TRP:HB3	2:593:B:ASP:HA	14	1.29
(1,2926)	2:653:B:VAL:HG13	1:44:A:LEU:HB2	3	1.28
(1,2138)	2:678:B:SER:H	2:677:B:LEU:HD21	5	1.28
(1,1215)	2:681:B:ASP:HB3	2:677:B:LEU:HD21	4	1.28
(1,1067)	2:582:B:GLN:HG2	2:580:B:ILE:HG21	5	1.28
(1,637)	2:658:B:TRP:HB2	2:672:B:LEU:HD23	10	1.28
(1,404)	2:648:B:GLU:HG3	2:669:B:LEU:HD11	13	1.28
(1,203)	2:609:B:LEU:HD11	2:609:B:LEU:HA	12	1.28
(1,2525)	2:611:B:ILE:HG21	1:37:A:TRP:HZ3	2	1.27
(1,1086)	2:609:B:LEU:HD21	1:37:A:TRP:HZ3	9	1.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,639)	2:658:B:TRP:HB3	2:593:B:ASP:HA	8	1.27
(1,639)	2:658:B:TRP:HB3	2:593:B:ASP:HA	9	1.27
(1,2596)	2:574:B:TYR:HB3	2:581:B:ILE:HD13	8	1.26
(1,2525)	2:611:B:ILE:HG21	1:37:A:TRP:HZ3	8	1.26
(1,2397)	2:629:B:VAL:HG21	2:641:B:VAL:HA	3	1.26
(1,420)	2:654:B:PHE:HB2	2:682:B:VAL:HB	15	1.26
(1,152)	2:595:B:LYS:HG2	2:658:B:TRP:HB3	14	1.26
(1,2431)	2:646:B:LEU:HD11	2:625:B:PRO:HA	12	1.25
(1,2431)	2:646:B:LEU:HD13	2:625:B:PRO:HA	14	1.25
(1,2380)	2:620:B:GLU:HB3	2:629:B:VAL:HG21	11	1.25
(1,642)	2:683:B:CYS:HB2	2:651:B:PHE:HB2	14	1.25
(1,639)	2:658:B:TRP:HB3	2:593:B:ASP:HA	15	1.25
(1,2577)	2:630:B:ILE:HD11	2:681:B:ASP:HB2	11	1.24
(1,2431)	2:646:B:LEU:HD13	2:625:B:PRO:HA	7	1.24
(1,2431)	2:646:B:LEU:HD11	2:625:B:PRO:HA	9	1.24
(1,2431)	2:646:B:LEU:HD11	2:625:B:PRO:HA	10	1.24
(1,1251)	2:594:B:LEU:HD13	2:658:B:TRP:HZ2	7	1.24
(1,1056)	2:666:B:THR:HG23	2:672:B:LEU:HD22	9	1.24
(1,639)	2:658:B:TRP:HB3	2:593:B:ASP:HA	10	1.24
(1,639)	2:658:B:TRP:HB3	2:593:B:ASP:HA	11	1.24
(1,637)	2:658:B:TRP:HB2	2:672:B:LEU:HD21	12	1.24
(1,2577)	2:630:B:ILE:HD12	2:681:B:ASP:HB2	3	1.23
(1,2577)	2:630:B:ILE:HD12	2:681:B:ASP:HB2	4	1.23
(1,2525)	2:611:B:ILE:HG21	1:37:A:TRP:HZ3	11	1.23
(1,2431)	2:646:B:LEU:HD13	2:625:B:PRO:HA	1	1.23
(1,2431)	2:646:B:LEU:HD13	2:625:B:PRO:HA	4	1.23
(1,2431)	2:646:B:LEU:HD12	2:625:B:PRO:HA	8	1.23
(1,2277)	2:639:B:ALA:HB2	1:48:A:GLN:HB3	6	1.23
(1,2267)	2:643:B:VAL:HG23	1:44:A:LEU:HD12	5	1.23
(1,639)	2:658:B:TRP:HB3	2:593:B:ASP:HA	3	1.23
(1,501)	2:677:B:LEU:HD13	2:630:B:ILE:HG23	15	1.23
(1,8)	2:568:B:PRO:HB3	2:569:B:PRO:HD3	3	1.23
(1,2596)	2:574:B:TYR:HB3	2:581:B:ILE:HD13	4	1.22
(1,2525)	2:611:B:ILE:HG21	1:37:A:TRP:HZ3	9	1.22
(1,2466)	2:618:B:ARG:HG3	2:679:B:VAL:HG12	4	1.22
(1,1251)	2:594:B:LEU:HD11	2:658:B:TRP:HZ2	2	1.22
(1,1086)	2:609:B:LEU:HD23	1:37:A:TRP:HZ3	10	1.22
(1,1067)	2:582:B:GLN:HG2	2:580:B:ILE:HG21	2	1.22
(1,637)	2:658:B:TRP:HB2	2:672:B:LEU:HD23	9	1.22
(1,423)	2:654:B:PHE:HB2	2:682:B:VAL:HG21	1	1.22
(1,2738)	2:679:B:VAL:H	2:619:B:ILE:HG12	4	1.21
(1,2577)	2:630:B:ILE:HD11	2:681:B:ASP:HB2	13	1.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2431)	2:646:B:LEU:HD11	2:625:B:PRO:HA	5	1.21
(1,2431)	2:646:B:LEU:HD13	2:625:B:PRO:HA	13	1.21
(1,2431)	2:646:B:LEU:HD13	2:625:B:PRO:HA	15	1.21
(1,2358)	2:616:B:VAL:HG13	2:617:B:GLU:HB3	2	1.21
(1,2358)	2:616:B:VAL:HG11	2:617:B:GLU:HB3	11	1.21
(1,2358)	2:616:B:VAL:HG12	2:617:B:GLU:HB3	13	1.21
(1,2358)	2:616:B:VAL:HG12	2:617:B:GLU:HB3	15	1.21
(1,2270)	2:641:B:VAL:HG12	1:44:A:LEU:HD13	12	1.21
(1,2930)	2:576:B:MET:HB3	1:39:A:SER:HG	8	1.2
(1,2431)	2:646:B:LEU:HD12	2:625:B:PRO:HA	6	1.2
(1,2431)	2:646:B:LEU:HD13	2:625:B:PRO:HA	11	1.2
(1,1403)	1:41:A:VAL:HG23	1:39:A:SER:H	13	1.2
(1,1086)	2:609:B:LEU:HD22	1:37:A:TRP:HZ3	14	1.2
(1,2926)	2:682:B:VAL:HG12	1:44:A:LEU:HB2	14	1.19
(1,2525)	2:611:B:ILE:HG21	1:37:A:TRP:HZ3	15	1.19
(1,2397)	2:629:B:VAL:HG23	2:641:B:VAL:HA	2	1.19
(1,2358)	2:616:B:VAL:HG12	2:617:B:GLU:HB3	8	1.19
(1,203)	2:609:B:LEU:HD13	2:609:B:LEU:HA	3	1.19
(1,2431)	2:646:B:LEU:HD12	2:625:B:PRO:HA	2	1.18
(1,2397)	2:629:B:VAL:HG21	2:641:B:VAL:HA	6	1.18
(1,489)	2:674:B:CYS:HB3	2:663:B:PRO:HB2	1	1.18
(1,203)	2:609:B:LEU:HD12	2:609:B:LEU:HA	1	1.18
(1,8)	2:568:B:PRO:HB3	2:569:B:PRO:HD3	14	1.18
(1,2942)	2:663:B:PRO:HG3	1:40:A:LEU:HB2	8	1.17
(1,2666)	2:591:B:VAL:HG11	2:658:B:TRP:HE3	2	1.17
(1,2525)	2:611:B:ILE:HG21	1:37:A:TRP:HZ3	3	1.17
(1,2397)	2:629:B:VAL:HG23	2:641:B:VAL:HA	11	1.17
(1,2358)	2:616:B:VAL:HG12	2:617:B:GLU:HB3	10	1.17
(1,2269)	2:629:B:VAL:HG21	1:44:A:LEU:HB2	10	1.17
(1,2143)	2:680:B:GLY:H	2:679:B:VAL:HG21	4	1.17
(1,1256)	2:592:B:GLU:HA	2:591:B:VAL:HG21	9	1.17
(1,1086)	2:609:B:LEU:HD22	1:37:A:TRP:HZ3	3	1.17
(1,641)	2:683:B:CYS:HB3	2:651:B:PHE:HB2	6	1.17
(1,2926)	2:653:B:VAL:HG13	1:44:A:LEU:HB2	7	1.16
(1,2577)	2:630:B:ILE:HD11	2:681:B:ASP:HB2	10	1.16
(1,2457)	2:674:B:CYS:HB3	2:666:B:THR:HA	11	1.16
(1,2397)	2:629:B:VAL:HG23	2:641:B:VAL:HA	14	1.16
(1,2358)	2:616:B:VAL:HG12	2:617:B:GLU:HB3	5	1.16
(1,2270)	2:641:B:VAL:HG13	1:44:A:LEU:HD11	6	1.16
(1,639)	2:658:B:TRP:HB3	2:593:B:ASP:HA	7	1.16
(1,98)	2:672:B:LEU:HD13	2:591:B:VAL:HG23	9	1.16
(1,2666)	2:591:B:VAL:HG12	2:658:B:TRP:HE3	3	1.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2622)	2:648:B:GLU:HG3	2:669:B:LEU:HD13	8	1.15
(1,2607)	2:659:B:SER:HA	2:673:B:PRO:HB2	8	1.15
(1,2270)	2:641:B:VAL:HG11	1:44:A:LEU:HD12	1	1.15
(1,1256)	2:592:B:GLU:HA	2:591:B:VAL:HG23	10	1.15
(1,1067)	2:582:B:GLN:HG2	2:580:B:ILE:HG23	10	1.15
(1,2666)	2:591:B:VAL:HG11	2:658:B:TRP:HE3	13	1.14
(1,2380)	2:620:B:GLU:HB3	2:629:B:VAL:HG22	15	1.14
(1,2358)	2:616:B:VAL:HG12	2:617:B:GLU:HB3	9	1.14
(1,404)	2:648:B:GLU:HG3	2:669:B:LEU:HD11	12	1.14
(1,2577)	2:630:B:ILE:HD13	2:681:B:ASP:HB2	1	1.13
(1,2397)	2:629:B:VAL:HG21	2:641:B:VAL:HA	15	1.13
(1,2358)	2:616:B:VAL:HG12	2:617:B:GLU:HB3	4	1.13
(1,775)	2:612:B:ASP:HB2	1:44:A:LEU:HD13	4	1.13
(1,642)	2:683:B:CYS:HB2	2:651:B:PHE:HB2	9	1.13
(1,510)	2:682:B:VAL:HG21	2:613:B:SER:HB2	1	1.13
(1,322)	2:629:B:VAL:HG21	1:44:A:LEU:HD23	12	1.13
(1,8)	2:568:B:PRO:HB3	2:569:B:PRO:HD3	5	1.13
(1,2930)	2:576:B:MET:HB3	1:39:A:SER:HG	9	1.12
(1,2666)	2:591:B:VAL:HG12	2:658:B:TRP:HE3	6	1.12
(1,2397)	2:629:B:VAL:HG23	2:641:B:VAL:HA	7	1.12
(1,2358)	2:616:B:VAL:HG11	2:617:B:GLU:HB3	1	1.12
(1,2270)	2:641:B:VAL:HG11	1:44:A:LEU:HD11	14	1.12
(1,1309)	2:579:B:SER:HB3	1:39:A:SER:HG	2	1.12
(1,2596)	2:574:B:TYR:HB3	2:581:B:ILE:HD11	14	1.11
(1,2397)	2:629:B:VAL:HG23	2:641:B:VAL:HA	1	1.11
(1,2397)	2:629:B:VAL:HG22	2:641:B:VAL:HA	4	1.11
(1,2269)	2:629:B:VAL:HG23	1:44:A:LEU:HB2	2	1.11
(1,2218)	2:666:B:THR:HG22	1:39:A:SER:HG	1	1.11
(1,2218)	2:666:B:THR:HG23	1:39:A:SER:HG	4	1.11
(1,2218)	2:666:B:THR:HG22	1:39:A:SER:HG	9	1.11
(1,489)	2:674:B:CYS:HB3	2:663:B:PRO:HB2	9	1.11
(1,152)	2:595:B:LYS:HG2	2:658:B:TRP:HB3	6	1.11
(1,2666)	2:591:B:VAL:HG13	2:658:B:TRP:HE3	1	1.1
(1,2577)	2:630:B:ILE:HD13	2:681:B:ASP:HB2	5	1.1
(1,2577)	2:630:B:ILE:HD13	2:683:B:CYS:HB3	6	1.1
(1,2454)	2:674:B:CYS:HB2	2:666:B:THR:HA	4	1.1
(1,2397)	2:629:B:VAL:HG21	2:641:B:VAL:HA	8	1.1
(1,521)	2:679:B:VAL:HG21	2:680:B:GLY:HA2	4	1.1
(1,510)	2:682:B:VAL:HG23	2:613:B:SER:HB2	5	1.1
(1,510)	2:682:B:VAL:HG22	2:613:B:SER:HB2	9	1.1
(1,2525)	2:611:B:ILE:HG22	1:37:A:TRP:HZ3	4	1.09
(1,2358)	2:616:B:VAL:HG12	2:617:B:GLU:HB3	12	1.09

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,501)	2:677:B:LEU:HD11	2:630:B:ILE:HG23	5	1.09
(1,489)	2:674:B:CYS:HB3	2:663:B:PRO:HB2	11	1.09
(1,322)	2:629:B:VAL:HG21	1:44:A:LEU:HD22	6	1.09
(1,2666)	2:591:B:VAL:HG12	2:658:B:TRP:HE3	8	1.08
(1,2577)	2:630:B:ILE:HD12	2:681:B:ASP:HB2	14	1.08
(1,2525)	2:611:B:ILE:HG21	1:37:A:TRP:HZ3	12	1.08
(1,2358)	2:616:B:VAL:HG13	2:617:B:GLU:HB3	14	1.08
(1,1352)	1:47:A:SER:HA	1:48:A:GLN:HG3	11	1.08
(1,1308)	2:579:B:SER:HB2	1:39:A:SER:HG	13	1.08
(1,1308)	2:579:B:SER:HB2	1:39:A:SER:HG	15	1.08
(1,322)	2:629:B:VAL:HG21	1:44:A:LEU:HD22	9	1.08
(1,152)	2:595:B:LYS:HG2	2:658:B:TRP:HB3	9	1.08
(1,1583)	2:596:B:THR:H	2:652:B:PHE:HZ	14	1.07
(1,501)	2:677:B:LEU:HD13	2:630:B:ILE:HG22	4	1.07
(1,2666)	2:591:B:VAL:HG13	2:658:B:TRP:HE3	12	1.06
(1,2622)	2:587:B:GLU:HB2	2:583:B:LEU:HD12	3	1.06
(1,2577)	2:630:B:ILE:HD12	2:681:B:ASP:HB2	15	1.06
(1,2457)	2:674:B:CYS:HB3	2:666:B:THR:HA	15	1.06
(1,2454)	2:674:B:CYS:HB2	2:666:B:THR:HA	10	1.06
(1,2270)	2:641:B:VAL:HG13	1:44:A:LEU:HD12	8	1.06
(1,1057)	2:650:B:PRO:HG2	2:666:B:THR:HG23	4	1.06
(1,977)	2:574:B:TYR:HB2	1:40:A:LEU:HD23	14	1.06
(1,510)	2:682:B:VAL:HG21	2:613:B:SER:HB2	14	1.06
(1,489)	2:674:B:CYS:HB3	2:663:B:PRO:HB2	15	1.06
(1,8)	2:568:B:PRO:HB3	2:569:B:PRO:HD3	4	1.06
(1,2942)	2:663:B:PRO:HG3	1:40:A:LEU:HB2	4	1.05
(1,2397)	2:629:B:VAL:HG21	2:641:B:VAL:HA	13	1.05
(1,1583)	2:596:B:THR:H	2:652:B:PHE:HZ	1	1.05
(1,322)	2:629:B:VAL:HG23	1:44:A:LEU:HD23	2	1.05
(1,322)	2:629:B:VAL:HG23	1:44:A:LEU:HD23	14	1.05
(1,8)	2:568:B:PRO:HB3	2:569:B:PRO:HD3	1	1.05
(1,8)	2:568:B:PRO:HB3	2:569:B:PRO:HD3	13	1.05
(1,2320)	2:617:B:GLU:HG3	2:679:B:VAL:HG13	4	1.04
(1,2272)	2:641:B:VAL:HG12	1:44:A:LEU:HB3	11	1.04
(1,2218)	2:666:B:THR:HG22	1:39:A:SER:HG	14	1.04
(1,1308)	2:579:B:SER:HB2	1:39:A:SER:HG	5	1.04
(1,1255)	2:672:B:LEU:HD13	2:592:B:GLU:HA	5	1.04
(1,977)	2:574:B:TYR:HB2	1:40:A:LEU:HD22	15	1.04
(1,523)	2:680:B:GLY:HA3	2:679:B:VAL:HG21	4	1.04
(1,2272)	2:641:B:VAL:HG13	1:44:A:LEU:HB3	8	1.03
(1,1560)	2:592:B:GLU:H	2:672:B:LEU:HD13	9	1.03
(1,1541)	2:590:B:LYS:H	2:589:B:LYS:HE2	3	1.03

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1309)	2:579:B:SER:HB3	1:39:A:SER:HG	5	1.03
(1,977)	2:574:B:TYR:HB2	1:40:A:LEU:HD23	2	1.03
(1,2666)	2:591:B:VAL:HG12	2:658:B:TRP:HE3	4	1.02
(1,2666)	2:591:B:VAL:HG12	2:658:B:TRP:HE3	10	1.02
(1,2666)	2:591:B:VAL:HG12	2:658:B:TRP:HE3	11	1.02
(1,2397)	2:629:B:VAL:HG21	2:641:B:VAL:HA	12	1.02
(1,2358)	2:616:B:VAL:HG13	2:617:B:GLU:HB3	3	1.02
(1,2358)	2:616:B:VAL:HG12	2:617:B:GLU:HB3	7	1.02
(1,1403)	1:41:A:VAL:HG23	1:39:A:SER:H	7	1.02
(1,1256)	2:592:B:GLU:HA	2:591:B:VAL:HG23	8	1.02
(1,977)	2:574:B:TYR:HB2	1:40:A:LEU:HD21	12	1.02
(1,152)	2:595:B:LYS:HG2	2:658:B:TRP:HB3	5	1.02
(1,2942)	2:663:B:PRO:HG3	1:40:A:LEU:HB2	15	1.01
(1,2930)	2:573:B:PRO:HB3	1:39:A:SER:HG	7	1.01
(1,2674)	2:571:B:LEU:HD13	2:568:B:PRO:HG2	14	1.01
(1,2666)	2:591:B:VAL:HG12	2:658:B:TRP:HE3	7	1.01
(1,2622)	2:587:B:GLU:HB2	2:583:B:LEU:HD13	13	1.01
(1,2397)	2:629:B:VAL:HG22	2:641:B:VAL:HA	5	1.01
(1,2358)	2:616:B:VAL:HG12	2:617:B:GLU:HB3	6	1.01
(1,2320)	2:617:B:GLU:HG3	2:679:B:VAL:HG22	8	1.01
(1,2320)	2:617:B:GLU:HG3	2:679:B:VAL:HG23	11	1.01
(1,2317)	2:587:B:GLU:HB3	2:589:B:LYS:HG3	11	1.01
(1,1468)	2:580:B:ILE:H	2:580:B:ILE:HG13	15	1.01
(1,1429)	2:576:B:MET:H	2:575:B:PHE:HZ	15	1.01
(1,977)	2:574:B:TYR:HB2	1:40:A:LEU:HD21	11	1.01
(1,404)	2:648:B:GLU:HG3	2:669:B:LEU:HD11	1	1.01
(1,322)	2:629:B:VAL:HG21	1:44:A:LEU:HD21	3	1.01
(1,8)	2:568:B:PRO:HB3	2:569:B:PRO:HD3	10	1.01
(1,2926)	2:682:B:VAL:HG11	1:44:A:LEU:HB2	1	1.0
(1,2926)	2:682:B:VAL:HG13	1:44:A:LEU:HB2	9	1.0
(1,2457)	2:674:B:CYS:HB3	2:667:B:SER:HA	5	1.0
(1,1353)	1:44:A:LEU:HA	1:44:A:LEU:HD12	4	1.0
(1,801)	2:680:B:GLY:HA3	2:615:B:THR:HG21	14	1.0
(1,394)	2:646:B:LEU:HD21	2:646:B:LEU:HA	3	1.0
(1,322)	2:629:B:VAL:HG21	1:44:A:LEU:HD23	8	1.0
(1,2397)	2:629:B:VAL:HG21	2:641:B:VAL:HA	9	0.99
(1,1583)	2:596:B:THR:H	2:652:B:PHE:HZ	12	0.99
(1,1429)	2:576:B:MET:H	2:575:B:PHE:HZ	2	0.99
(1,1429)	2:576:B:MET:H	2:575:B:PHE:HZ	3	0.99
(1,1429)	2:576:B:MET:H	2:575:B:PHE:HZ	11	0.99
(1,1113)	2:674:B:CYS:HA	2:663:B:PRO:HB2	10	0.99
(1,977)	2:574:B:TYR:HB2	1:40:A:LEU:HD22	1	0.99

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,489)	2:674:B:CYS:HB3	2:663:B:PRO:HB2	6	0.99
(1,2930)	2:573:B:PRO:HB3	1:39:A:SER:HG	5	0.98
(1,2454)	2:674:B:CYS:HB2	2:677:B:LEU:HA	5	0.98
(1,2207)	2:674:B:CYS:HB2	1:40:A:LEU:HB2	5	0.98
(1,1429)	2:576:B:MET:H	2:575:B:PHE:HZ	6	0.98
(1,1429)	2:576:B:MET:H	2:575:B:PHE:HZ	7	0.98
(1,1429)	2:576:B:MET:H	2:575:B:PHE:HZ	12	0.98
(1,1429)	2:576:B:MET:H	2:575:B:PHE:HZ	13	0.98
(1,1113)	2:674:B:CYS:HA	2:663:B:PRO:HB2	8	0.98
(1,931)	2:639:B:ALA:HB2	2:634:B:VAL:HG23	4	0.98
(1,552)	2:686:B:LEU:HD13	2:611:B:ILE:HA	10	0.98
(1,552)	2:686:B:LEU:HD12	2:611:B:ILE:HA	14	0.98
(1,322)	2:629:B:VAL:HG23	1:44:A:LEU:HD22	11	0.98
(1,103)	2:672:B:LEU:HD11	2:672:B:LEU:HA	9	0.98
(1,22)	2:571:B:LEU:HD23	2:571:B:LEU:HA	1	0.98
(1,8)	2:568:B:PRO:HB3	2:569:B:PRO:HD3	12	0.98
(1,2942)	2:688:B:LEU:HG	1:40:A:LEU:HB2	2	0.97
(1,2666)	2:591:B:VAL:HG13	2:658:B:TRP:HE3	14	0.97
(1,2622)	2:587:B:GLU:HB2	2:583:B:LEU:HD12	15	0.97
(1,2577)	2:630:B:ILE:HD13	2:681:B:ASP:HB2	2	0.97
(1,2525)	2:611:B:ILE:HG21	1:37:A:TRP:HZ3	5	0.97
(1,2525)	2:611:B:ILE:HG22	1:37:A:TRP:HZ3	13	0.97
(1,2267)	2:643:B:VAL:HG23	1:44:A:LEU:HD13	7	0.97
(1,1429)	2:576:B:MET:H	2:575:B:PHE:HZ	5	0.97
(1,1403)	1:41:A:VAL:HG22	1:39:A:SER:H	12	0.97
(1,977)	2:574:B:TYR:HB2	1:40:A:LEU:HD22	6	0.97
(1,425)	2:654:B:PHE:HB3	2:682:B:VAL:HG21	2	0.97
(1,204)	2:609:B:LEU:HD13	2:688:B:LEU:HA	3	0.97
(1,2271)	2:641:B:VAL:HG13	1:44:A:LEU:HD22	4	0.96
(1,1774)	2:621:B:ASP:H	2:620:B:GLU:HB2	5	0.96
(1,1774)	2:621:B:ASP:H	2:620:B:GLU:HB2	13	0.96
(1,1709)	2:614:B:SER:H	2:682:B:VAL:HG22	5	0.96
(1,1429)	2:576:B:MET:H	2:575:B:PHE:HZ	10	0.96
(1,1288)	2:581:B:ILE:HG21	1:34:A:VAL:HA	9	0.96
(1,977)	2:574:B:TYR:HB2	1:40:A:LEU:HD23	3	0.96
(1,977)	2:574:B:TYR:HB2	1:40:A:LEU:HD21	7	0.96
(1,977)	2:574:B:TYR:HB2	1:40:A:LEU:HD23	13	0.96
(1,797)	2:660:B:SER:HB2	1:40:A:LEU:HA	15	0.96
(1,642)	2:683:B:CYS:HB2	2:651:B:PHE:HB2	7	0.96
(1,64)	2:587:B:GLU:HB2	2:583:B:LEU:HD12	8	0.96
(1,2926)	2:653:B:VAL:HG11	1:44:A:LEU:HB2	11	0.95
(1,2622)	2:587:B:GLU:HB2	2:583:B:LEU:HD12	6	0.95

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1583)	2:596:B:THR:H	2:652:B:PHE:HZ	4	0.95
(1,1583)	2:596:B:THR:H	2:652:B:PHE:HZ	11	0.95
(1,1518)	2:587:B:GLU:H	2:587:B:GLU:HB2	8	0.95
(1,1353)	1:44:A:LEU:HA	1:44:A:LEU:HD12	1	0.95
(1,641)	2:683:B:CYS:HB3	2:651:B:PHE:HB2	9	0.95
(1,8)	2:568:B:PRO:HB3	2:569:B:PRO:HD3	9	0.95
(2,6)	2:590:B:LYS:HD2	2:589:B:LYS:HA	11	0.94
(1,2622)	2:587:B:GLU:HB2	2:583:B:LEU:HD13	10	0.94
(1,2320)	2:617:B:GLU:HG3	2:679:B:VAL:HG22	13	0.94
(1,1518)	2:587:B:GLU:H	2:587:B:GLU:HB2	6	0.94
(1,1429)	2:576:B:MET:H	2:575:B:PHE:HZ	1	0.94
(1,1168)	2:686:B:LEU:HD13	2:609:B:LEU:HB2	8	0.94
(1,977)	2:574:B:TYR:HB2	1:40:A:LEU:HD22	8	0.94
(1,2942)	2:688:B:LEU:HG	1:40:A:LEU:HB2	14	0.93
(1,2525)	2:611:B:ILE:HG22	1:37:A:TRP:HZ3	6	0.93
(1,2320)	2:617:B:GLU:HG3	2:679:B:VAL:HG23	15	0.93
(1,2269)	2:629:B:VAL:HG21	1:44:A:LEU:HB2	13	0.93
(1,1518)	2:587:B:GLU:H	2:587:B:GLU:HB2	3	0.93
(1,1518)	2:587:B:GLU:H	2:587:B:GLU:HB2	10	0.93
(1,1518)	2:587:B:GLU:H	2:587:B:GLU:HB2	15	0.93
(1,1429)	2:576:B:MET:H	2:575:B:PHE:HZ	4	0.93
(1,1308)	2:579:B:SER:HB2	1:39:A:SER:HG	3	0.93
(1,977)	2:574:B:TYR:HB2	1:40:A:LEU:HD21	4	0.93
(1,801)	2:680:B:GLY:HA3	2:615:B:THR:HG21	2	0.93
(1,801)	2:680:B:GLY:HA3	2:615:B:THR:HG23	9	0.93
(1,487)	2:674:B:CYS:HB2	2:659:B:SER:HA	15	0.93
(1,204)	2:609:B:LEU:HD12	2:688:B:LEU:HA	1	0.93
(1,2942)	2:688:B:LEU:HG	1:40:A:LEU:HB2	12	0.92
(1,2926)	2:653:B:VAL:HG12	1:44:A:LEU:HB2	4	0.92
(1,2397)	2:629:B:VAL:HG21	2:641:B:VAL:HA	10	0.92
(1,2320)	2:617:B:GLU:HG3	2:679:B:VAL:HG22	2	0.92
(1,2218)	2:666:B:THR:HG21	1:39:A:SER:HG	8	0.92
(1,2082)	2:670:B:PHE:H	2:575:B:PHE:HZ	10	0.92
(1,1709)	2:614:B:SER:H	2:682:B:VAL:HG23	2	0.92
(1,1518)	2:587:B:GLU:H	2:587:B:GLU:HB2	11	0.92
(1,1468)	2:580:B:ILE:H	2:580:B:ILE:HG13	2	0.92
(1,797)	2:660:B:SER:HB2	1:40:A:LEU:HA	11	0.92
(1,423)	2:654:B:PHE:HB2	2:682:B:VAL:HG21	14	0.92
(1,2622)	2:587:B:GLU:HB2	2:583:B:LEU:HD11	4	0.91
(1,2320)	2:617:B:GLU:HG3	2:679:B:VAL:HG23	10	0.91
(1,2082)	2:670:B:PHE:H	2:575:B:PHE:HZ	8	0.91
(1,2045)	2:664:B:GLU:H	2:664:B:GLU:HG2	7	0.91

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1583)	2:596:B:THR:H	2:652:B:PHE:HZ	15	0.91
(1,1429)	2:576:B:MET:H	2:575:B:PHE:HZ	14	0.91
(1,1113)	2:674:B:CYS:HA	2:663:B:PRO:HB2	2	0.91
(1,977)	2:574:B:TYR:HB2	1:40:A:LEU:HD21	9	0.91
(1,642)	2:683:B:CYS:HB2	2:651:B:PHE:HB2	4	0.91
(1,2942)	2:688:B:LEU:HG	1:40:A:LEU:HB2	1	0.9
(1,2942)	2:688:B:LEU:HG	1:40:A:LEU:HB2	11	0.9
(1,2577)	2:630:B:ILE:HD11	2:681:B:ASP:HB2	8	0.9
(1,2272)	2:641:B:VAL:HG11	1:44:A:LEU:HB3	1	0.9
(1,2272)	2:641:B:VAL:HG13	1:44:A:LEU:HB3	9	0.9
(1,2045)	2:664:B:GLU:H	2:664:B:GLU:HG3	1	0.9
(1,1583)	2:596:B:THR:H	2:652:B:PHE:HZ	6	0.9
(1,1468)	2:580:B:ILE:H	2:580:B:ILE:HG13	1	0.9
(1,1288)	2:581:B:ILE:HG21	1:34:A:VAL:HA	10	0.9
(1,801)	2:680:B:GLY:HA3	2:615:B:THR:HG22	7	0.9
(1,322)	2:629:B:VAL:HG21	1:44:A:LEU:HD21	13	0.9
(2,6)	2:590:B:LYS:HD2	2:589:B:LYS:HA	2	0.89
(1,2930)	2:576:B:MET:HB3	1:39:A:SER:HG	1	0.89
(1,2457)	2:674:B:CYS:HB3	2:667:B:SER:HA	4	0.89
(1,2272)	2:641:B:VAL:HG11	1:44:A:LEU:HB3	3	0.89
(1,1709)	2:614:B:SER:H	2:682:B:VAL:HG23	1	0.89
(1,1429)	2:576:B:MET:H	2:575:B:PHE:HZ	8	0.89
(1,1308)	2:579:B:SER:HB2	1:39:A:SER:HG	10	0.89
(1,1288)	2:581:B:ILE:HG23	1:34:A:VAL:HA	1	0.89
(1,801)	2:680:B:GLY:HA3	2:615:B:THR:HG23	11	0.89
(1,552)	2:686:B:LEU:HD13	2:611:B:ILE:HA	2	0.89
(1,515)	2:679:B:VAL:HG13	2:618:B:ARG:HA	11	0.89
(2,6)	2:590:B:LYS:HD2	2:589:B:LYS:HA	8	0.88
(2,6)	2:590:B:LYS:HD2	2:589:B:LYS:HA	10	0.88
(1,1774)	2:621:B:ASP:H	2:620:B:GLU:HB2	10	0.88
(1,1698)	2:610:B:LYS:H	2:609:B:LEU:HD12	13	0.88
(1,1583)	2:596:B:THR:H	2:652:B:PHE:HZ	7	0.88
(1,1541)	2:590:B:LYS:H	2:589:B:LYS:HE2	10	0.88
(1,1518)	2:587:B:GLU:H	2:587:B:GLU:HB2	4	0.88
(1,1518)	2:587:B:GLU:H	2:587:B:GLU:HB2	13	0.88
(1,1468)	2:580:B:ILE:H	2:580:B:ILE:HG13	4	0.88
(1,1288)	2:581:B:ILE:HG23	1:34:A:VAL:HA	15	0.88
(1,1113)	2:674:B:CYS:HA	2:663:B:PRO:HB2	5	0.88
(1,977)	2:574:B:TYR:HB2	1:40:A:LEU:HD22	10	0.88
(1,801)	2:680:B:GLY:HA3	2:615:B:THR:HG22	15	0.88
(1,642)	2:683:B:CYS:HB2	2:651:B:PHE:HB2	6	0.88
(1,2930)	2:573:B:PRO:HB3	1:39:A:SER:HG	11	0.87

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2353)	2:609:B:LEU:HD12	1:38:A:HIS:H	4	0.87
(1,2209)	2:576:B:MET:HB2	1:39:A:SER:HG	14	0.87
(1,1583)	2:596:B:THR:H	2:652:B:PHE:HZ	13	0.87
(1,1468)	2:580:B:ILE:H	2:580:B:ILE:HG13	5	0.87
(1,1216)	2:681:B:ASP:HB2	2:677:B:LEU:HD21	5	0.87
(1,152)	2:595:B:LYS:HG2	2:658:B:TRP:HB3	13	0.87
(2,6)	2:590:B:LYS:HD2	2:589:B:LYS:HA	3	0.86
(1,2385)	2:656:B:GLN:HG2	2:682:B:VAL:HA	12	0.86
(1,2272)	2:641:B:VAL:HG13	1:44:A:LEU:HB3	4	0.86
(1,1605)	2:598:B:ASP:H	2:597:B:GLU:HG2	8	0.86
(1,1583)	2:596:B:THR:H	2:652:B:PHE:HZ	3	0.86
(1,1468)	2:580:B:ILE:H	2:580:B:ILE:HG13	6	0.86
(1,1468)	2:580:B:ILE:H	2:580:B:ILE:HG13	12	0.86
(2,6)	2:590:B:LYS:HD2	2:589:B:LYS:HA	6	0.85
(2,2)	2:595:B:LYS:HD2	2:658:B:TRP:HB3	8	0.85
(1,2804)	2:619:B:ILE:H	2:679:B:VAL:HG13	5	0.85
(1,2519)	2:608:B:ASP:HB3	2:688:B:LEU:HD21	4	0.85
(1,2082)	2:670:B:PHE:H	2:575:B:PHE:HZ	9	0.85
(1,1774)	2:621:B:ASP:H	2:620:B:GLU:HB2	1	0.85
(1,1774)	2:621:B:ASP:H	2:620:B:GLU:HB2	9	0.85
(1,1774)	2:621:B:ASP:H	2:620:B:GLU:HB2	14	0.85
(1,1774)	2:621:B:ASP:H	2:620:B:GLU:HB2	15	0.85
(1,1605)	2:598:B:ASP:H	2:597:B:GLU:HG2	12	0.85
(1,1353)	1:44:A:LEU:HA	1:44:A:LEU:HD12	13	0.85
(1,1353)	1:44:A:LEU:HA	1:44:A:LEU:HD11	15	0.85
(1,1288)	2:581:B:ILE:HG21	1:34:A:VAL:HA	11	0.85
(1,801)	2:680:B:GLY:HA3	2:615:B:THR:HG22	4	0.85
(1,553)	2:686:B:LEU:HD12	2:686:B:LEU:HA	8	0.85
(1,420)	2:654:B:PHE:HB2	2:682:B:VAL:HB	11	0.85
(2,6)	2:590:B:LYS:HD2	2:589:B:LYS:HA	7	0.84
(1,2942)	2:663:B:PRO:HG3	1:40:A:LEU:HB2	13	0.84
(1,2525)	2:611:B:ILE:HG23	1:37:A:TRP:HZ3	7	0.84
(1,2082)	2:670:B:PHE:H	2:575:B:PHE:HZ	11	0.84
(1,1774)	2:621:B:ASP:H	2:620:B:GLU:HB2	8	0.84
(1,1605)	2:598:B:ASP:H	2:597:B:GLU:HG2	10	0.84
(1,801)	2:680:B:GLY:HA3	2:615:B:THR:HG23	1	0.84
(1,552)	2:686:B:LEU:HD13	2:611:B:ILE:HA	3	0.84
(1,416)	2:653:B:VAL:HB	2:656:B:GLN:HB3	4	0.84
(1,8)	2:568:B:PRO:HB3	2:569:B:PRO:HD3	8	0.84
(1,8)	2:568:B:PRO:HB3	2:569:B:PRO:HD3	11	0.84
(1,2654)	2:674:B:CYS:HB2	2:676:B:LYS:HD3	11	0.83
(1,1698)	2:610:B:LYS:H	2:609:B:LEU:HD11	7	0.83

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1698)	2:610:B:LYS:H	2:609:B:LEU:HD13	12	0.83
(1,1583)	2:596:B:THR:H	2:652:B:PHE:HZ	8	0.83
(1,1468)	2:580:B:ILE:H	2:580:B:ILE:HG13	10	0.83
(1,996)	2:647:B:VAL:HG22	2:625:B:PRO:HA	11	0.83
(1,801)	2:680:B:GLY:HA3	2:615:B:THR:HG22	12	0.83
(1,797)	2:660:B:SER:HB2	1:40:A:LEU:HA	7	0.83
(1,257)	2:617:B:GLU:HG3	2:615:B:THR:HG22	2	0.83
(1,64)	2:587:B:GLU:HB2	2:583:B:LEU:HD12	3	0.83
(1,2654)	2:674:B:CYS:HB2	2:676:B:LYS:HD3	1	0.82
(1,2490)	2:625:B:PRO:HB3	2:623:B:HIS:HA	12	0.82
(1,2272)	2:641:B:VAL:HG12	1:44:A:LEU:HB3	15	0.82
(1,2082)	2:670:B:PHE:H	2:575:B:PHE:HZ	12	0.82
(1,1928)	2:645:B:VAL:H	2:645:B:VAL:HG11	4	0.82
(1,1541)	2:590:B:LYS:H	2:589:B:LYS:HE2	2	0.82
(1,1468)	2:580:B:ILE:H	2:580:B:ILE:HG13	7	0.82
(1,1468)	2:580:B:ILE:H	2:580:B:ILE:HG13	8	0.82
(1,1468)	2:580:B:ILE:H	2:580:B:ILE:HG13	11	0.82
(1,1353)	1:44:A:LEU:HA	1:44:A:LEU:HD12	3	0.82
(1,515)	2:679:B:VAL:HG12	2:618:B:ARG:HA	6	0.82
(1,515)	2:679:B:VAL:HG11	2:618:B:ARG:HA	12	0.82
(1,8)	2:568:B:PRO:HB3	2:569:B:PRO:HD3	6	0.82
(1,2209)	2:576:B:MET:HB2	1:39:A:SER:HG	4	0.81
(1,1774)	2:621:B:ASP:H	2:620:B:GLU:HB2	7	0.81
(1,1605)	2:598:B:ASP:H	2:597:B:GLU:HG2	2	0.81
(1,1541)	2:590:B:LYS:H	2:589:B:LYS:HE2	5	0.81
(1,1468)	2:580:B:ILE:H	2:580:B:ILE:HG13	14	0.81
(1,1403)	1:41:A:VAL:HG22	1:39:A:SER:H	4	0.81
(1,1353)	1:44:A:LEU:HA	1:44:A:LEU:HD12	2	0.81
(1,641)	2:683:B:CYS:HB3	2:651:B:PHE:HB2	2	0.81
(1,1928)	2:645:B:VAL:H	2:645:B:VAL:HG12	8	0.8
(1,1709)	2:614:B:SER:H	2:682:B:VAL:HG23	14	0.8
(1,1468)	2:580:B:ILE:H	2:580:B:ILE:HG13	3	0.8
(1,1309)	2:579:B:SER:HB3	1:39:A:SER:HG	3	0.8
(1,996)	2:647:B:VAL:HG22	2:625:B:PRO:HA	9	0.8
(1,801)	2:680:B:GLY:HA3	2:615:B:THR:HG22	8	0.8
(1,510)	2:682:B:VAL:HG21	2:613:B:SER:HB2	6	0.8
(2,6)	2:590:B:LYS:HD2	2:589:B:LYS:HA	14	0.79
(1,2926)	2:653:B:VAL:HG13	1:44:A:LEU:HB2	8	0.79
(1,2222)	2:686:B:LEU:HD21	1:38:A:HIS:HB2	3	0.79
(1,1774)	2:621:B:ASP:H	2:620:B:GLU:HB2	3	0.79
(1,1429)	2:576:B:MET:H	2:575:B:PHE:HZ	9	0.79
(1,1288)	2:581:B:ILE:HG22	1:34:A:VAL:HA	2	0.79

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1288)	2:581:B:ILE:HG21	1:34:A:VAL:HA	3	0.79
(1,801)	2:680:B:GLY:HA3	2:615:B:THR:HG21	6	0.79
(1,641)	2:683:B:CYS:HB3	2:651:B:PHE:HB2	5	0.79
(1,553)	2:686:B:LEU:HD13	2:686:B:LEU:HA	1	0.79
(1,257)	2:617:B:GLU:HG3	2:615:B:THR:HG23	4	0.79
(1,8)	2:568:B:PRO:HB3	2:569:B:PRO:HD3	2	0.79
(1,2942)	2:688:B:LEU:HG	1:40:A:LEU:HB2	7	0.78
(1,2942)	2:688:B:LEU:HG	1:40:A:LEU:HB2	9	0.78
(1,2866)	2:661:B:CYS:H	2:674:B:CYS:HB2	1	0.78
(1,2866)	2:651:B:PHE:H	2:674:B:CYS:HB2	11	0.78
(1,2454)	2:674:B:CYS:HB2	2:666:B:THR:HA	2	0.78
(1,2269)	2:629:B:VAL:HG21	1:44:A:LEU:HB2	15	0.78
(1,1774)	2:621:B:ASP:H	2:620:B:GLU:HB2	2	0.78
(1,1605)	2:598:B:ASP:H	2:597:B:GLU:HG2	3	0.78
(1,1559)	2:592:B:GLU:H	2:591:B:VAL:HG21	6	0.78
(1,1518)	2:587:B:GLU:H	2:587:B:GLU:HB2	9	0.78
(1,1353)	1:44:A:LEU:HA	1:44:A:LEU:HD12	14	0.78
(1,1251)	2:594:B:LEU:HD13	2:658:B:TRP:HZ2	10	0.78
(1,996)	2:647:B:VAL:HG23	2:625:B:PRO:HA	8	0.78
(1,931)	2:639:B:ALA:HB2	2:634:B:VAL:HG21	15	0.78
(1,801)	2:680:B:GLY:HA3	2:615:B:THR:HG23	5	0.78
(1,404)	2:648:B:GLU:HG3	2:669:B:LEU:HD13	2	0.78
(1,64)	2:587:B:GLU:HB2	2:583:B:LEU:HD13	13	0.78
(2,6)	2:590:B:LYS:HD2	2:589:B:LYS:HA	5	0.77
(1,2930)	2:573:B:PRO:HB3	1:39:A:SER:HG	2	0.77
(1,2666)	2:591:B:VAL:HG11	2:658:B:TRP:HE3	5	0.77
(1,2082)	2:670:B:PHE:H	2:575:B:PHE:HZ	1	0.77
(1,2082)	2:670:B:PHE:H	2:575:B:PHE:HZ	6	0.77
(1,1544)	2:590:B:LYS:H	2:590:B:LYS:HG2	9	0.77
(1,1113)	2:674:B:CYS:HA	2:663:B:PRO:HB2	4	0.77
(1,487)	2:674:B:CYS:HB2	2:659:B:SER:HA	9	0.77
(1,487)	2:674:B:CYS:HB2	2:659:B:SER:HA	11	0.77
(1,420)	2:654:B:PHE:HB2	2:682:B:VAL:HB	8	0.77
(1,2675)	2:571:B:LEU:HD23	2:569:B:PRO:HB3	2	0.76
(1,2454)	2:674:B:CYS:HB2	2:666:B:THR:HA	8	0.76
(1,2388)	2:628:B:ALA:HB1	2:629:B:VAL:HA	14	0.76
(1,2082)	2:670:B:PHE:H	2:575:B:PHE:HZ	5	0.76
(1,1774)	2:621:B:ASP:H	2:620:B:GLU:HB2	12	0.76
(1,1353)	1:44:A:LEU:HA	1:44:A:LEU:HD13	7	0.76
(1,1288)	2:581:B:ILE:HG23	1:34:A:VAL:HA	14	0.76
(1,996)	2:647:B:VAL:HG23	2:625:B:PRO:HA	12	0.76
(1,801)	2:680:B:GLY:HA3	2:615:B:THR:HG23	13	0.76

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,552)	2:686:B:LEU:HD12	2:611:B:ILE:HA	6	0.76
(1,513)	2:679:B:VAL:HG12	2:616:B:VAL:HG21	11	0.76
(1,2942)	2:688:B:LEU:HG	1:40:A:LEU:HB2	3	0.75
(1,2866)	2:651:B:PHE:H	2:674:B:CYS:HB2	9	0.75
(1,2209)	2:576:B:MET:HB2	1:39:A:SER:HG	8	0.75
(1,1709)	2:614:B:SER:H	2:682:B:VAL:HG21	9	0.75
(1,1605)	2:598:B:ASP:H	2:597:B:GLU:HG2	9	0.75
(1,1583)	2:596:B:THR:H	2:652:B:PHE:HZ	2	0.75
(1,1559)	2:592:B:GLU:H	2:591:B:VAL:HG22	14	0.75
(1,1403)	1:41:A:VAL:HG21	1:39:A:SER:H	15	0.75
(1,1353)	1:44:A:LEU:HA	1:44:A:LEU:HD13	8	0.75
(1,1288)	2:581:B:ILE:HG21	1:34:A:VAL:HA	8	0.75
(1,1113)	2:674:B:CYS:HA	2:663:B:PRO:HB2	13	0.75
(1,1109)	2:672:B:LEU:HG	2:673:B:PRO:HD3	4	0.75
(1,996)	2:647:B:VAL:HG21	2:625:B:PRO:HA	4	0.75
(1,996)	2:647:B:VAL:HG21	2:625:B:PRO:HA	15	0.75
(1,977)	2:574:B:TYR:HB2	1:40:A:LEU:HD22	5	0.75
(1,641)	2:683:B:CYS:HB3	2:651:B:PHE:HB2	10	0.75
(1,8)	2:568:B:PRO:HB3	2:569:B:PRO:HD3	15	0.75
(2,6)	2:590:B:LYS:HD2	2:589:B:LYS:HA	12	0.74
(1,2388)	2:628:B:ALA:HB1	2:629:B:VAL:HA	1	0.74
(1,1605)	2:598:B:ASP:H	2:597:B:GLU:HG2	7	0.74
(1,1559)	2:592:B:GLU:H	2:591:B:VAL:HG23	3	0.74
(1,1353)	1:44:A:LEU:HA	1:44:A:LEU:HD12	6	0.74
(1,1353)	1:44:A:LEU:HA	1:44:A:LEU:HD13	9	0.74
(1,1288)	2:581:B:ILE:HG21	1:34:A:VAL:HA	5	0.74
(1,1073)	2:579:B:SER:HB3	2:581:B:ILE:HD12	15	0.74
(1,996)	2:647:B:VAL:HG22	2:625:B:PRO:HA	14	0.74
(1,801)	2:680:B:GLY:HA3	2:615:B:THR:HG22	3	0.74
(1,513)	2:679:B:VAL:HG11	2:616:B:VAL:HG21	6	0.74
(1,152)	2:595:B:LYS:HG2	2:658:B:TRP:HB3	12	0.74
(1,64)	2:587:B:GLU:HB2	2:583:B:LEU:HD12	15	0.74
(1,2866)	2:651:B:PHE:H	2:674:B:CYS:HB2	15	0.73
(1,2654)	2:674:B:CYS:HB2	2:676:B:LYS:HD3	9	0.73
(1,2630)	2:672:B:LEU:HB3	2:673:B:PRO:HD3	4	0.73
(1,2490)	2:656:B:GLN:HB2	2:682:B:VAL:HA	13	0.73
(1,2473)	2:688:B:LEU:HG	1:38:A:HIS:H	4	0.73
(1,2454)	2:674:B:CYS:HB2	2:666:B:THR:HA	12	0.73
(1,2388)	2:628:B:ALA:HB2	2:629:B:VAL:HA	7	0.73
(1,2388)	2:628:B:ALA:HB2	2:629:B:VAL:HA	12	0.73
(1,2171)	2:683:B:CYS:H	2:682:B:VAL:HG22	5	0.73
(1,2082)	2:670:B:PHE:H	2:575:B:PHE:HZ	7	0.73

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1774)	2:621:B:ASP:H	2:620:B:GLU:HB2	6	0.73
(1,1605)	2:598:B:ASP:H	2:597:B:GLU:HG2	5	0.73
(1,1543)	2:590:B:LYS:H	2:590:B:LYS:HB3	3	0.73
(1,1543)	2:590:B:LYS:H	2:590:B:LYS:HB3	6	0.73
(1,1113)	2:674:B:CYS:HA	2:663:B:PRO:HB2	3	0.73
(1,1113)	2:674:B:CYS:HA	2:663:B:PRO:HB2	7	0.73
(1,1113)	2:674:B:CYS:HA	2:663:B:PRO:HB2	14	0.73
(1,996)	2:647:B:VAL:HG22	2:625:B:PRO:HA	10	0.73
(1,896)	2:630:B:ILE:HD12	2:651:B:PHE:HE1	11	0.73
(1,801)	2:680:B:GLY:HA3	2:615:B:THR:HG21	10	0.73
(1,515)	2:679:B:VAL:HG13	2:618:B:ARG:HA	3	0.73
(1,513)	2:679:B:VAL:HG12	2:616:B:VAL:HG21	2	0.73
(1,404)	2:648:B:GLU:HG3	2:669:B:LEU:HD11	14	0.73
(1,322)	2:629:B:VAL:HG21	1:44:A:LEU:HD21	15	0.73
(1,64)	2:587:B:GLU:HB2	2:583:B:LEU:HD11	11	0.73
(1,2171)	2:683:B:CYS:H	2:682:B:VAL:HG23	1	0.72
(1,2152)	2:681:B:ASP:H	2:681:B:ASP:HB2	7	0.72
(1,1605)	2:598:B:ASP:H	2:597:B:GLU:HG2	1	0.72
(1,1559)	2:592:B:GLU:H	2:591:B:VAL:HG23	12	0.72
(1,1543)	2:590:B:LYS:H	2:590:B:LYS:HB3	5	0.72
(1,1543)	2:590:B:LYS:H	2:590:B:LYS:HB3	7	0.72
(1,1309)	2:579:B:SER:HB3	1:39:A:SER:HG	10	0.72
(1,1308)	2:579:B:SER:HB2	1:39:A:SER:HG	7	0.72
(1,996)	2:647:B:VAL:HG22	2:625:B:PRO:HA	3	0.72
(1,515)	2:679:B:VAL:HG11	2:618:B:ARG:HA	7	0.72
(1,513)	2:679:B:VAL:HG13	2:616:B:VAL:HG22	12	0.72
(1,487)	2:674:B:CYS:HB2	2:659:B:SER:HA	6	0.72
(1,404)	2:648:B:GLU:HG3	2:669:B:LEU:HD12	7	0.72
(1,85)	2:588:B:LEU:HD21	2:582:B:GLN:HB3	5	0.72
(1,64)	2:587:B:GLU:HB2	2:583:B:LEU:HD12	6	0.72
(1,22)	2:571:B:LEU:HD23	2:571:B:LEU:HA	2	0.72
(1,2846)	2:649:B:TYR:H	2:645:B:VAL:HB	5	0.71
(1,2738)	2:679:B:VAL:H	2:619:B:ILE:HG12	6	0.71
(1,2388)	2:628:B:ALA:HB1	2:629:B:VAL:HA	13	0.71
(1,2082)	2:670:B:PHE:H	2:575:B:PHE:HZ	4	0.71
(1,1988)	2:656:B:GLN:H	2:656:B:GLN:HB3	2	0.71
(1,1928)	2:645:B:VAL:H	2:645:B:VAL:HG13	6	0.71
(1,1605)	2:598:B:ASP:H	2:597:B:GLU:HG2	14	0.71
(1,1559)	2:592:B:GLU:H	2:591:B:VAL:HG21	2	0.71
(1,1543)	2:590:B:LYS:H	2:590:B:LYS:HB3	8	0.71
(1,1543)	2:590:B:LYS:H	2:590:B:LYS:HB3	9	0.71
(1,1543)	2:590:B:LYS:H	2:590:B:LYS:HB3	12	0.71

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1543)	2:590:B:LYS:H	2:590:B:LYS:HB3	14	0.71
(1,1468)	2:580:B:ILE:H	2:580:B:ILE:HG13	13	0.71
(1,1353)	1:44:A:LEU:HA	1:44:A:LEU:HD12	5	0.71
(1,1309)	2:579:B:SER:HB3	1:39:A:SER:HG	7	0.71
(1,1269)	2:672:B:LEU:HD23	2:575:B:PHE:HB2	5	0.71
(1,1216)	2:681:B:ASP:HB2	2:677:B:LEU:HD21	4	0.71
(1,1109)	2:672:B:LEU:HG	2:673:B:PRO:HD3	14	0.71
(1,996)	2:647:B:VAL:HG23	2:625:B:PRO:HA	1	0.71
(1,641)	2:683:B:CYS:HB3	2:651:B:PHE:HB2	8	0.71
(1,566)	2:688:B:LEU:HD23	1:38:A:HIS:H	11	0.71
(1,515)	2:679:B:VAL:HG13	2:618:B:ARG:HA	8	0.71
(1,515)	2:679:B:VAL:HG11	2:618:B:ARG:HA	10	0.71
(1,64)	2:587:B:GLU:HB2	2:583:B:LEU:HD13	10	0.71
(1,2942)	2:663:B:PRO:HG3	1:40:A:LEU:HB2	6	0.7
(1,2630)	2:672:B:LEU:HB3	2:673:B:PRO:HD3	7	0.7
(1,2490)	2:656:B:GLN:HB2	2:682:B:VAL:HA	6	0.7
(1,2457)	2:674:B:CYS:HB3	2:667:B:SER:HA	10	0.7
(1,2454)	2:674:B:CYS:HB2	2:666:B:THR:HA	14	0.7
(1,2082)	2:670:B:PHE:H	2:575:B:PHE:HZ	15	0.7
(1,1774)	2:621:B:ASP:H	2:620:B:GLU:HB2	4	0.7
(1,1605)	2:598:B:ASP:H	2:597:B:GLU:HG2	15	0.7
(1,1583)	2:596:B:THR:H	2:652:B:PHE:HZ	9	0.7
(1,1557)	2:592:B:GLU:H	2:590:B:LYS:HB2	15	0.7
(1,1543)	2:590:B:LYS:H	2:590:B:LYS:HB3	2	0.7
(1,996)	2:647:B:VAL:HG22	2:625:B:PRO:HA	5	0.7
(1,996)	2:647:B:VAL:HG22	2:625:B:PRO:HA	13	0.7
(1,896)	2:630:B:ILE:HD13	2:651:B:PHE:HE1	15	0.7
(1,642)	2:683:B:CYS:HB2	2:651:B:PHE:HB2	11	0.7
(1,513)	2:679:B:VAL:HG12	2:616:B:VAL:HG22	1	0.7
(1,416)	2:653:B:VAL:HB	2:656:B:GLN:HB3	14	0.7
(1,2930)	2:573:B:PRO:HB3	1:39:A:SER:HG	13	0.69
(1,2846)	2:649:B:TYR:H	2:645:B:VAL:HB	1	0.69
(1,2846)	2:649:B:TYR:H	2:645:B:VAL:HB	14	0.69
(1,2675)	2:571:B:LEU:HD23	2:572:B:PRO:HG2	14	0.69
(1,2388)	2:628:B:ALA:HB2	2:629:B:VAL:HA	6	0.69
(1,2388)	2:628:B:ALA:HB2	2:629:B:VAL:HA	9	0.69
(1,2209)	2:576:B:MET:HB2	1:39:A:SER:HG	9	0.69
(1,2171)	2:683:B:CYS:H	2:682:B:VAL:HG23	14	0.69
(1,2082)	2:670:B:PHE:H	2:575:B:PHE:HZ	2	0.69
(1,2082)	2:670:B:PHE:H	2:575:B:PHE:HZ	3	0.69
(1,1628)	2:600:B:ILE:H	2:600:B:ILE:HG12	7	0.69
(1,1628)	2:600:B:ILE:H	2:600:B:ILE:HG12	13	0.69

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1605)	2:598:B:ASP:H	2:597:B:GLU:HG2	4	0.69
(1,1605)	2:598:B:ASP:H	2:597:B:GLU:HG2	6	0.69
(1,1559)	2:592:B:GLU:H	2:591:B:VAL:HG22	5	0.69
(1,1543)	2:590:B:LYS:H	2:590:B:LYS:HB3	10	0.69
(1,1543)	2:590:B:LYS:H	2:590:B:LYS:HB3	11	0.69
(1,1543)	2:590:B:LYS:H	2:590:B:LYS:HB3	13	0.69
(1,1269)	2:672:B:LEU:HD22	2:575:B:PHE:HB2	8	0.69
(1,1113)	2:674:B:CYS:HA	2:663:B:PRO:HB2	15	0.69
(1,1073)	2:579:B:SER:HB3	2:581:B:ILE:HD12	13	0.69
(1,996)	2:647:B:VAL:HG23	2:625:B:PRO:HA	2	0.69
(1,931)	2:639:B:ALA:HB2	2:634:B:VAL:HG21	6	0.69
(1,515)	2:679:B:VAL:HG11	2:618:B:ARG:HA	13	0.69
(1,513)	2:679:B:VAL:HG12	2:616:B:VAL:HG23	8	0.69
(1,416)	2:653:B:VAL:HB	2:656:B:GLN:HB3	5	0.69
(1,404)	2:648:B:GLU:HG3	2:669:B:LEU:HD11	5	0.69
(1,8)	2:568:B:PRO:HB3	2:569:B:PRO:HD3	7	0.69
(1,2630)	2:672:B:LEU:HB3	2:673:B:PRO:HD3	6	0.68
(1,2272)	2:641:B:VAL:HG11	1:44:A:LEU:HB3	10	0.68
(1,2171)	2:683:B:CYS:H	2:682:B:VAL:HG23	2	0.68
(1,2171)	2:683:B:CYS:H	2:682:B:VAL:HG21	9	0.68
(1,2082)	2:670:B:PHE:H	2:575:B:PHE:HZ	13	0.68
(1,1628)	2:600:B:ILE:H	2:600:B:ILE:HG12	10	0.68
(1,1628)	2:600:B:ILE:H	2:600:B:ILE:HG12	12	0.68
(1,1605)	2:598:B:ASP:H	2:597:B:GLU:HG2	11	0.68
(1,1583)	2:596:B:THR:H	2:652:B:PHE:HZ	5	0.68
(1,996)	2:647:B:VAL:HG21	2:625:B:PRO:HA	6	0.68
(1,931)	2:639:B:ALA:HB1	2:634:B:VAL:HG21	11	0.68
(1,552)	2:686:B:LEU:HD12	2:611:B:ILE:HA	11	0.68
(1,404)	2:648:B:GLU:HG3	2:669:B:LEU:HD11	10	0.68
(1,245)	2:616:B:VAL:HG11	2:630:B:ILE:HG22	4	0.68
(1,64)	2:587:B:GLU:HB2	2:583:B:LEU:HD11	4	0.68
(1,2846)	2:649:B:TYR:H	2:645:B:VAL:HB	9	0.67
(1,2804)	2:619:B:ILE:H	2:679:B:VAL:HG13	9	0.67
(1,2804)	2:619:B:ILE:H	2:679:B:VAL:HG21	12	0.67
(1,2738)	2:679:B:VAL:H	2:619:B:ILE:HG12	1	0.67
(1,2622)	2:648:B:GLU:HG3	2:669:B:LEU:HD12	11	0.67
(1,2596)	2:574:B:TYR:HB3	2:581:B:ILE:HD11	12	0.67
(1,2517)	2:605:B:ILE:HG23	2:604:B:GLU:HB3	7	0.67
(1,2388)	2:628:B:ALA:HB3	2:629:B:VAL:HA	5	0.67
(1,2388)	2:628:B:ALA:HB3	2:629:B:VAL:HA	10	0.67
(1,2380)	2:620:B:GLU:HB3	2:629:B:VAL:HG22	8	0.67
(1,2209)	2:576:B:MET:HB2	1:39:A:SER:HG	11	0.67

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2200)	2:689:B:LYS:H	2:609:B:LEU:HD11	13	0.67
(1,1628)	2:600:B:ILE:H	2:600:B:ILE:HG12	6	0.67
(1,1543)	2:590:B:LYS:H	2:590:B:LYS:HB3	1	0.67
(1,1541)	2:590:B:LYS:H	2:589:B:LYS:HE2	1	0.67
(1,1288)	2:581:B:ILE:HG21	1:34:A:VAL:HA	6	0.67
(1,1109)	2:672:B:LEU:HG	2:673:B:PRO:HD3	7	0.67
(1,1057)	2:650:B:PRO:HG2	2:666:B:THR:HG21	6	0.67
(1,515)	2:679:B:VAL:HG13	2:618:B:ARG:HA	5	0.67
(1,404)	2:648:B:GLU:HG3	2:669:B:LEU:HD12	15	0.67
(1,192)	2:585:B:ASN:HB3	2:605:B:ILE:HD13	9	0.67
(1,149)	2:596:B:THR:H	2:595:B:LYS:HB2	10	0.67
(1,85)	2:588:B:LEU:HD23	2:582:B:GLN:HB3	9	0.67
(1,2866)	2:651:B:PHE:H	2:674:B:CYS:HB2	6	0.66
(1,2846)	2:649:B:TYR:H	2:645:B:VAL:HB	7	0.66
(1,2846)	2:649:B:TYR:H	2:645:B:VAL:HB	12	0.66
(1,2804)	2:619:B:ILE:H	2:679:B:VAL:HG13	1	0.66
(1,2630)	2:672:B:LEU:HB3	2:673:B:PRO:HD3	14	0.66
(1,2596)	2:574:B:TYR:HB3	2:581:B:ILE:HD11	3	0.66
(1,2517)	2:605:B:ILE:HG21	2:604:B:GLU:HB3	15	0.66
(1,2388)	2:628:B:ALA:HB2	2:629:B:VAL:HA	2	0.66
(1,2317)	2:587:B:GLU:HB3	2:589:B:LYS:HG3	3	0.66
(1,2200)	2:689:B:LYS:H	2:609:B:LEU:HD12	12	0.66
(1,1988)	2:656:B:GLN:H	2:656:B:GLN:HB3	1	0.66
(1,1928)	2:645:B:VAL:H	2:645:B:VAL:HG12	10	0.66
(1,1628)	2:600:B:ILE:H	2:600:B:ILE:HG12	2	0.66
(1,1628)	2:600:B:ILE:H	2:600:B:ILE:HG12	9	0.66
(1,1559)	2:592:B:GLU:H	2:591:B:VAL:HG21	11	0.66
(1,1070)	2:581:B:ILE:HD12	2:594:B:LEU:HD11	7	0.66
(1,797)	2:660:B:SER:HB2	1:40:A:LEU:HA	14	0.66
(1,591)	2:580:B:ILE:HD12	2:590:B:LYS:HE3	4	0.66
(1,513)	2:679:B:VAL:HG12	2:616:B:VAL:HG21	3	0.66
(1,513)	2:679:B:VAL:HG12	2:616:B:VAL:HG23	5	0.66
(1,487)	2:674:B:CYS:HB2	2:659:B:SER:HA	1	0.66
(1,2930)	2:573:B:PRO:HB3	1:39:A:SER:HG	6	0.65
(1,2388)	2:628:B:ALA:HB3	2:629:B:VAL:HA	4	0.65
(1,1583)	2:596:B:THR:H	2:652:B:PHE:HZ	10	0.65
(1,1353)	1:44:A:LEU:HA	1:44:A:LEU:HD13	11	0.65
(1,1353)	1:44:A:LEU:HA	1:44:A:LEU:HD13	12	0.65
(1,1222)	2:601:B:GLN:HG3	2:605:B:ILE:HD12	14	0.65
(1,1070)	2:581:B:ILE:HD12	2:594:B:LEU:HD12	6	0.65
(1,999)	2:669:B:LEU:HD11	2:648:B:GLU:HB2	13	0.65
(1,931)	2:639:B:ALA:HB2	2:634:B:VAL:HG23	5	0.65

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,515)	2:679:B:VAL:HG13	2:618:B:ARG:HA	1	0.65
(1,515)	2:679:B:VAL:HG13	2:618:B:ARG:HA	2	0.65
(1,85)	2:588:B:LEU:HD23	2:582:B:GLN:HB3	10	0.65
(1,2942)	2:688:B:LEU:HG	1:40:A:LEU:HB2	10	0.64
(1,2930)	2:573:B:PRO:HB3	1:39:A:SER:HG	15	0.64
(1,2738)	2:679:B:VAL:H	2:619:B:ILE:HG12	12	0.64
(1,2646)	2:687:B:THR:HB	2:611:B:ILE:HA	8	0.64
(1,2630)	2:672:B:LEU:HB3	2:673:B:PRO:HD3	3	0.64
(1,2622)	2:587:B:GLU:HB2	2:583:B:LEU:HD12	9	0.64
(1,2388)	2:628:B:ALA:HB1	2:629:B:VAL:HA	3	0.64
(1,2388)	2:628:B:ALA:HB3	2:629:B:VAL:HA	8	0.64
(1,2272)	2:641:B:VAL:HG12	1:44:A:LEU:HB3	13	0.64
(1,2082)	2:670:B:PHE:H	2:575:B:PHE:HZ	14	0.64
(1,1560)	2:592:B:GLU:H	2:672:B:LEU:HD12	8	0.64
(1,1559)	2:592:B:GLU:H	2:591:B:VAL:HG21	1	0.64
(1,1559)	2:592:B:GLU:H	2:591:B:VAL:HG23	4	0.64
(1,1541)	2:590:B:LYS:H	2:589:B:LYS:HE2	7	0.64
(1,1070)	2:581:B:ILE:HD11	2:594:B:LEU:HD12	15	0.64
(1,996)	2:647:B:VAL:HG22	2:625:B:PRO:HA	7	0.64
(1,641)	2:683:B:CYS:HB3	2:651:B:PHE:HB2	13	0.64
(1,513)	2:679:B:VAL:HG13	2:616:B:VAL:HG22	14	0.64
(1,510)	2:682:B:VAL:HG23	2:613:B:SER:HB2	10	0.64
(1,133)	2:591:B:VAL:HG21	2:579:B:SER:HB2	13	0.64
(1,2926)	2:682:B:VAL:HG13	1:44:A:LEU:HB2	5	0.63
(1,2738)	2:679:B:VAL:H	2:619:B:ILE:HG12	13	0.63
(1,2388)	2:628:B:ALA:HB1	2:629:B:VAL:HA	11	0.63
(1,2209)	2:576:B:MET:HB2	1:39:A:SER:HG	6	0.63
(1,2001)	2:658:B:TRP:HE1	2:594:B:LEU:HB2	5	0.63
(1,1988)	2:656:B:GLN:H	2:656:B:GLN:HB3	4	0.63
(1,1988)	2:656:B:GLN:H	2:656:B:GLN:HB3	12	0.63
(1,1628)	2:600:B:ILE:H	2:600:B:ILE:HG12	3	0.63
(1,1628)	2:600:B:ILE:H	2:600:B:ILE:HG12	4	0.63
(1,1628)	2:600:B:ILE:H	2:600:B:ILE:HG12	11	0.63
(1,1559)	2:592:B:GLU:H	2:591:B:VAL:HG22	15	0.63
(1,1216)	2:681:B:ASP:HB2	2:677:B:LEU:HD22	15	0.63
(1,978)	2:574:B:TYR:HB3	1:40:A:LEU:HD22	8	0.63
(1,2930)	2:573:B:PRO:HB3	1:39:A:SER:HG	12	0.62
(1,2738)	2:679:B:VAL:H	2:619:B:ILE:HG12	5	0.62
(1,2675)	2:571:B:LEU:HD23	2:572:B:PRO:HG2	11	0.62
(1,2490)	2:656:B:GLN:HB2	2:682:B:VAL:HA	10	0.62
(1,2451)	2:674:B:CYS:HB2	2:673:B:PRO:HB2	2	0.62
(1,2209)	2:576:B:MET:HB2	1:39:A:SER:HG	12	0.62

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1988)	2:656:B:GLN:H	2:656:B:GLN:HB3	11	0.62
(1,1988)	2:656:B:GLN:H	2:656:B:GLN:HB3	14	0.62
(1,1468)	2:580:B:ILE:H	2:580:B:ILE:HG13	9	0.62
(1,1312)	2:654:B:PHE:HB3	2:684:B:ILE:HG12	3	0.62
(1,1070)	2:581:B:ILE:HD13	2:594:B:LEU:HD13	4	0.62
(1,1070)	2:581:B:ILE:HD13	2:594:B:LEU:HD11	8	0.62
(1,797)	2:660:B:SER:HB2	1:40:A:LEU:HA	1	0.62
(1,513)	2:679:B:VAL:HG12	2:616:B:VAL:HG23	9	0.62
(1,513)	2:679:B:VAL:HG13	2:616:B:VAL:HG22	13	0.62
(1,510)	2:682:B:VAL:HG21	2:613:B:SER:HB2	8	0.62
(1,420)	2:654:B:PHE:HB2	2:682:B:VAL:HB	4	0.62
(1,420)	2:654:B:PHE:HB2	2:682:B:VAL:HB	13	0.62
(1,2738)	2:679:B:VAL:H	2:619:B:ILE:HG12	9	0.61
(1,2654)	2:674:B:CYS:HB2	2:676:B:LYS:HD3	15	0.61
(1,2630)	2:673:B:PRO:HD3	2:577:B:LYS:HG2	12	0.61
(1,2596)	2:574:B:TYR:HB3	2:581:B:ILE:HD11	2	0.61
(1,2454)	2:674:B:CYS:HB2	2:667:B:SER:HA	13	0.61
(1,2222)	2:686:B:LEU:HD21	1:38:A:HIS:HB2	10	0.61
(1,2203)	2:609:B:LEU:HD11	1:37:A:TRP:HZ3	4	0.61
(1,1988)	2:656:B:GLN:H	2:656:B:GLN:HB3	8	0.61
(1,1988)	2:656:B:GLN:H	2:656:B:GLN:HB3	13	0.61
(1,1628)	2:600:B:ILE:H	2:600:B:ILE:HG12	8	0.61
(1,1399)	1:41:A:VAL:HG21	1:41:A:VAL:H	4	0.61
(1,1288)	2:581:B:ILE:HG23	1:34:A:VAL:HA	13	0.61
(1,797)	2:660:B:SER:HB2	1:40:A:LEU:HA	3	0.61
(1,566)	2:688:B:LEU:HD22	1:38:A:HIS:H	7	0.61
(1,566)	2:688:B:LEU:HD22	1:38:A:HIS:H	12	0.61
(1,515)	2:679:B:VAL:HG12	2:618:B:ARG:HA	15	0.61
(1,513)	2:679:B:VAL:HG13	2:616:B:VAL:HG23	10	0.61
(1,245)	2:616:B:VAL:HG12	2:630:B:ILE:HG21	3	0.61
(1,116)	2:578:B:GLY:HA3	2:590:B:LYS:HD3	13	0.61
(1,2804)	2:619:B:ILE:H	2:679:B:VAL:HG11	14	0.6
(1,2738)	2:679:B:VAL:H	2:619:B:ILE:HG12	15	0.6
(1,2646)	2:687:B:THR:HB	2:611:B:ILE:HA	12	0.6
(1,2517)	2:605:B:ILE:HG22	2:604:B:GLU:HB3	8	0.6
(1,2454)	2:674:B:CYS:HB2	2:666:B:THR:HA	3	0.6
(1,2388)	2:628:B:ALA:HB2	2:629:B:VAL:HA	15	0.6
(1,1988)	2:656:B:GLN:H	2:656:B:GLN:HB3	15	0.6
(1,1931)	2:679:B:VAL:H	2:678:B:SER:HB2	5	0.6
(1,1928)	2:645:B:VAL:H	2:645:B:VAL:HG11	13	0.6
(1,1219)	2:659:B:SER:HB2	2:677:B:LEU:HD23	4	0.6
(1,1070)	2:581:B:ILE:HD11	2:594:B:LEU:HD11	5	0.6

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,896)	2:630:B:ILE:HD11	2:651:B:PHE:HE1	9	0.6
(1,566)	2:688:B:LEU:HD23	1:38:A:HIS:H	5	0.6
(1,404)	2:648:B:GLU:HG3	2:669:B:LEU:HD13	8	0.6
(1,85)	2:588:B:LEU:HD21	2:582:B:GLN:HB3	11	0.6
(1,2898)	2:675:B:SER:H	2:673:B:PRO:HB2	4	0.59
(1,2679)	1:34:A:VAL:HA	1:34:A:VAL:HG22	12	0.59
(1,2317)	2:587:B:GLU:HB3	2:589:B:LYS:HG3	10	0.59
(1,2272)	2:641:B:VAL:HG12	1:44:A:LEU:HB3	6	0.59
(1,2203)	2:609:B:LEU:HD11	1:37:A:TRP:HZ3	10	0.59
(1,1605)	2:598:B:ASP:H	2:597:B:GLU:HG2	13	0.59
(1,1288)	2:581:B:ILE:HG22	1:34:A:VAL:HA	7	0.59
(1,1109)	2:672:B:LEU:HG	2:673:B:PRO:HD3	12	0.59
(1,931)	2:639:B:ALA:HB3	2:634:B:VAL:HG23	1	0.59
(1,887)	2:630:B:ILE:HG21	2:643:B:VAL:HG12	13	0.59
(1,641)	2:683:B:CYS:HB3	2:651:B:PHE:HB2	15	0.59
(1,513)	2:679:B:VAL:HG11	2:616:B:VAL:HG22	15	0.59
(1,85)	2:588:B:LEU:HD23	2:582:B:GLN:HB3	1	0.59
(1,85)	2:588:B:LEU:HD21	2:582:B:GLN:HB3	4	0.59
(1,85)	2:588:B:LEU:HD23	2:582:B:GLN:HB3	13	0.59
(1,2675)	2:571:B:LEU:HD21	2:572:B:PRO:HG2	12	0.58
(1,2646)	2:687:B:THR:HB	2:611:B:ILE:HA	11	0.58
(1,2517)	2:605:B:ILE:HG21	2:604:B:GLU:HB3	1	0.58
(1,2517)	2:605:B:ILE:HG22	2:604:B:GLU:HB3	10	0.58
(1,2517)	2:605:B:ILE:HG21	2:604:B:GLU:HB3	14	0.58
(1,2490)	2:656:B:GLN:HB2	2:682:B:VAL:HA	8	0.58
(1,2454)	2:674:B:CYS:HB2	2:666:B:THR:HA	7	0.58
(1,2272)	2:641:B:VAL:HG11	1:44:A:LEU:HB3	14	0.58
(1,2208)	2:674:B:CYS:HB3	1:40:A:LEU:HB2	1	0.58
(1,2208)	2:674:B:CYS:HB3	1:40:A:LEU:HB2	15	0.58
(1,1988)	2:656:B:GLN:H	2:656:B:GLN:HB3	5	0.58
(1,1944)	2:646:B:LEU:H	2:646:B:LEU:HD22	3	0.58
(1,1774)	2:621:B:ASP:H	2:620:B:GLU:HB2	11	0.58
(1,1763)	2:620:B:GLU:H	2:620:B:GLU:HB3	7	0.58
(1,1628)	2:600:B:ILE:H	2:600:B:ILE:HG12	1	0.58
(1,1117)	2:589:B:LYS:HB2	2:589:B:LYS:HE2	3	0.58
(1,1070)	2:581:B:ILE:HD13	2:594:B:LEU:HD11	3	0.58
(1,1070)	2:581:B:ILE:HD13	2:594:B:LEU:HD12	14	0.58
(1,896)	2:630:B:ILE:HD12	2:651:B:PHE:HE1	8	0.58
(1,638)	2:658:B:TRP:HB2	2:593:B:ASP:HA	1	0.58
(1,638)	2:658:B:TRP:HB2	2:593:B:ASP:HA	5	0.58
(1,515)	2:679:B:VAL:HG11	2:618:B:ARG:HA	14	0.58
(1,510)	2:682:B:VAL:HG22	2:613:B:SER:HB2	3	0.58

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,510)	2:682:B:VAL:HG22	2:613:B:SER:HB2	4	0.58
(1,425)	2:654:B:PHE:HB3	2:682:B:VAL:HG23	5	0.58
(1,245)	2:616:B:VAL:HG11	2:630:B:ILE:HG21	9	0.58
(1,245)	2:616:B:VAL:HG12	2:630:B:ILE:HG21	14	0.58
(1,85)	2:588:B:LEU:HD21	2:582:B:GLN:HB3	2	0.58
(1,85)	2:588:B:LEU:HD21	2:582:B:GLN:HB3	6	0.58
(1,2804)	2:619:B:ILE:H	2:679:B:VAL:HG11	10	0.57
(1,2738)	2:679:B:VAL:H	2:619:B:ILE:HG12	3	0.57
(1,2596)	2:574:B:TYR:HB3	2:581:B:ILE:HD12	13	0.57
(1,2499)	2:619:B:ILE:H	2:619:B:ILE:HG12	9	0.57
(1,2499)	2:619:B:ILE:H	2:619:B:ILE:HG12	12	0.57
(1,2490)	2:656:B:GLN:HB2	2:682:B:VAL:HA	4	0.57
(1,1988)	2:656:B:GLN:H	2:656:B:GLN:HB3	9	0.57
(1,1763)	2:620:B:GLU:H	2:620:B:GLU:HB3	11	0.57
(1,1250)	2:619:B:ILE:HG12	2:618:B:ARG:H	15	0.57
(1,1205)	2:569:B:PRO:HA	2:568:B:PRO:HG2	7	0.57
(1,1113)	2:674:B:CYS:HA	2:663:B:PRO:HB2	1	0.57
(1,1113)	2:674:B:CYS:HA	2:663:B:PRO:HB2	11	0.57
(1,1113)	2:674:B:CYS:HA	2:663:B:PRO:HB2	12	0.57
(1,1070)	2:581:B:ILE:HD11	2:594:B:LEU:HD13	11	0.57
(1,978)	2:574:B:TYR:HB3	1:40:A:LEU:HD23	14	0.57
(1,931)	2:639:B:ALA:HB1	2:634:B:VAL:HG21	12	0.57
(1,797)	2:660:B:SER:HB2	1:40:A:LEU:HA	12	0.57
(1,576)	2:577:B:LYS:HD2	2:671:B:ASP:HB2	7	0.57
(1,552)	2:686:B:LEU:HD11	2:611:B:ILE:HA	5	0.57
(1,552)	2:686:B:LEU:HD13	2:611:B:ILE:HA	13	0.57
(1,257)	2:617:B:GLU:HG3	2:615:B:THR:HG23	15	0.57
(1,103)	2:672:B:LEU:HD11	2:672:B:LEU:HA	5	0.57
(1,85)	2:588:B:LEU:HD21	2:582:B:GLN:HB3	14	0.57
(2,6)	2:590:B:LYS:HD2	2:589:B:LYS:HA	1	0.56
(2,2)	2:595:B:LYS:HD2	2:658:B:TRP:HB3	14	0.56
(1,2846)	2:649:B:TYR:H	2:645:B:VAL:HB	6	0.56
(1,2679)	1:34:A:VAL:HA	1:34:A:VAL:HG22	1	0.56
(1,2679)	1:34:A:VAL:HA	1:34:A:VAL:HG21	2	0.56
(1,2679)	1:34:A:VAL:HA	1:34:A:VAL:HG22	10	0.56
(1,2596)	2:574:B:TYR:HB3	2:581:B:ILE:HD12	15	0.56
(1,2499)	2:619:B:ILE:H	2:619:B:ILE:HG12	1	0.56
(1,2208)	2:674:B:CYS:HB3	1:40:A:LEU:HB2	11	0.56
(1,2001)	2:658:B:TRP:HE1	2:594:B:LEU:HB2	9	0.56
(1,1205)	2:569:B:PRO:HA	2:568:B:PRO:HG2	3	0.56
(1,1205)	2:569:B:PRO:HA	2:568:B:PRO:HG2	14	0.56
(1,1109)	2:672:B:LEU:HG	2:673:B:PRO:HD3	13	0.56

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1070)	2:581:B:ILE:HD13	2:594:B:LEU:HD11	10	0.56
(1,638)	2:658:B:TRP:HB2	2:593:B:ASP:HA	9	0.56
(1,245)	2:616:B:VAL:HG11	2:630:B:ILE:HG22	13	0.56
(1,105)	2:672:B:LEU:HD21	2:591:B:VAL:HB	7	0.56
(1,99)	2:672:B:LEU:HD13	2:672:B:LEU:HB3	7	0.56
(1,99)	2:672:B:LEU:HD12	2:672:B:LEU:HB3	14	0.56
(1,2804)	2:619:B:ILE:H	2:679:B:VAL:HG11	13	0.55
(1,2679)	1:34:A:VAL:HA	1:34:A:VAL:HG21	5	0.55
(1,2679)	1:34:A:VAL:HA	1:34:A:VAL:HG23	6	0.55
(1,2679)	1:34:A:VAL:HA	1:34:A:VAL:HG21	11	0.55
(1,2647)	2:687:B:THR:HG23	2:689:B:LYS:HB2	7	0.55
(1,2630)	2:672:B:LEU:HB3	2:673:B:PRO:HD3	2	0.55
(1,2499)	2:619:B:ILE:H	2:619:B:ILE:HG12	5	0.55
(1,2499)	2:619:B:ILE:H	2:619:B:ILE:HG12	14	0.55
(1,2272)	2:641:B:VAL:HG11	1:44:A:LEU:HB3	7	0.55
(1,2210)	2:579:B:SER:HA	1:39:A:SER:HG	9	0.55
(1,2200)	2:689:B:LYS:H	2:609:B:LEU:HD13	7	0.55
(1,1763)	2:620:B:GLU:H	2:620:B:GLU:HB3	12	0.55
(1,1560)	2:592:B:GLU:H	2:672:B:LEU:HD13	5	0.55
(1,1399)	1:41:A:VAL:HG23	1:41:A:VAL:H	3	0.55
(1,1399)	1:41:A:VAL:HG23	1:41:A:VAL:H	6	0.55
(1,1250)	2:619:B:ILE:HG12	2:618:B:ARG:H	3	0.55
(1,1250)	2:619:B:ILE:HG12	2:618:B:ARG:H	9	0.55
(1,1205)	2:569:B:PRO:HA	2:568:B:PRO:HG2	1	0.55
(1,1109)	2:672:B:LEU:HG	2:673:B:PRO:HD3	2	0.55
(1,978)	2:574:B:TYR:HB3	1:40:A:LEU:HD21	4	0.55
(1,515)	2:679:B:VAL:HG13	2:618:B:ARG:HA	9	0.55
(1,420)	2:654:B:PHE:HB2	2:682:B:VAL:HB	7	0.55
(1,420)	2:654:B:PHE:HB2	2:682:B:VAL:HB	10	0.55
(1,387)	2:646:B:LEU:HB3	2:646:B:LEU:HD13	3	0.55
(1,128)	2:591:B:VAL:HG12	2:591:B:VAL:H	12	0.55
(1,99)	2:672:B:LEU:HD11	2:672:B:LEU:HB3	1	0.55
(1,99)	2:672:B:LEU:HD13	2:672:B:LEU:HB3	3	0.55
(1,99)	2:672:B:LEU:HD11	2:672:B:LEU:HB3	6	0.55
(1,99)	2:672:B:LEU:HD12	2:672:B:LEU:HB3	10	0.55
(1,99)	2:672:B:LEU:HD12	2:672:B:LEU:HB3	11	0.55
(1,99)	2:672:B:LEU:HD12	2:672:B:LEU:HB3	12	0.55
(1,85)	2:588:B:LEU:HD22	2:582:B:GLN:HB3	12	0.55
(2,2)	2:595:B:LYS:HD2	2:658:B:TRP:HB3	11	0.54
(1,2679)	1:34:A:VAL:HA	1:34:A:VAL:HG22	15	0.54
(1,2675)	2:571:B:LEU:HD21	2:572:B:PRO:HG2	5	0.54
(1,2654)	2:674:B:CYS:HB2	2:676:B:LYS:HD3	7	0.54

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2608)	2:660:B:SER:HA	2:662:B:CYS:HA	4	0.54
(1,2596)	2:574:B:TYR:HB3	2:581:B:ILE:HD13	6	0.54
(1,2517)	2:605:B:ILE:HG22	2:604:B:GLU:HB3	4	0.54
(1,2490)	2:656:B:GLN:HB2	2:682:B:VAL:HA	3	0.54
(1,2317)	2:587:B:GLU:HB3	2:589:B:LYS:HG3	6	0.54
(1,2263)	2:614:B:SER:HB2	1:47:A:SER:HB3	15	0.54
(1,2209)	2:576:B:MET:HB2	1:39:A:SER:HG	5	0.54
(1,1763)	2:620:B:GLU:H	2:620:B:GLU:HB3	1	0.54
(1,1543)	2:590:B:LYS:H	2:590:B:LYS:HB3	4	0.54
(1,1399)	1:41:A:VAL:HG23	1:41:A:VAL:H	9	0.54
(1,1399)	1:41:A:VAL:HG23	1:41:A:VAL:H	10	0.54
(1,1399)	1:41:A:VAL:HG22	1:41:A:VAL:H	14	0.54
(1,1109)	2:672:B:LEU:HG	2:673:B:PRO:HD3	3	0.54
(1,1070)	2:581:B:ILE:HD13	2:594:B:LEU:HD11	12	0.54
(1,638)	2:658:B:TRP:HB2	2:593:B:ASP:HA	14	0.54
(1,513)	2:679:B:VAL:HG13	2:616:B:VAL:HG21	7	0.54
(1,510)	2:682:B:VAL:HG22	2:613:B:SER:HB2	11	0.54
(1,422)	2:654:B:PHE:HB2	2:682:B:VAL:HG11	15	0.54
(1,232)	2:611:B:ILE:HG21	2:684:B:ILE:HD12	9	0.54
(1,152)	2:595:B:LYS:HG2	2:658:B:TRP:HB3	10	0.54
(1,128)	2:591:B:VAL:HG11	2:591:B:VAL:H	11	0.54
(1,99)	2:672:B:LEU:HD11	2:672:B:LEU:HB3	2	0.54
(1,99)	2:672:B:LEU:HD13	2:672:B:LEU:HB3	4	0.54
(1,85)	2:588:B:LEU:HD22	2:582:B:GLN:HB3	8	0.54
(1,2930)	2:573:B:PRO:HB3	1:39:A:SER:HG	3	0.53
(1,2930)	2:573:B:PRO:HB3	1:39:A:SER:HG	10	0.53
(1,2738)	2:679:B:VAL:H	2:619:B:ILE:HG12	10	0.53
(1,2738)	2:679:B:VAL:H	2:619:B:ILE:HG12	11	0.53
(1,2738)	2:679:B:VAL:H	2:619:B:ILE:HG12	14	0.53
(1,2263)	2:614:B:SER:HB2	1:47:A:SER:HB3	14	0.53
(1,1988)	2:656:B:GLN:H	2:656:B:GLN:HB3	10	0.53
(1,1931)	2:679:B:VAL:H	2:678:B:SER:HB2	7	0.53
(1,1763)	2:620:B:GLU:H	2:620:B:GLU:HB3	2	0.53
(1,1763)	2:620:B:GLU:H	2:620:B:GLU:HB3	3	0.53
(1,1763)	2:620:B:GLU:H	2:620:B:GLU:HB3	6	0.53
(1,1763)	2:620:B:GLU:H	2:620:B:GLU:HB3	9	0.53
(1,1763)	2:620:B:GLU:H	2:620:B:GLU:HB3	14	0.53
(1,1399)	1:41:A:VAL:HG21	1:41:A:VAL:H	2	0.53
(1,1109)	2:672:B:LEU:HG	2:673:B:PRO:HD3	10	0.53
(1,1086)	2:609:B:LEU:HD22	1:37:A:TRP:HZ3	7	0.53
(1,1070)	2:581:B:ILE:HD13	2:594:B:LEU:HD12	2	0.53
(1,1070)	2:581:B:ILE:HD12	2:594:B:LEU:HD13	9	0.53

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1006)	2:652:B:PHE:HA	1:41:A:VAL:HA	7	0.53
(1,638)	2:658:B:TRP:HB2	2:593:B:ASP:HA	12	0.53
(1,591)	2:580:B:ILE:HD12	2:590:B:LYS:HE2	15	0.53
(1,552)	2:686:B:LEU:HD12	2:611:B:ILE:HA	15	0.53
(1,101)	2:672:B:LEU:HD13	2:591:B:VAL:HB	5	0.53
(1,99)	2:672:B:LEU:HD11	2:672:B:LEU:HB3	13	0.53
(1,85)	2:588:B:LEU:HD22	2:582:B:GLN:HB3	3	0.53
(1,85)	2:588:B:LEU:HD21	2:582:B:GLN:HB3	7	0.53
(1,2804)	2:619:B:ILE:H	2:679:B:VAL:HG13	8	0.52
(1,2738)	2:679:B:VAL:H	2:619:B:ILE:HG12	8	0.52
(1,2665)	2:591:B:VAL:HG11	2:658:B:TRP:HH2	15	0.52
(1,2630)	2:673:B:PRO:HD3	2:577:B:LYS:HG2	1	0.52
(1,2630)	2:672:B:LEU:HB3	2:673:B:PRO:HD3	13	0.52
(1,2596)	2:574:B:TYR:HB3	2:581:B:ILE:HD12	11	0.52
(1,2517)	2:605:B:ILE:HG23	2:604:B:GLU:HB3	9	0.52
(1,2517)	2:605:B:ILE:HG23	2:604:B:GLU:HB3	13	0.52
(1,2499)	2:619:B:ILE:H	2:619:B:ILE:HG12	7	0.52
(1,2490)	2:656:B:GLN:HB2	2:682:B:VAL:HA	7	0.52
(1,2210)	2:579:B:SER:HA	1:39:A:SER:HG	8	0.52
(1,1988)	2:656:B:GLN:H	2:656:B:GLN:HB3	3	0.52
(1,1763)	2:620:B:GLU:H	2:620:B:GLU:HB3	15	0.52
(1,1543)	2:590:B:LYS:H	2:590:B:LYS:HB3	15	0.52
(1,1399)	1:41:A:VAL:HG23	1:41:A:VAL:H	8	0.52
(1,1399)	1:41:A:VAL:HG23	1:41:A:VAL:H	11	0.52
(1,1399)	1:41:A:VAL:HG23	1:41:A:VAL:H	15	0.52
(1,1250)	2:619:B:ILE:HG12	2:618:B:ARG:H	1	0.52
(1,1222)	2:601:B:GLN:HG3	2:605:B:ILE:HD11	7	0.52
(1,978)	2:574:B:TYR:HB3	1:40:A:LEU:HD22	1	0.52
(1,638)	2:658:B:TRP:HB2	2:593:B:ASP:HA	8	0.52
(1,638)	2:658:B:TRP:HB2	2:593:B:ASP:HA	13	0.52
(1,534)	2:684:B:ILE:HG23	2:611:B:ILE:HB	9	0.52
(1,534)	2:684:B:ILE:HG21	2:611:B:ILE:HB	15	0.52
(1,128)	2:591:B:VAL:HG12	2:591:B:VAL:H	14	0.52
(1,2942)	2:688:B:LEU:HG	1:40:A:LEU:HB2	5	0.51
(1,2926)	2:653:B:VAL:HG12	1:44:A:LEU:HB2	10	0.51
(1,2804)	2:619:B:ILE:H	2:679:B:VAL:HG13	3	0.51
(1,2530)	2:642:B:SER:HB3	2:629:B:VAL:HG12	1	0.51
(1,2511)	2:600:B:ILE:HA	2:600:B:ILE:HD12	2	0.51
(1,2511)	2:600:B:ILE:HA	2:600:B:ILE:HD13	9	0.51
(1,2511)	2:600:B:ILE:HA	2:600:B:ILE:HD12	13	0.51
(1,2317)	2:587:B:GLU:HB3	2:589:B:LYS:HG3	4	0.51
(1,2222)	2:686:B:LEU:HD22	1:38:A:HIS:HB2	6	0.51

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2210)	2:579:B:SER:HA	1:39:A:SER:HG	14	0.51
(1,1931)	2:679:B:VAL:H	2:678:B:SER:HB2	15	0.51
(1,1763)	2:620:B:GLU:H	2:620:B:GLU:HB3	4	0.51
(1,1628)	2:600:B:ILE:H	2:600:B:ILE:HG12	14	0.51
(1,1604)	2:598:B:ASP:H	2:598:B:ASP:HB2	10	0.51
(1,1559)	2:592:B:GLU:H	2:591:B:VAL:HG22	7	0.51
(1,1559)	2:592:B:GLU:H	2:591:B:VAL:HG23	13	0.51
(1,1454)	2:579:B:SER:H	2:579:B:SER:HB2	15	0.51
(1,1312)	2:654:B:PHE:HB3	2:684:B:ILE:HG12	11	0.51
(1,1250)	2:619:B:ILE:HG12	2:618:B:ARG:H	7	0.51
(1,1250)	2:619:B:ILE:HG12	2:618:B:ARG:H	8	0.51
(1,1250)	2:619:B:ILE:HG12	2:618:B:ARG:H	14	0.51
(1,1109)	2:672:B:LEU:HG	2:673:B:PRO:HD3	1	0.51
(1,1109)	2:672:B:LEU:HG	2:673:B:PRO:HD3	6	0.51
(1,1109)	2:672:B:LEU:HG	2:673:B:PRO:HD3	11	0.51
(1,1006)	2:652:B:PHE:HA	1:41:A:VAL:HA	5	0.51
(1,638)	2:658:B:TRP:HB2	2:593:B:ASP:HA	2	0.51
(1,638)	2:658:B:TRP:HB2	2:593:B:ASP:HA	3	0.51
(1,638)	2:658:B:TRP:HB2	2:593:B:ASP:HA	4	0.51
(1,638)	2:658:B:TRP:HB2	2:593:B:ASP:HA	11	0.51
(1,552)	2:686:B:LEU:HD11	2:611:B:ILE:HA	9	0.51
(1,552)	2:686:B:LEU:HD12	2:611:B:ILE:HA	12	0.51
(1,534)	2:684:B:ILE:HG23	2:611:B:ILE:HB	6	0.51
(1,416)	2:653:B:VAL:HB	2:656:B:GLN:HB3	8	0.51
(1,416)	2:653:B:VAL:HB	2:656:B:GLN:HB3	11	0.51
(1,245)	2:616:B:VAL:HG11	2:630:B:ILE:HG23	5	0.51
(1,128)	2:591:B:VAL:HG12	2:591:B:VAL:H	1	0.51
(1,105)	2:672:B:LEU:HD21	2:591:B:VAL:HB	6	0.51
(1,105)	2:672:B:LEU:HD21	2:591:B:VAL:HB	11	0.51
(1,2804)	2:619:B:ILE:H	2:679:B:VAL:HG21	7	0.5
(1,2738)	2:679:B:VAL:H	2:619:B:ILE:HG12	2	0.5
(1,2511)	2:600:B:ILE:HA	2:600:B:ILE:HD12	6	0.5
(1,2511)	2:600:B:ILE:HA	2:600:B:ILE:HD13	7	0.5
(1,2511)	2:600:B:ILE:HA	2:600:B:ILE:HD11	12	0.5
(1,2490)	2:656:B:GLN:HB2	2:682:B:VAL:HA	11	0.5
(1,2069)	2:668:B:GLN:H	2:667:B:SER:HB3	12	0.5
(1,1789)	2:624:B:SER:H	2:624:B:SER:HB3	4	0.5
(1,1789)	2:624:B:SER:H	2:624:B:SER:HB3	6	0.5
(1,1557)	2:592:B:GLU:H	2:590:B:LYS:HB2	4	0.5
(1,1454)	2:579:B:SER:H	2:579:B:SER:HB2	13	0.5
(1,1312)	2:654:B:PHE:HB3	2:684:B:ILE:HG12	8	0.5
(1,1250)	2:619:B:ILE:HG12	2:618:B:ARG:H	6	0.5

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1250)	2:619:B:ILE:HG12	2:618:B:ARG:H	12	0.5
(1,1070)	2:581:B:ILE:HD11	2:594:B:LEU:HD12	13	0.5
(1,887)	2:630:B:ILE:HG21	2:643:B:VAL:HG11	1	0.5
(1,887)	2:630:B:ILE:HG21	2:643:B:VAL:HG12	4	0.5
(1,638)	2:658:B:TRP:HB2	2:593:B:ASP:HA	7	0.5
(1,591)	2:580:B:ILE:HD11	2:590:B:LYS:HE3	13	0.5
(1,534)	2:684:B:ILE:HG21	2:611:B:ILE:HB	4	0.5
(1,534)	2:684:B:ILE:HG22	2:611:B:ILE:HB	8	0.5
(1,425)	2:654:B:PHE:HB3	2:682:B:VAL:HG22	9	0.5
(1,365)	2:665:B:ARG:HD3	2:647:B:VAL:HG23	6	0.5
(1,149)	2:596:B:THR:H	2:595:B:LYS:HB2	4	0.5
(1,128)	2:591:B:VAL:HG11	2:591:B:VAL:H	3	0.5
(1,128)	2:591:B:VAL:HG13	2:591:B:VAL:H	5	0.5
(1,116)	2:578:B:GLY:HA3	2:590:B:LYS:HD3	3	0.5
(1,105)	2:672:B:LEU:HD21	2:591:B:VAL:HB	1	0.5
(1,2804)	2:619:B:ILE:H	2:679:B:VAL:HG12	15	0.49
(1,2630)	2:672:B:LEU:HB3	2:673:B:PRO:HD3	8	0.49
(1,2511)	2:600:B:ILE:HA	2:600:B:ILE:HD12	1	0.49
(1,2511)	2:600:B:ILE:HA	2:600:B:ILE:HD13	3	0.49
(1,2511)	2:600:B:ILE:HA	2:600:B:ILE:HD11	4	0.49
(1,2511)	2:600:B:ILE:HA	2:600:B:ILE:HD11	11	0.49
(1,2499)	2:619:B:ILE:H	2:619:B:ILE:HG12	13	0.49
(1,2317)	2:587:B:GLU:HB3	2:589:B:LYS:HG3	15	0.49
(1,2209)	2:576:B:MET:HB2	1:39:A:SER:HG	10	0.49
(1,2208)	2:674:B:CYS:HB3	1:40:A:LEU:HB2	6	0.49
(1,2200)	2:689:B:LYS:H	2:609:B:LEU:HD11	1	0.49
(1,1403)	1:41:A:VAL:HG23	1:39:A:SER:H	6	0.49
(1,1312)	2:654:B:PHE:HB3	2:684:B:ILE:HG12	4	0.49
(1,1250)	2:619:B:ILE:HG12	2:618:B:ARG:H	10	0.49
(1,1250)	2:619:B:ILE:HG12	2:618:B:ARG:H	11	0.49
(1,1211)	2:630:B:ILE:HA	2:619:B:ILE:HG13	5	0.49
(1,1113)	2:674:B:CYS:HA	2:663:B:PRO:HB2	9	0.49
(1,576)	2:577:B:LYS:HD2	2:671:B:ASP:HB2	10	0.49
(1,534)	2:684:B:ILE:HG21	2:611:B:ILE:HB	3	0.49
(1,257)	2:617:B:GLU:HG3	2:615:B:THR:HG21	13	0.49
(1,133)	2:591:B:VAL:HG23	2:579:B:SER:HB2	15	0.49
(1,2898)	2:675:B:SER:H	2:673:B:PRO:HB2	7	0.48
(1,2898)	2:675:B:SER:H	2:673:B:PRO:HB2	9	0.48
(1,2511)	2:600:B:ILE:HA	2:600:B:ILE:HD12	8	0.48
(1,2511)	2:600:B:ILE:HA	2:600:B:ILE:HD12	10	0.48
(1,2499)	2:619:B:ILE:H	2:619:B:ILE:HG12	3	0.48
(1,2455)	2:674:B:CYS:HB3	2:673:B:PRO:HB2	9	0.48

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2317)	2:587:B:GLU:HB3	2:589:B:LYS:HG3	8	0.48
(1,2263)	2:614:B:SER:HB2	1:47:A:SER:HB3	8	0.48
(1,2209)	2:576:B:MET:HB2	1:39:A:SER:HG	13	0.48
(1,2208)	2:674:B:CYS:HB3	1:40:A:LEU:HB2	9	0.48
(1,2001)	2:658:B:TRP:HE1	2:594:B:LEU:HB2	2	0.48
(1,1988)	2:656:B:GLN:H	2:656:B:GLN:HB3	7	0.48
(1,1559)	2:592:B:GLU:H	2:591:B:VAL:HG21	9	0.48
(1,1541)	2:590:B:LYS:H	2:589:B:LYS:HE2	8	0.48
(1,1250)	2:619:B:ILE:HG12	2:618:B:ARG:H	5	0.48
(1,1222)	2:601:B:GLN:HG3	2:605:B:ILE:HD12	8	0.48
(1,1222)	2:601:B:GLN:HG3	2:605:B:ILE:HD13	12	0.48
(1,1117)	2:589:B:LYS:HB2	2:589:B:LYS:HE2	2	0.48
(1,638)	2:658:B:TRP:HB2	2:593:B:ASP:HA	15	0.48
(1,534)	2:684:B:ILE:HG23	2:611:B:ILE:HB	2	0.48
(1,534)	2:684:B:ILE:HG23	2:611:B:ILE:HB	5	0.48
(1,534)	2:684:B:ILE:HG23	2:611:B:ILE:HB	7	0.48
(1,245)	2:616:B:VAL:HG13	2:630:B:ILE:HG22	1	0.48
(1,245)	2:616:B:VAL:HG12	2:630:B:ILE:HG21	2	0.48
(1,245)	2:616:B:VAL:HG11	2:630:B:ILE:HG23	12	0.48
(1,128)	2:591:B:VAL:HG13	2:591:B:VAL:H	2	0.48
(1,128)	2:591:B:VAL:HG11	2:591:B:VAL:H	6	0.48
(1,105)	2:672:B:LEU:HD23	2:591:B:VAL:HB	12	0.48
(1,99)	2:672:B:LEU:HD11	2:672:B:LEU:HB3	15	0.48
(1,2898)	2:675:B:SER:H	2:673:B:PRO:HB2	12	0.47
(1,2804)	2:619:B:ILE:H	2:679:B:VAL:HG13	2	0.47
(1,2646)	2:687:B:THR:HB	2:611:B:ILE:HA	10	0.47
(1,2608)	2:660:B:SER:HA	2:662:B:CYS:HA	15	0.47
(1,2517)	2:605:B:ILE:HG22	2:604:B:GLU:HB3	12	0.47
(1,2499)	2:619:B:ILE:H	2:619:B:ILE:HG12	6	0.47
(1,2209)	2:576:B:MET:HB2	1:39:A:SER:HG	2	0.47
(1,1988)	2:656:B:GLN:H	2:656:B:GLN:HB3	6	0.47
(1,1928)	2:645:B:VAL:H	2:645:B:VAL:HG12	7	0.47
(1,1789)	2:624:B:SER:H	2:624:B:SER:HB3	5	0.47
(1,1773)	2:621:B:ASP:H	2:621:B:ASP:HB3	7	0.47
(1,1753)	2:619:B:ILE:H	2:619:B:ILE:HG12	9	0.47
(1,1753)	2:619:B:ILE:H	2:619:B:ILE:HG12	12	0.47
(1,1250)	2:619:B:ILE:HG12	2:618:B:ARG:H	2	0.47
(1,1250)	2:619:B:ILE:HG12	2:618:B:ARG:H	13	0.47
(1,1219)	2:659:B:SER:HB2	2:677:B:LEU:HD21	15	0.47
(1,1211)	2:630:B:ILE:HA	2:619:B:ILE:HG13	10	0.47
(1,1117)	2:589:B:LYS:HB2	2:589:B:LYS:HE2	13	0.47
(1,1076)	2:581:B:ILE:HD12	1:35:A:PHE:HD1	10	0.47

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,931)	2:639:B:ALA:HB1	2:634:B:VAL:HG21	8	0.47
(1,931)	2:639:B:ALA:HB1	2:634:B:VAL:HG21	10	0.47
(1,896)	2:630:B:ILE:HD11	2:651:B:PHE:HE1	2	0.47
(1,638)	2:658:B:TRP:HB2	2:593:B:ASP:HA	6	0.47
(1,515)	2:679:B:VAL:HG13	2:618:B:ARG:HA	4	0.47
(1,425)	2:654:B:PHE:HB3	2:682:B:VAL:HG21	1	0.47
(1,245)	2:616:B:VAL:HG11	2:630:B:ILE:HG22	10	0.47
(1,128)	2:591:B:VAL:HG11	2:591:B:VAL:H	4	0.47
(1,116)	2:578:B:GLY:HA3	2:590:B:LYS:HD3	11	0.47
(1,101)	2:672:B:LEU:HD11	2:591:B:VAL:HB	8	0.47
(1,98)	2:672:B:LEU:HD11	2:591:B:VAL:HG23	6	0.47
(1,2898)	2:675:B:SER:H	2:673:B:PRO:HB2	14	0.46
(1,2709)	2:580:B:ILE:H	2:580:B:ILE:HG21	13	0.46
(1,2675)	2:571:B:LEU:HD21	2:572:B:PRO:HG2	6	0.46
(1,2654)	2:674:B:CYS:HB2	2:676:B:LYS:HD3	12	0.46
(1,2596)	2:574:B:TYR:HB3	2:581:B:ILE:HD13	7	0.46
(1,2499)	2:619:B:ILE:H	2:619:B:ILE:HG12	2	0.46
(1,2499)	2:619:B:ILE:H	2:619:B:ILE:HG12	8	0.46
(1,2272)	2:641:B:VAL:HG11	1:44:A:LEU:HB3	5	0.46
(1,2070)	2:668:B:GLN:H	2:668:B:GLN:HG2	10	0.46
(1,2069)	2:668:B:GLN:H	2:667:B:SER:HB3	4	0.46
(1,2065)	2:667:B:SER:H	2:667:B:SER:HB3	8	0.46
(1,2065)	2:667:B:SER:H	2:667:B:SER:HB3	13	0.46
(1,1928)	2:645:B:VAL:H	2:645:B:VAL:HG13	14	0.46
(1,1763)	2:620:B:GLU:H	2:620:B:GLU:HB3	8	0.46
(1,1753)	2:619:B:ILE:H	2:619:B:ILE:HG12	1	0.46
(1,1449)	2:577:B:LYS:H	2:672:B:LEU:HB3	4	0.46
(1,1399)	1:41:A:VAL:HG22	1:41:A:VAL:H	5	0.46
(1,1399)	1:41:A:VAL:HG21	1:41:A:VAL:H	12	0.46
(1,1399)	1:41:A:VAL:HG22	1:41:A:VAL:H	13	0.46
(1,1250)	2:619:B:ILE:HG12	2:618:B:ARG:H	4	0.46
(1,1194)	2:689:B:LYS:HA	2:610:B:LYS:HE2	4	0.46
(1,1117)	2:589:B:LYS:HB2	2:589:B:LYS:HE2	1	0.46
(1,1117)	2:589:B:LYS:HB2	2:589:B:LYS:HE2	5	0.46
(1,1117)	2:589:B:LYS:HB2	2:589:B:LYS:HE2	10	0.46
(1,1117)	2:589:B:LYS:HB2	2:589:B:LYS:HE2	11	0.46
(1,1117)	2:589:B:LYS:HB2	2:589:B:LYS:HE2	12	0.46
(1,1117)	2:589:B:LYS:HB2	2:589:B:LYS:HE2	15	0.46
(1,1070)	2:581:B:ILE:HD13	2:594:B:LEU:HD13	1	0.46
(1,931)	2:639:B:ALA:HB1	2:634:B:VAL:HG22	7	0.46
(1,638)	2:658:B:TRP:HB2	2:593:B:ASP:HA	10	0.46
(1,552)	2:686:B:LEU:HD13	2:611:B:ILE:HA	1	0.46

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,534)	2:684:B:ILE:HG23	2:611:B:ILE:HB	10	0.46
(1,534)	2:684:B:ILE:HG21	2:611:B:ILE:HB	12	0.46
(1,416)	2:653:B:VAL:HB	2:656:B:GLN:HB3	13	0.46
(1,245)	2:616:B:VAL:HG11	2:630:B:ILE:HG23	15	0.46
(1,149)	2:596:B:THR:H	2:595:B:LYS:HB2	11	0.46
(1,116)	2:578:B:GLY:HA3	2:590:B:LYS:HD3	2	0.46
(1,98)	2:672:B:LEU:HD12	2:591:B:VAL:HG22	10	0.46
(1,98)	2:672:B:LEU:HD12	2:591:B:VAL:HG22	12	0.46
(1,2898)	2:675:B:SER:H	2:673:B:PRO:HB2	6	0.45
(1,2674)	2:571:B:LEU:HD13	2:568:B:PRO:HG2	3	0.45
(1,2666)	2:591:B:VAL:HG11	2:658:B:TRP:HE3	9	0.45
(1,2530)	2:682:B:VAL:HG21	2:613:B:SER:HB3	2	0.45
(1,2499)	2:619:B:ILE:H	2:619:B:ILE:HG12	10	0.45
(1,2499)	2:619:B:ILE:H	2:619:B:ILE:HG12	15	0.45
(1,2455)	2:674:B:CYS:HB3	2:673:B:PRO:HB2	11	0.45
(1,2263)	2:614:B:SER:HB2	1:47:A:SER:HB2	10	0.45
(1,2217)	2:583:B:LEU:HD21	1:38:A:HIS:HA	13	0.45
(1,2210)	2:579:B:SER:HA	1:39:A:SER:HG	11	0.45
(1,2209)	2:576:B:MET:HB2	1:39:A:SER:HG	15	0.45
(1,2065)	2:667:B:SER:H	2:667:B:SER:HB3	2	0.45
(1,2065)	2:667:B:SER:H	2:667:B:SER:HB3	7	0.45
(1,2065)	2:667:B:SER:H	2:667:B:SER:HB3	10	0.45
(1,2001)	2:658:B:TRP:HE1	2:594:B:LEU:HB2	11	0.45
(1,1928)	2:645:B:VAL:H	2:645:B:VAL:HG12	1	0.45
(1,1773)	2:621:B:ASP:H	2:621:B:ASP:HB3	13	0.45
(1,1763)	2:620:B:GLU:H	2:620:B:GLU:HB3	13	0.45
(1,1753)	2:619:B:ILE:H	2:619:B:ILE:HG12	5	0.45
(1,1753)	2:619:B:ILE:H	2:619:B:ILE:HG12	14	0.45
(1,1402)	1:40:A:LEU:HD12	1:39:A:SER:H	11	0.45
(1,1399)	1:41:A:VAL:HG22	1:41:A:VAL:H	7	0.45
(1,1113)	2:674:B:CYS:HA	2:663:B:PRO:HB2	6	0.45
(1,931)	2:639:B:ALA:HB2	2:634:B:VAL:HG22	13	0.45
(1,574)	2:576:B:MET:HB2	2:575:B:PHE:HD1	5	0.45
(1,552)	2:686:B:LEU:HD13	2:611:B:ILE:HA	4	0.45
(1,420)	2:654:B:PHE:HB2	2:682:B:VAL:HB	6	0.45
(1,245)	2:616:B:VAL:HG11	2:630:B:ILE:HG23	6	0.45
(1,128)	2:591:B:VAL:HG13	2:591:B:VAL:H	13	0.45
(1,2898)	2:675:B:SER:H	2:673:B:PRO:HB2	11	0.44
(1,2665)	2:591:B:VAL:HG12	2:594:B:LEU:H	3	0.44
(1,2665)	2:591:B:VAL:HG13	2:594:B:LEU:H	12	0.44
(1,2654)	2:674:B:CYS:HB2	2:676:B:LYS:HD3	10	0.44
(1,2654)	2:674:B:CYS:HB2	2:676:B:LYS:HD3	14	0.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2608)	2:660:B:SER:HA	2:662:B:CYS:HA	2	0.44
(1,2499)	2:619:B:ILE:H	2:619:B:ILE:HG12	11	0.44
(1,2277)	2:639:B:ALA:HB1	1:48:A:GLN:HB3	10	0.44
(1,2270)	2:641:B:VAL:HG11	1:44:A:LEU:HD13	7	0.44
(1,2263)	2:614:B:SER:HB2	1:47:A:SER:HB3	13	0.44
(1,2209)	2:576:B:MET:HB2	1:39:A:SER:HG	1	0.44
(1,2069)	2:668:B:GLN:H	2:667:B:SER:HB3	15	0.44
(1,1789)	2:624:B:SER:H	2:624:B:SER:HB3	15	0.44
(1,1763)	2:620:B:GLU:H	2:620:B:GLU:HB3	10	0.44
(1,1730)	2:617:B:GLU:H	2:617:B:GLU:HB3	3	0.44
(1,1730)	2:617:B:GLU:H	2:617:B:GLU:HB3	12	0.44
(1,1541)	2:590:B:LYS:H	2:589:B:LYS:HE2	12	0.44
(1,1399)	1:41:A:VAL:HG23	1:41:A:VAL:H	1	0.44
(1,1222)	2:601:B:GLN:HG3	2:605:B:ILE:HD11	10	0.44
(1,1211)	2:630:B:ILE:HA	2:619:B:ILE:HG13	4	0.44
(1,534)	2:684:B:ILE:HG22	2:611:B:ILE:HB	13	0.44
(1,425)	2:654:B:PHE:HB3	2:682:B:VAL:HG21	14	0.44
(1,420)	2:654:B:PHE:HB2	2:682:B:VAL:HB	12	0.44
(1,257)	2:617:B:GLU:HG3	2:615:B:THR:HG22	10	0.44
(1,128)	2:591:B:VAL:HG11	2:591:B:VAL:H	10	0.44
(1,98)	2:672:B:LEU:HD11	2:591:B:VAL:HG23	2	0.44
(1,2935)	2:583:B:LEU:HD22	1:39:A:SER:HB3	10	0.43
(1,2646)	2:687:B:THR:HB	2:610:B:LYS:HA	2	0.43
(1,2289)	2:575:B:PHE:HE2	1:39:A:SER:HB3	4	0.43
(1,2217)	2:583:B:LEU:HD21	1:38:A:HIS:HA	4	0.43
(1,2209)	2:576:B:MET:HB2	1:39:A:SER:HG	7	0.43
(1,2001)	2:658:B:TRP:HE1	2:594:B:LEU:HB2	1	0.43
(1,1977)	2:654:B:PHE:H	2:682:B:VAL:HG22	2	0.43
(1,1389)	1:37:A:TRP:HB3	1:37:A:TRP:HE3	12	0.43
(1,1389)	1:37:A:TRP:HB3	1:37:A:TRP:HE3	15	0.43
(1,1211)	2:630:B:ILE:HA	2:619:B:ILE:HG13	15	0.43
(1,1117)	2:589:B:LYS:HB2	2:589:B:LYS:HE2	4	0.43
(1,1076)	2:581:B:ILE:HD13	1:35:A:PHE:HD1	15	0.43
(1,887)	2:630:B:ILE:HG23	2:643:B:VAL:HG11	14	0.43
(1,534)	2:684:B:ILE:HG21	2:611:B:ILE:HB	14	0.43
(1,128)	2:591:B:VAL:HG11	2:591:B:VAL:H	7	0.43
(1,105)	2:672:B:LEU:HD22	2:591:B:VAL:HB	10	0.43
(1,101)	2:672:B:LEU:HD13	2:591:B:VAL:HB	9	0.43
(1,98)	2:672:B:LEU:HD13	2:591:B:VAL:HG22	3	0.43
(2,2)	2:595:B:LYS:HD2	2:658:B:TRP:HB3	7	0.42
(1,2935)	2:583:B:LEU:HD22	1:39:A:SER:HB3	12	0.42
(1,2935)	2:583:B:LEU:HD22	1:39:A:SER:HB3	15	0.42

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2709)	2:580:B:ILE:H	2:580:B:ILE:HG23	11	0.42
(1,2665)	2:591:B:VAL:HG11	2:658:B:TRP:HH2	13	0.42
(1,2608)	2:660:B:SER:HA	2:662:B:CYS:HA	11	0.42
(1,2490)	2:656:B:GLN:HB2	2:682:B:VAL:HA	15	0.42
(1,2457)	2:674:B:CYS:HB3	2:667:B:SER:HA	2	0.42
(1,2455)	2:674:B:CYS:HB3	2:673:B:PRO:HB2	12	0.42
(1,2451)	2:674:B:CYS:HB2	2:673:B:PRO:HB2	5	0.42
(1,2451)	2:674:B:CYS:HB2	2:673:B:PRO:HB2	10	0.42
(1,2317)	2:587:B:GLU:HB3	2:589:B:LYS:HG3	13	0.42
(1,2289)	2:575:B:PHE:HE2	1:39:A:SER:HB3	14	0.42
(1,2217)	2:583:B:LEU:HD23	1:38:A:HIS:HA	7	0.42
(1,2200)	2:689:B:LYS:H	2:609:B:LEU:HD12	3	0.42
(1,1753)	2:619:B:ILE:H	2:619:B:ILE:HG12	7	0.42
(1,1730)	2:617:B:GLU:H	2:617:B:GLU:HB3	7	0.42
(1,1559)	2:592:B:GLU:H	2:591:B:VAL:HG23	8	0.42
(1,1403)	1:41:A:VAL:HG23	1:39:A:SER:H	11	0.42
(1,1364)	1:47:A:SER:HA	1:48:A:GLN:HB3	10	0.42
(1,1222)	2:601:B:GLN:HG3	2:605:B:ILE:HD11	3	0.42
(1,1117)	2:589:B:LYS:HB2	2:589:B:LYS:HE2	14	0.42
(1,896)	2:630:B:ILE:HD13	2:651:B:PHE:HE1	3	0.42
(1,797)	2:660:B:SER:HB2	1:40:A:LEU:HA	13	0.42
(1,534)	2:684:B:ILE:HG23	2:611:B:ILE:HB	1	0.42
(1,416)	2:653:B:VAL:HB	2:656:B:GLN:HB3	15	0.42
(1,257)	2:617:B:GLU:HG3	2:615:B:THR:HG23	8	0.42
(1,149)	2:596:B:THR:H	2:595:B:LYS:HB2	8	0.42
(1,128)	2:591:B:VAL:HG11	2:591:B:VAL:H	8	0.42
(1,116)	2:578:B:GLY:HA3	2:590:B:LYS:HD3	10	0.42
(1,98)	2:672:B:LEU:HD11	2:591:B:VAL:HG22	13	0.42
(2,2)	2:595:B:LYS:HD2	2:658:B:TRP:HB3	5	0.41
(1,2935)	2:583:B:LEU:HD21	1:39:A:SER:HB3	6	0.41
(1,2804)	2:619:B:ILE:H	2:679:B:VAL:HG21	6	0.41
(1,2738)	2:679:B:VAL:H	2:619:B:ILE:HG12	7	0.41
(1,2709)	2:580:B:ILE:H	2:580:B:ILE:HG21	4	0.41
(1,2709)	2:580:B:ILE:H	2:580:B:ILE:HG22	9	0.41
(1,2646)	2:687:B:THR:HB	2:611:B:ILE:HA	6	0.41
(1,2455)	2:674:B:CYS:HB3	2:673:B:PRO:HB2	7	0.41
(1,2289)	2:575:B:PHE:HE2	1:39:A:SER:HB3	7	0.41
(1,2263)	2:614:B:SER:HB2	1:47:A:SER:HB3	2	0.41
(1,2217)	2:583:B:LEU:HD21	1:38:A:HIS:HA	14	0.41
(1,1730)	2:617:B:GLU:H	2:617:B:GLU:HB3	6	0.41
(1,1730)	2:617:B:GLU:H	2:617:B:GLU:HB3	9	0.41
(1,1559)	2:592:B:GLU:H	2:591:B:VAL:HG23	10	0.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1389)	1:37:A:TRP:HB3	1:37:A:TRP:HE3	10	0.41
(1,1389)	1:37:A:TRP:HB3	1:37:A:TRP:HE3	11	0.41
(1,1312)	2:654:B:PHE:HB3	2:684:B:ILE:HG12	1	0.41
(1,1312)	2:654:B:PHE:HB3	2:684:B:ILE:HG12	6	0.41
(1,1295)	2:589:B:LYS:HB2	2:590:B:LYS:H	7	0.41
(1,1211)	2:630:B:ILE:HA	2:619:B:ILE:HG13	3	0.41
(1,1117)	2:589:B:LYS:HB2	2:589:B:LYS:HE2	8	0.41
(1,404)	2:648:B:GLU:HG3	2:669:B:LEU:HD13	6	0.41
(1,257)	2:617:B:GLU:HG3	2:615:B:THR:HG21	11	0.41
(1,132)	2:591:B:VAL:HG23	2:577:B:LYS:HA	8	0.41
(1,128)	2:591:B:VAL:HG13	2:591:B:VAL:H	15	0.41
(1,124)	2:596:B:THR:HG21	2:684:B:ILE:HD11	6	0.41
(1,116)	2:578:B:GLY:HA3	2:590:B:LYS:HD3	1	0.41
(1,116)	2:578:B:GLY:HA3	2:590:B:LYS:HD3	5	0.41
(1,105)	2:672:B:LEU:HD23	2:591:B:VAL:HB	15	0.41
(1,64)	2:587:B:GLU:HB2	2:583:B:LEU:HD12	9	0.41
(1,2898)	2:675:B:SER:H	2:673:B:PRO:HB2	13	0.4
(1,2665)	2:591:B:VAL:HG12	2:594:B:LEU:H	6	0.4
(1,2608)	2:660:B:SER:HA	2:662:B:CYS:HA	10	0.4
(1,2530)	2:642:B:SER:HB3	2:629:B:VAL:HG13	5	0.4
(1,2517)	2:605:B:ILE:HG23	2:604:B:GLU:HB3	5	0.4
(1,2465)	2:686:B:LEU:HD23	1:37:A:TRP:HE3	4	0.4
(1,2263)	2:614:B:SER:HB2	1:47:A:SER:HB3	6	0.4
(1,2203)	2:609:B:LEU:HD11	1:37:A:TRP:HZ3	6	0.4
(1,2132)	2:678:B:SER:H	2:678:B:SER:HB3	4	0.4
(1,1931)	2:679:B:VAL:H	2:678:B:SER:HB2	6	0.4
(1,1697)	2:610:B:LYS:H	2:610:B:LYS:HG2	10	0.4
(1,1389)	1:37:A:TRP:HB3	1:37:A:TRP:HE3	1	0.4
(1,1389)	1:37:A:TRP:HB3	1:37:A:TRP:HE3	2	0.4
(1,1389)	1:37:A:TRP:HB3	1:37:A:TRP:HE3	5	0.4
(1,1389)	1:37:A:TRP:HB3	1:37:A:TRP:HE3	6	0.4
(1,1312)	2:654:B:PHE:HB3	2:684:B:ILE:HG12	14	0.4
(1,1222)	2:601:B:GLN:HG3	2:605:B:ILE:HD11	9	0.4
(1,1205)	2:569:B:PRO:HA	2:568:B:PRO:HG2	2	0.4
(1,1188)	2:687:B:THR:H	2:687:B:THR:HG23	7	0.4
(1,712)	2:603:B:ALA:HA	2:606:B:SER:HA	6	0.4
(1,259)	2:617:B:GLU:HG3	2:617:B:GLU:HA	10	0.4
(1,149)	2:596:B:THR:H	2:595:B:LYS:HB2	1	0.4
(1,149)	2:596:B:THR:H	2:595:B:LYS:HB2	14	0.4
(1,124)	2:596:B:THR:HG21	2:684:B:ILE:HD11	12	0.4
(1,116)	2:578:B:GLY:HA3	2:590:B:LYS:HD3	6	0.4
(1,98)	2:672:B:LEU:HD12	2:591:B:VAL:HG22	4	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,98)	2:672:B:LEU:HD12	2:591:B:VAL:HG21	7	0.4
(2,2)	2:595:B:LYS:HD2	2:658:B:TRP:HB3	6	0.39
(1,2866)	2:661:B:CYS:H	2:674:B:CYS:HB2	3	0.39
(1,2846)	2:649:B:TYR:H	2:645:B:VAL:HB	13	0.39
(1,2804)	2:619:B:ILE:H	2:679:B:VAL:HG22	11	0.39
(1,2709)	2:580:B:ILE:H	2:580:B:ILE:HG23	10	0.39
(1,2665)	2:591:B:VAL:HG11	2:658:B:TRP:HH2	2	0.39
(1,2665)	2:591:B:VAL:HG12	2:594:B:LEU:H	11	0.39
(1,2517)	2:605:B:ILE:HG22	2:604:B:GLU:HB3	11	0.39
(1,2512)	2:598:B:ASP:HA	2:601:B:GLN:HG2	6	0.39
(1,2490)	2:656:B:GLN:HB2	2:682:B:VAL:HA	14	0.39
(1,2455)	2:674:B:CYS:HB3	2:673:B:PRO:HB2	6	0.39
(1,2455)	2:674:B:CYS:HB3	2:673:B:PRO:HB2	14	0.39
(1,2380)	2:620:B:GLU:HB3	2:629:B:VAL:HG23	5	0.39
(1,2217)	2:583:B:LEU:HD21	1:38:A:HIS:HA	9	0.39
(1,2132)	2:678:B:SER:H	2:678:B:SER:HB3	7	0.39
(1,1967)	2:653:B:VAL:H	1:41:A:VAL:HA	5	0.39
(1,1967)	2:653:B:VAL:H	1:41:A:VAL:HA	7	0.39
(1,1763)	2:620:B:GLU:H	2:620:B:GLU:HB3	5	0.39
(1,1753)	2:619:B:ILE:H	2:619:B:ILE:HG12	13	0.39
(1,1730)	2:617:B:GLU:H	2:617:B:GLU:HB3	1	0.39
(1,1730)	2:617:B:GLU:H	2:617:B:GLU:HB3	14	0.39
(1,1541)	2:590:B:LYS:H	2:589:B:LYS:HE2	14	0.39
(1,1288)	2:581:B:ILE:HG21	1:34:A:VAL:HA	12	0.39
(1,1222)	2:601:B:GLN:HG3	2:605:B:ILE:HD11	5	0.39
(1,1205)	2:569:B:PRO:HA	2:568:B:PRO:HG2	9	0.39
(1,887)	2:630:B:ILE:HG21	2:643:B:VAL:HG11	10	0.39
(1,576)	2:577:B:LYS:HD2	2:671:B:ASP:HB2	5	0.39
(1,534)	2:684:B:ILE:HG22	2:611:B:ILE:HB	11	0.39
(1,416)	2:653:B:VAL:HB	2:656:B:GLN:HB3	10	0.39
(1,276)	2:619:B:ILE:HG21	2:628:B:ALA:HB2	12	0.39
(1,276)	2:619:B:ILE:HG23	2:628:B:ALA:HB2	15	0.39
(1,259)	2:617:B:GLU:HG3	2:617:B:GLU:HA	4	0.39
(1,259)	2:617:B:GLU:HG3	2:617:B:GLU:HA	13	0.39
(1,245)	2:616:B:VAL:HG11	2:630:B:ILE:HG23	8	0.39
(1,116)	2:578:B:GLY:HA3	2:590:B:LYS:HD3	12	0.39
(1,98)	2:672:B:LEU:HD12	2:591:B:VAL:HG21	14	0.39
(1,2903)	2:678:B:SER:H	2:676:B:LYS:HG3	13	0.38
(1,2898)	2:675:B:SER:H	2:673:B:PRO:HB2	2	0.38
(1,2898)	2:675:B:SER:H	2:673:B:PRO:HB2	3	0.38
(1,2866)	2:651:B:PHE:H	2:674:B:CYS:HB2	7	0.38
(1,2866)	2:661:B:CYS:H	2:674:B:CYS:HB2	12	0.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2866)	2:651:B:PHE:H	2:674:B:CYS:HB2	13	0.38
(1,2709)	2:580:B:ILE:H	2:580:B:ILE:HG22	3	0.38
(1,2709)	2:580:B:ILE:H	2:580:B:ILE:HG21	12	0.38
(1,2709)	2:580:B:ILE:H	2:580:B:ILE:HG21	15	0.38
(1,2665)	2:591:B:VAL:HG13	2:658:B:TRP:HH2	14	0.38
(1,2608)	2:660:B:SER:HA	2:662:B:CYS:HA	5	0.38
(1,2608)	2:660:B:SER:HA	2:662:B:CYS:HA	8	0.38
(1,2517)	2:605:B:ILE:HG21	2:604:B:GLU:HB3	3	0.38
(1,2499)	2:619:B:ILE:H	2:619:B:ILE:HG12	4	0.38
(1,2353)	2:609:B:LEU:HD12	1:38:A:HIS:H	6	0.38
(1,2289)	2:575:B:PHE:HE2	1:39:A:SER:HB3	3	0.38
(1,2132)	2:678:B:SER:H	2:678:B:SER:HB3	15	0.38
(1,2108)	2:674:B:CYS:H	2:673:B:PRO:HB2	2	0.38
(1,2001)	2:658:B:TRP:HE1	2:594:B:LEU:HB2	12	0.38
(1,2001)	2:658:B:TRP:HE1	2:594:B:LEU:HB2	14	0.38
(1,1753)	2:619:B:ILE:H	2:619:B:ILE:HG12	3	0.38
(1,1389)	1:37:A:TRP:HB3	1:37:A:TRP:HE3	13	0.38
(1,1222)	2:601:B:GLN:HG3	2:605:B:ILE:HD12	15	0.38
(1,1194)	2:689:B:LYS:HA	2:610:B:LYS:HE2	1	0.38
(1,1188)	2:687:B:THR:H	2:687:B:THR:HG21	13	0.38
(1,578)	2:577:B:LYS:HD3	2:671:B:ASP:HB2	5	0.38
(1,576)	2:577:B:LYS:HD2	2:671:B:ASP:HB2	1	0.38
(1,276)	2:619:B:ILE:HG23	2:628:B:ALA:HB1	3	0.38
(1,259)	2:617:B:GLU:HG3	2:617:B:GLU:HA	11	0.38
(1,245)	2:616:B:VAL:HG13	2:630:B:ILE:HG23	11	0.38
(1,149)	2:596:B:THR:H	2:595:B:LYS:HB2	13	0.38
(1,124)	2:596:B:THR:HG23	2:684:B:ILE:HD13	7	0.38
(1,105)	2:672:B:LEU:HD23	2:591:B:VAL:HB	13	0.38
(1,98)	2:672:B:LEU:HD13	2:591:B:VAL:HG23	1	0.38
(1,2935)	2:583:B:LEU:HD23	1:39:A:SER:HB3	11	0.37
(1,2898)	2:675:B:SER:H	2:673:B:PRO:HB2	1	0.37
(1,2675)	2:571:B:LEU:HD22	2:568:B:PRO:HG2	3	0.37
(1,2646)	2:687:B:THR:HB	2:611:B:ILE:HA	4	0.37
(1,2630)	2:673:B:PRO:HD3	2:577:B:LYS:HG2	5	0.37
(1,2608)	2:660:B:SER:HA	2:662:B:CYS:HA	7	0.37
(1,2451)	2:674:B:CYS:HB2	2:673:B:PRO:HB2	4	0.37
(1,2320)	2:617:B:GLU:HG3	2:679:B:VAL:HG21	5	0.37
(1,2272)	2:641:B:VAL:HG13	1:44:A:LEU:HB3	2	0.37
(1,2217)	2:583:B:LEU:HD21	1:38:A:HIS:HA	3	0.37
(1,2019)	2:660:B:SER:H	2:663:B:PRO:HB2	10	0.37
(1,2001)	2:658:B:TRP:HE1	2:594:B:LEU:HB2	7	0.37
(1,1931)	2:679:B:VAL:H	2:678:B:SER:HB2	13	0.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1928)	2:645:B:VAL:H	2:645:B:VAL:HG11	12	0.37
(1,1753)	2:619:B:ILE:H	2:619:B:ILE:HG12	6	0.37
(1,1730)	2:617:B:GLU:H	2:617:B:GLU:HB3	5	0.37
(1,1389)	1:37:A:TRP:HB3	1:37:A:TRP:HE3	3	0.37
(1,1389)	1:37:A:TRP:HB3	1:37:A:TRP:HE3	14	0.37
(1,1222)	2:601:B:GLN:HG3	2:605:B:ILE:HD12	13	0.37
(1,1188)	2:687:B:THR:H	2:687:B:THR:HG22	14	0.37
(1,1171)	2:677:B:LEU:HD12	2:678:B:SER:HA	15	0.37
(1,375)	2:644:B:GLU:H	2:643:B:VAL:HB	6	0.37
(1,276)	2:619:B:ILE:HG22	2:628:B:ALA:HB3	5	0.37
(1,276)	2:619:B:ILE:HG22	2:628:B:ALA:HB3	8	0.37
(1,276)	2:619:B:ILE:HG23	2:628:B:ALA:HB1	11	0.37
(1,259)	2:617:B:GLU:HG3	2:617:B:GLU:HA	2	0.37
(1,259)	2:617:B:GLU:HG3	2:617:B:GLU:HA	8	0.37
(1,259)	2:617:B:GLU:HG3	2:617:B:GLU:HA	15	0.37
(1,132)	2:591:B:VAL:HG23	2:577:B:LYS:HA	4	0.37
(1,124)	2:596:B:THR:HG22	2:684:B:ILE:HD12	13	0.37
(1,116)	2:578:B:GLY:HA3	2:590:B:LYS:HD3	7	0.37
(1,105)	2:672:B:LEU:HD22	2:591:B:VAL:HB	2	0.37
(1,2958)	2:641:B:VAL:HG21	1:44:A:LEU:HD22	4	0.36
(1,2935)	2:583:B:LEU:HD23	1:39:A:SER:HB3	1	0.36
(1,2935)	2:583:B:LEU:HD21	1:39:A:SER:HB3	5	0.36
(1,2898)	2:675:B:SER:H	2:673:B:PRO:HB2	5	0.36
(1,2709)	2:580:B:ILE:H	2:580:B:ILE:HG23	7	0.36
(1,2675)	2:571:B:LEU:HD22	2:572:B:PRO:HG2	10	0.36
(1,2654)	2:674:B:CYS:HB2	2:676:B:LYS:HD3	8	0.36
(1,2455)	2:674:B:CYS:HB3	2:673:B:PRO:HB2	3	0.36
(1,2217)	2:583:B:LEU:HD22	1:38:A:HIS:HA	8	0.36
(1,2217)	2:583:B:LEU:HD23	1:38:A:HIS:HA	11	0.36
(1,2132)	2:678:B:SER:H	2:678:B:SER:HB3	14	0.36
(1,2070)	2:668:B:GLN:H	2:668:B:GLN:HG2	12	0.36
(1,2001)	2:658:B:TRP:HE1	2:594:B:LEU:HB2	15	0.36
(1,1902)	2:640:B:GLN:H	2:640:B:GLN:HG3	4	0.36
(1,1753)	2:619:B:ILE:H	2:619:B:ILE:HG12	2	0.36
(1,1753)	2:619:B:ILE:H	2:619:B:ILE:HG12	8	0.36
(1,1698)	2:610:B:LYS:H	2:609:B:LEU:HD13	15	0.36
(1,1649)	2:602:B:SER:H	2:602:B:SER:HB2	11	0.36
(1,1540)	2:590:B:LYS:H	2:590:B:LYS:HE2	11	0.36
(1,1222)	2:601:B:GLN:HG3	2:605:B:ILE:HD12	1	0.36
(1,1222)	2:601:B:GLN:HG3	2:605:B:ILE:HD12	4	0.36
(1,1205)	2:569:B:PRO:HA	2:568:B:PRO:HG2	15	0.36
(1,1194)	2:689:B:LYS:HA	2:610:B:LYS:HE2	3	0.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1188)	2:687:B:THR:H	2:687:B:THR:HG21	3	0.36
(1,383)	2:646:B:LEU:H	2:645:B:VAL:HB	5	0.36
(1,375)	2:644:B:GLU:H	2:643:B:VAL:HB	7	0.36
(1,276)	2:619:B:ILE:HG21	2:628:B:ALA:HB2	6	0.36
(1,149)	2:596:B:THR:H	2:595:B:LYS:HB2	15	0.36
(1,128)	2:591:B:VAL:HG13	2:591:B:VAL:H	9	0.36
(1,116)	2:578:B:GLY:HA3	2:590:B:LYS:HD3	8	0.36
(1,105)	2:672:B:LEU:HD23	2:591:B:VAL:HB	4	0.36
(1,85)	2:588:B:LEU:HD23	2:582:B:GLN:HB3	15	0.36
(1,2935)	2:583:B:LEU:HD21	1:39:A:SER:HB3	13	0.35
(1,2709)	2:580:B:ILE:H	2:580:B:ILE:HG22	6	0.35
(1,2675)	2:571:B:LEU:HD22	2:572:B:PRO:HG2	4	0.35
(1,2630)	2:673:B:PRO:HD3	2:577:B:LYS:HG2	10	0.35
(1,2608)	2:660:B:SER:HA	2:662:B:CYS:HA	1	0.35
(1,2608)	2:660:B:SER:HA	2:662:B:CYS:HA	9	0.35
(1,2517)	2:605:B:ILE:HG21	2:604:B:GLU:HB3	2	0.35
(1,2270)	2:641:B:VAL:HG11	1:44:A:LEU:HD12	5	0.35
(1,2270)	2:641:B:VAL:HG12	1:44:A:LEU:HD13	15	0.35
(1,2070)	2:668:B:GLN:H	2:668:B:GLN:HG2	5	0.35
(1,2001)	2:658:B:TRP:HE1	2:594:B:LEU:HB2	3	0.35
(1,1982)	2:655:B:GLY:H	2:596:B:THR:HG22	2	0.35
(1,1979)	2:655:B:GLY:H	2:654:B:PHE:HA	3	0.35
(1,1979)	2:655:B:GLY:H	2:654:B:PHE:HA	4	0.35
(1,1753)	2:619:B:ILE:H	2:619:B:ILE:HG12	10	0.35
(1,1753)	2:619:B:ILE:H	2:619:B:ILE:HG12	15	0.35
(1,1389)	1:37:A:TRP:HB3	1:37:A:TRP:HE3	4	0.35
(1,1389)	1:37:A:TRP:HB3	1:37:A:TRP:HE3	8	0.35
(1,1389)	1:37:A:TRP:HB3	1:37:A:TRP:HE3	9	0.35
(1,1211)	2:630:B:ILE:HA	2:619:B:ILE:HG13	11	0.35
(1,1194)	2:689:B:LYS:HA	2:610:B:LYS:HE2	8	0.35
(1,1194)	2:689:B:LYS:HA	2:610:B:LYS:HE2	11	0.35
(1,1117)	2:589:B:LYS:HB2	2:589:B:LYS:HE2	9	0.35
(1,375)	2:644:B:GLU:H	2:643:B:VAL:HB	11	0.35
(1,276)	2:619:B:ILE:HG21	2:628:B:ALA:HB1	1	0.35
(1,245)	2:616:B:VAL:HG11	2:630:B:ILE:HG22	7	0.35
(1,149)	2:596:B:THR:H	2:595:B:LYS:HB2	12	0.35
(1,132)	2:591:B:VAL:HG23	2:577:B:LYS:HA	10	0.35
(1,124)	2:596:B:THR:HG22	2:684:B:ILE:HD11	9	0.35
(1,116)	2:578:B:GLY:HA3	2:590:B:LYS:HD3	14	0.35
(1,2866)	2:661:B:CYS:H	2:674:B:CYS:HB2	14	0.34
(1,2709)	2:580:B:ILE:H	2:580:B:ILE:HG22	1	0.34
(1,2709)	2:580:B:ILE:H	2:580:B:ILE:HG21	5	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2709)	2:580:B:ILE:H	2:580:B:ILE:HG21	14	0.34
(1,2455)	2:674:B:CYS:HB3	2:673:B:PRO:HB2	15	0.34
(1,2313)	2:583:B:LEU:HD12	2:589:B:LYS:HE2	11	0.34
(1,2289)	2:575:B:PHE:HE1	1:39:A:SER:HB3	12	0.34
(1,2217)	2:583:B:LEU:HD21	1:38:A:HIS:HA	5	0.34
(1,2209)	2:576:B:MET:HB2	1:39:A:SER:HG	3	0.34
(1,2134)	2:678:B:SER:H	2:681:B:ASP:HB2	7	0.34
(1,2132)	2:678:B:SER:H	2:678:B:SER:HB3	10	0.34
(1,2132)	2:678:B:SER:H	2:678:B:SER:HB3	13	0.34
(1,2107)	2:674:B:CYS:H	2:674:B:CYS:HB3	13	0.34
(1,2070)	2:668:B:GLN:H	2:668:B:GLN:HG2	6	0.34
(1,2070)	2:668:B:GLN:H	2:668:B:GLN:HG2	15	0.34
(1,2019)	2:660:B:SER:H	2:663:B:PRO:HB2	1	0.34
(1,1979)	2:655:B:GLY:H	2:654:B:PHE:HA	1	0.34
(1,1979)	2:655:B:GLY:H	2:654:B:PHE:HA	8	0.34
(1,1979)	2:655:B:GLY:H	2:654:B:PHE:HA	14	0.34
(1,1931)	2:679:B:VAL:H	2:678:B:SER:HB2	3	0.34
(1,1931)	2:679:B:VAL:H	2:678:B:SER:HB2	9	0.34
(1,1928)	2:645:B:VAL:H	2:645:B:VAL:HG12	5	0.34
(1,1902)	2:640:B:GLN:H	2:640:B:GLN:HG3	12	0.34
(1,1789)	2:624:B:SER:H	2:624:B:SER:HB3	11	0.34
(1,1753)	2:619:B:ILE:H	2:619:B:ILE:HG12	11	0.34
(1,1730)	2:617:B:GLU:H	2:617:B:GLU:HB3	4	0.34
(1,1730)	2:617:B:GLU:H	2:617:B:GLU:HB3	10	0.34
(1,1425)	2:571:B:LEU:H	2:571:B:LEU:HB2	3	0.34
(1,1424)	2:571:B:LEU:H	2:570:B:THR:HA	4	0.34
(1,1389)	1:37:A:TRP:HB3	1:37:A:TRP:HE3	7	0.34
(1,1222)	2:601:B:GLN:HG3	2:605:B:ILE:HD13	2	0.34
(1,1205)	2:569:B:PRO:HA	2:568:B:PRO:HG2	5	0.34
(1,1060)	2:666:B:THR:HG22	1:40:A:LEU:HA	4	0.34
(1,887)	2:630:B:ILE:HG23	2:643:B:VAL:HG13	3	0.34
(1,578)	2:577:B:LYS:HD3	2:671:B:ASP:HB2	15	0.34
(1,416)	2:653:B:VAL:HB	2:656:B:GLN:HB3	12	0.34
(1,383)	2:646:B:LEU:H	2:645:B:VAL:HB	9	0.34
(1,375)	2:644:B:GLU:H	2:643:B:VAL:HB	5	0.34
(1,375)	2:644:B:GLU:H	2:643:B:VAL:HB	12	0.34
(1,102)	2:672:B:LEU:HD12	2:673:B:PRO:HD3	8	0.34
(1,2935)	2:583:B:LEU:HD21	1:39:A:SER:HB3	3	0.33
(1,2928)	2:645:B:VAL:HG23	1:44:A:LEU:HD13	9	0.33
(1,2675)	2:571:B:LEU:HD21	2:572:B:PRO:HG2	8	0.33
(1,2665)	2:591:B:VAL:HG13	2:594:B:LEU:H	1	0.33
(1,2451)	2:674:B:CYS:HB2	2:673:B:PRO:HB2	8	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2317)	2:587:B:GLU:HB3	2:589:B:LYS:HG3	9	0.33
(1,2289)	2:575:B:PHE:HE2	1:39:A:SER:HB3	13	0.33
(1,2132)	2:678:B:SER:H	2:678:B:SER:HB3	8	0.33
(1,2019)	2:660:B:SER:H	2:663:B:PRO:HB2	2	0.33
(1,2019)	2:660:B:SER:H	2:663:B:PRO:HB2	4	0.33
(1,1979)	2:655:B:GLY:H	2:654:B:PHE:HA	11	0.33
(1,1730)	2:617:B:GLU:H	2:617:B:GLU:HB3	2	0.33
(1,1649)	2:602:B:SER:H	2:602:B:SER:HB2	15	0.33
(1,1402)	1:40:A:LEU:HD13	1:39:A:SER:H	6	0.33
(1,1402)	1:40:A:LEU:HD13	1:39:A:SER:H	15	0.33
(1,1288)	2:581:B:ILE:HG23	1:34:A:VAL:HA	4	0.33
(1,1211)	2:630:B:ILE:HA	2:619:B:ILE:HG13	2	0.33
(1,1194)	2:689:B:LYS:HA	2:610:B:LYS:HE2	13	0.33
(1,1188)	2:687:B:THR:H	2:687:B:THR:HG22	1	0.33
(1,1171)	2:677:B:LEU:HD12	2:678:B:SER:HA	4	0.33
(1,375)	2:644:B:GLU:H	2:643:B:VAL:HB	1	0.33
(1,124)	2:596:B:THR:HG22	2:684:B:ILE:HD12	1	0.33
(1,105)	2:672:B:LEU:HD21	2:591:B:VAL:HB	3	0.33
(1,2935)	2:583:B:LEU:HD21	1:39:A:SER:HB3	9	0.32
(1,2665)	2:591:B:VAL:HG12	2:658:B:TRP:HH2	4	0.32
(1,2654)	2:674:B:CYS:HB2	2:676:B:LYS:HD3	13	0.32
(1,2630)	2:673:B:PRO:HD3	2:577:B:LYS:HG2	9	0.32
(1,2608)	2:660:B:SER:HA	2:662:B:CYS:HA	13	0.32
(1,2457)	2:674:B:CYS:HB3	2:666:B:THR:HA	8	0.32
(1,2455)	2:674:B:CYS:HB3	2:673:B:PRO:HB2	1	0.32
(1,2320)	2:617:B:GLU:HG3	2:679:B:VAL:HG23	14	0.32
(1,2289)	2:575:B:PHE:HE1	1:39:A:SER:HB3	6	0.32
(1,2267)	2:643:B:VAL:HG21	1:44:A:LEU:HD12	4	0.32
(1,2217)	2:583:B:LEU:HD22	1:38:A:HIS:HA	12	0.32
(1,2176)	2:684:B:ILE:H	2:684:B:ILE:HG12	6	0.32
(1,2019)	2:660:B:SER:H	2:663:B:PRO:HB2	8	0.32
(1,1789)	2:624:B:SER:H	2:624:B:SER:HB3	8	0.32
(1,1730)	2:617:B:GLU:H	2:617:B:GLU:HB3	8	0.32
(1,1730)	2:617:B:GLU:H	2:617:B:GLU:HB3	11	0.32
(1,1730)	2:617:B:GLU:H	2:617:B:GLU:HB3	13	0.32
(1,1698)	2:610:B:LYS:H	2:609:B:LEU:HD12	1	0.32
(1,1697)	2:610:B:LYS:H	2:610:B:LYS:HG2	7	0.32
(1,1649)	2:602:B:SER:H	2:602:B:SER:HB2	2	0.32
(1,1649)	2:602:B:SER:H	2:602:B:SER:HB2	10	0.32
(1,1638)	2:601:B:GLN:H	2:601:B:GLN:HG2	14	0.32
(1,1607)	2:598:B:ASP:H	2:595:B:LYS:HB3	10	0.32
(1,1188)	2:687:B:THR:H	2:687:B:THR:HG21	5	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1188)	2:687:B:THR:H	2:687:B:THR:HG23	9	0.32
(1,576)	2:577:B:LYS:HD2	2:671:B:ASP:HB2	14	0.32
(1,552)	2:686:B:LEU:HD12	2:611:B:ILE:HA	7	0.32
(1,420)	2:654:B:PHE:HB2	2:682:B:VAL:HB	3	0.32
(1,375)	2:644:B:GLU:H	2:643:B:VAL:HB	9	0.32
(1,375)	2:644:B:GLU:H	2:643:B:VAL:HB	14	0.32
(1,276)	2:619:B:ILE:HG23	2:628:B:ALA:HB3	4	0.32
(1,276)	2:619:B:ILE:HG22	2:628:B:ALA:HB3	10	0.32
(1,124)	2:596:B:THR:HG22	2:684:B:ILE:HD12	11	0.32
(2,2)	2:595:B:LYS:HD2	2:658:B:TRP:HB3	12	0.31
(1,2935)	2:583:B:LEU:HD23	1:39:A:SER:HB3	2	0.31
(1,2898)	2:675:B:SER:H	2:673:B:PRO:HB2	10	0.31
(1,2709)	2:580:B:ILE:H	2:580:B:ILE:HG21	2	0.31
(1,2608)	2:660:B:SER:HA	2:662:B:CYS:HA	6	0.31
(1,2488)	2:590:B:LYS:HB3	2:592:B:GLU:HA	9	0.31
(1,2320)	2:617:B:GLU:HG3	2:679:B:VAL:HG22	1	0.31
(1,2289)	2:575:B:PHE:HE1	1:39:A:SER:HB3	2	0.31
(1,2263)	2:614:B:SER:HB2	1:47:A:SER:HB3	9	0.31
(1,2217)	2:583:B:LEU:HD22	1:38:A:HIS:HA	10	0.31
(1,2108)	2:674:B:CYS:H	2:673:B:PRO:HB2	13	0.31
(1,2019)	2:660:B:SER:H	2:663:B:PRO:HB2	9	0.31
(1,2019)	2:660:B:SER:H	2:663:B:PRO:HB2	15	0.31
(1,2001)	2:658:B:TRP:HE1	2:594:B:LEU:HB2	4	0.31
(1,1931)	2:679:B:VAL:H	2:678:B:SER:HB2	1	0.31
(1,1835)	2:627:B:VAL:H	2:646:B:LEU:HA	5	0.31
(1,1789)	2:624:B:SER:H	2:624:B:SER:HB3	2	0.31
(1,1730)	2:617:B:GLU:H	2:617:B:GLU:HB3	15	0.31
(1,1649)	2:602:B:SER:H	2:602:B:SER:HB2	14	0.31
(1,1211)	2:630:B:ILE:HA	2:619:B:ILE:HG13	6	0.31
(1,1211)	2:630:B:ILE:HA	2:619:B:ILE:HG13	12	0.31
(1,1194)	2:689:B:LYS:HA	2:610:B:LYS:HE2	7	0.31
(1,1188)	2:687:B:THR:H	2:687:B:THR:HG21	15	0.31
(1,1086)	2:609:B:LEU:HD22	1:37:A:TRP:HZ3	12	0.31
(1,950)	2:572:B:PRO:HB2	2:573:B:PRO:HD3	14	0.31
(1,896)	2:630:B:ILE:HD13	2:651:B:PHE:HE1	7	0.31
(1,686)	2:600:B:ILE:HG13	2:600:B:ILE:HG22	13	0.31
(1,375)	2:644:B:GLU:H	2:643:B:VAL:HB	8	0.31
(1,375)	2:644:B:GLU:H	2:643:B:VAL:HB	10	0.31
(1,375)	2:644:B:GLU:H	2:643:B:VAL:HB	13	0.31
(1,375)	2:644:B:GLU:H	2:643:B:VAL:HB	15	0.31
(1,276)	2:619:B:ILE:HG23	2:628:B:ALA:HB2	2	0.31
(1,232)	2:611:B:ILE:HG22	2:684:B:ILE:HD12	6	0.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	2:596:B:THR:H	2:595:B:LYS:HB2	6	0.31
(2,2)	2:595:B:LYS:HD2	2:658:B:TRP:HB3	15	0.3
(1,2709)	2:580:B:ILE:H	2:580:B:ILE:HG21	8	0.3
(1,2654)	2:674:B:CYS:HB2	2:676:B:LYS:HD3	5	0.3
(1,2608)	2:660:B:SER:HA	2:662:B:CYS:HA	12	0.3
(1,2599)	2:645:B:VAL:HG12	2:629:B:VAL:HA	2	0.3
(1,2353)	2:609:B:LEU:HD13	1:38:A:HIS:H	5	0.3
(1,2318)	2:665:B:ARG:HB2	2:669:B:LEU:HD12	13	0.3
(1,2263)	2:614:B:SER:HB2	1:47:A:SER:HB2	12	0.3
(1,2217)	2:583:B:LEU:HD21	1:38:A:HIS:HA	6	0.3
(1,2217)	2:583:B:LEU:HD22	1:38:A:HIS:HA	15	0.3
(1,2176)	2:684:B:ILE:H	2:684:B:ILE:HG12	11	0.3
(1,2107)	2:674:B:CYS:H	2:674:B:CYS:HB3	3	0.3
(1,1977)	2:654:B:PHE:H	2:682:B:VAL:HG22	1	0.3
(1,1649)	2:602:B:SER:H	2:602:B:SER:HB2	12	0.3
(1,1628)	2:600:B:ILE:H	2:600:B:ILE:HG12	15	0.3
(1,1533)	2:589:B:LYS:H	2:589:B:LYS:HB3	11	0.3
(1,1533)	2:589:B:LYS:H	2:589:B:LYS:HB3	15	0.3
(1,1449)	2:577:B:LYS:H	2:672:B:LEU:HB3	14	0.3
(1,1222)	2:601:B:GLN:HG3	2:605:B:ILE:HD12	6	0.3
(1,1222)	2:601:B:GLN:HG3	2:605:B:ILE:HD11	11	0.3
(1,1219)	2:659:B:SER:HB2	2:677:B:LEU:HD23	5	0.3
(1,1205)	2:569:B:PRO:HA	2:568:B:PRO:HG2	10	0.3
(1,1205)	2:569:B:PRO:HA	2:568:B:PRO:HG2	11	0.3
(1,686)	2:600:B:ILE:HG13	2:600:B:ILE:HG23	3	0.3
(1,686)	2:600:B:ILE:HG13	2:600:B:ILE:HG23	9	0.3
(1,686)	2:600:B:ILE:HG13	2:600:B:ILE:HG21	11	0.3
(1,686)	2:600:B:ILE:HG13	2:600:B:ILE:HG23	12	0.3
(1,375)	2:644:B:GLU:H	2:643:B:VAL:HB	3	0.3
(1,375)	2:644:B:GLU:H	2:643:B:VAL:HB	4	0.3
(1,105)	2:672:B:LEU:HD21	2:591:B:VAL:HB	14	0.3
(1,98)	2:672:B:LEU:HD12	2:591:B:VAL:HG23	11	0.3
(1,27)	2:577:B:LYS:HE3	2:577:B:LYS:HG3	7	0.3
(1,2674)	2:571:B:LEU:HD11	2:569:B:PRO:HB3	11	0.29
(1,2654)	2:674:B:CYS:HB2	2:676:B:LYS:HD3	4	0.29
(1,2608)	2:660:B:SER:HA	2:662:B:CYS:HA	3	0.29
(1,2517)	2:605:B:ILE:HG22	2:604:B:GLU:HB3	6	0.29
(1,2217)	2:583:B:LEU:HD23	1:38:A:HIS:HA	2	0.29
(1,2176)	2:684:B:ILE:H	2:684:B:ILE:HG12	3	0.29
(1,2132)	2:678:B:SER:H	2:678:B:SER:HB3	1	0.29
(1,2019)	2:660:B:SER:H	2:663:B:PRO:HB2	5	0.29
(1,2019)	2:660:B:SER:H	2:663:B:PRO:HB2	11	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1255)	2:672:B:LEU:HD12	2:592:B:GLU:HA	8	0.29
(1,887)	2:630:B:ILE:HG22	2:643:B:VAL:HG12	12	0.29
(1,686)	2:600:B:ILE:HG13	2:600:B:ILE:HG22	2	0.29
(1,686)	2:600:B:ILE:HG13	2:600:B:ILE:HG23	6	0.29
(1,686)	2:600:B:ILE:HG13	2:600:B:ILE:HG22	8	0.29
(1,132)	2:591:B:VAL:HG21	2:577:B:LYS:HA	14	0.29
(1,2898)	2:675:B:SER:H	2:673:B:PRO:HB2	15	0.28
(1,2647)	2:687:B:THR:HG22	2:610:B:LYS:HD3	5	0.28
(1,2608)	2:660:B:SER:HA	2:662:B:CYS:HA	14	0.28
(1,2535)	2:660:B:SER:HB2	2:662:B:CYS:HA	9	0.28
(1,2455)	2:674:B:CYS:HB3	2:673:B:PRO:HB2	13	0.28
(1,2379)	2:583:B:LEU:H	2:587:B:GLU:HG2	2	0.28
(1,2217)	2:583:B:LEU:HD23	1:38:A:HIS:HA	1	0.28
(1,2176)	2:684:B:ILE:H	2:684:B:ILE:HG12	7	0.28
(1,2132)	2:678:B:SER:H	2:678:B:SER:HB3	3	0.28
(1,2132)	2:678:B:SER:H	2:678:B:SER:HB3	11	0.28
(1,2107)	2:674:B:CYS:H	2:674:B:CYS:HB3	7	0.28
(1,2019)	2:660:B:SER:H	2:663:B:PRO:HB2	12	0.28
(1,1928)	2:645:B:VAL:H	2:645:B:VAL:HG13	9	0.28
(1,1870)	2:636:B:GLU:H	2:636:B:GLU:HG3	7	0.28
(1,1835)	2:627:B:VAL:H	2:646:B:LEU:HA	1	0.28
(1,1835)	2:627:B:VAL:H	2:646:B:LEU:HA	7	0.28
(1,1835)	2:627:B:VAL:H	2:646:B:LEU:HA	9	0.28
(1,1835)	2:627:B:VAL:H	2:646:B:LEU:HA	15	0.28
(1,1753)	2:619:B:ILE:H	2:619:B:ILE:HG12	4	0.28
(1,1533)	2:589:B:LYS:H	2:589:B:LYS:HB3	10	0.28
(1,1525)	2:588:B:LEU:H	2:587:B:GLU:HB3	15	0.28
(1,1430)	2:575:B:PHE:H	2:576:B:MET:H	9	0.28
(1,1424)	2:571:B:LEU:H	2:570:B:THR:HA	11	0.28
(1,1205)	2:569:B:PRO:HA	2:568:B:PRO:HG2	12	0.28
(1,1205)	2:569:B:PRO:HA	2:568:B:PRO:HG2	13	0.28
(1,1194)	2:689:B:LYS:HA	2:610:B:LYS:HE2	15	0.28
(1,950)	2:572:B:PRO:HB2	2:573:B:PRO:HD3	3	0.28
(1,950)	2:572:B:PRO:HB2	2:573:B:PRO:HD3	13	0.28
(1,686)	2:600:B:ILE:HG13	2:600:B:ILE:HG23	7	0.28
(1,686)	2:600:B:ILE:HG13	2:600:B:ILE:HG23	10	0.28
(1,671)	2:596:B:THR:HG23	2:596:B:THR:HA	1	0.28
(1,671)	2:596:B:THR:HG23	2:596:B:THR:HA	2	0.28
(1,671)	2:596:B:THR:HG21	2:596:B:THR:HA	4	0.28
(1,578)	2:577:B:LYS:HD3	2:671:B:ASP:HB2	9	0.28
(1,2675)	2:571:B:LEU:HD21	2:572:B:PRO:HG2	7	0.27
(1,2488)	2:590:B:LYS:HB3	2:592:B:GLU:HA	6	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2320)	2:617:B:GLU:HG3	2:679:B:VAL:HG22	12	0.27
(1,2276)	2:643:B:VAL:HG12	1:44:A:LEU:HD12	2	0.27
(1,2272)	2:641:B:VAL:HG12	1:44:A:LEU:HB3	12	0.27
(1,2176)	2:684:B:ILE:H	2:684:B:ILE:HG12	1	0.27
(1,2176)	2:684:B:ILE:H	2:684:B:ILE:HG12	4	0.27
(1,2176)	2:684:B:ILE:H	2:684:B:ILE:HG12	14	0.27
(1,2018)	2:660:B:SER:H	2:674:B:CYS:HB2	15	0.27
(1,2001)	2:658:B:TRP:HE1	2:594:B:LEU:HB2	13	0.27
(1,1982)	2:655:B:GLY:H	2:596:B:THR:HG22	3	0.27
(1,1835)	2:627:B:VAL:H	2:646:B:LEU:HA	14	0.27
(1,1533)	2:589:B:LYS:H	2:589:B:LYS:HB3	13	0.27
(1,1194)	2:689:B:LYS:HA	2:610:B:LYS:HE2	2	0.27
(1,1194)	2:689:B:LYS:HA	2:610:B:LYS:HE2	5	0.27
(1,1076)	2:581:B:ILE:HD13	1:35:A:PHE:HD1	5	0.27
(1,1057)	2:650:B:PRO:HG2	2:666:B:THR:HG21	5	0.27
(1,671)	2:596:B:THR:HG21	2:596:B:THR:HA	3	0.27
(1,671)	2:596:B:THR:HG22	2:596:B:THR:HA	8	0.27
(1,671)	2:596:B:THR:HG23	2:596:B:THR:HA	9	0.27
(1,671)	2:596:B:THR:HG23	2:596:B:THR:HA	11	0.27
(1,578)	2:577:B:LYS:HD3	2:671:B:ASP:HB2	1	0.27
(1,503)	2:677:B:LEU:HB2	2:677:B:LEU:HD12	7	0.27
(1,426)	2:654:B:PHE:HB3	2:656:B:GLN:HE22	4	0.27
(1,426)	2:654:B:PHE:HB3	2:656:B:GLN:HE22	8	0.27
(1,375)	2:644:B:GLU:H	2:643:B:VAL:HB	2	0.27
(1,149)	2:596:B:THR:H	2:595:B:LYS:HB2	5	0.27
(1,149)	2:596:B:THR:H	2:595:B:LYS:HB2	7	0.27
(1,132)	2:591:B:VAL:HG23	2:577:B:LYS:HA	9	0.27
(1,124)	2:596:B:THR:HG21	2:684:B:ILE:HD12	5	0.27
(1,2926)	2:653:B:VAL:HG13	1:44:A:LEU:HB2	13	0.26
(1,2675)	2:571:B:LEU:HD22	2:572:B:PRO:HG2	13	0.26
(1,2630)	2:673:B:PRO:HD3	2:577:B:LYS:HG2	11	0.26
(1,2609)	2:660:B:SER:HA	2:677:B:LEU:HB3	5	0.26
(1,2465)	2:677:B:LEU:HD13	2:651:B:PHE:HD1	8	0.26
(1,2380)	2:620:B:GLU:HB3	2:629:B:VAL:HG22	10	0.26
(1,2353)	2:609:B:LEU:HD11	1:38:A:HIS:H	11	0.26
(1,2270)	2:641:B:VAL:HG12	1:44:A:LEU:HD11	13	0.26
(1,2176)	2:684:B:ILE:H	2:684:B:ILE:HG12	8	0.26
(1,2176)	2:684:B:ILE:H	2:684:B:ILE:HG12	12	0.26
(1,2132)	2:678:B:SER:H	2:678:B:SER:HB3	9	0.26
(1,2107)	2:674:B:CYS:H	2:674:B:CYS:HB3	12	0.26
(1,2107)	2:674:B:CYS:H	2:674:B:CYS:HB3	14	0.26
(1,2019)	2:660:B:SER:H	2:663:B:PRO:HB2	14	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2001)	2:658:B:TRP:HE1	2:594:B:LEU:HB2	8	0.26
(1,1931)	2:679:B:VAL:H	2:678:B:SER:HB2	11	0.26
(1,1835)	2:627:B:VAL:H	2:646:B:LEU:HA	4	0.26
(1,1533)	2:589:B:LYS:H	2:589:B:LYS:HB3	5	0.26
(1,1533)	2:589:B:LYS:H	2:589:B:LYS:HB3	8	0.26
(1,1533)	2:589:B:LYS:H	2:589:B:LYS:HB3	12	0.26
(1,1465)	2:580:B:ILE:H	2:579:B:SER:HB3	13	0.26
(1,1430)	2:575:B:PHE:H	2:576:B:MET:H	8	0.26
(1,1312)	2:654:B:PHE:HB3	2:684:B:ILE:HG12	13	0.26
(1,1205)	2:569:B:PRO:HA	2:568:B:PRO:HG2	4	0.26
(1,1205)	2:569:B:PRO:HA	2:568:B:PRO:HG2	8	0.26
(1,1130)	2:580:B:ILE:HG21	2:580:B:ILE:HG12	6	0.26
(1,1130)	2:580:B:ILE:HG22	2:580:B:ILE:HG12	10	0.26
(1,1130)	2:580:B:ILE:HG22	2:580:B:ILE:HG12	12	0.26
(1,854)	2:638:B:ARG:HG2	2:638:B:ARG:HD3	7	0.26
(1,686)	2:600:B:ILE:HG13	2:600:B:ILE:HG21	4	0.26
(1,671)	2:596:B:THR:HG21	2:596:B:THR:HA	14	0.26
(1,276)	2:619:B:ILE:HG21	2:628:B:ALA:HB1	13	0.26
(1,232)	2:611:B:ILE:HG23	2:684:B:ILE:HD11	7	0.26
(1,22)	2:571:B:LEU:HD23	2:571:B:LEU:HA	14	0.26
(1,2935)	2:583:B:LEU:HD21	1:39:A:SER:HB3	4	0.25
(1,2860)	2:659:B:SER:H	2:675:B:SER:HA	12	0.25
(1,2846)	2:649:B:TYR:H	2:645:B:VAL:HB	10	0.25
(1,2654)	2:674:B:CYS:HB2	2:676:B:LYS:HD3	6	0.25
(1,2647)	2:687:B:THR:HG23	2:610:B:LYS:HD3	14	0.25
(1,2630)	2:673:B:PRO:HD3	2:577:B:LYS:HG2	15	0.25
(1,2529)	2:613:B:SER:HB2	2:682:B:VAL:HG13	8	0.25
(1,2411)	2:679:B:VAL:H	2:679:B:VAL:HG23	8	0.25
(1,2320)	2:617:B:GLU:HG3	2:679:B:VAL:HG21	3	0.25
(1,2318)	2:587:B:GLU:HB3	2:583:B:LEU:HD12	15	0.25
(1,2176)	2:684:B:ILE:H	2:684:B:ILE:HG12	9	0.25
(1,2001)	2:658:B:TRP:HE1	2:594:B:LEU:HB2	6	0.25
(1,1980)	2:655:B:GLY:H	2:654:B:PHE:HB2	13	0.25
(1,1697)	2:610:B:LYS:H	2:610:B:LYS:HG2	2	0.25
(1,1533)	2:589:B:LYS:H	2:589:B:LYS:HB3	1	0.25
(1,1533)	2:589:B:LYS:H	2:589:B:LYS:HB3	2	0.25
(1,1533)	2:589:B:LYS:H	2:589:B:LYS:HB3	9	0.25
(1,1525)	2:588:B:LEU:H	2:587:B:GLU:HB3	6	0.25
(1,1430)	2:575:B:PHE:H	2:576:B:MET:H	14	0.25
(1,1370)	1:44:A:LEU:HA	1:44:A:LEU:HD21	10	0.25
(1,1211)	2:630:B:ILE:HA	2:619:B:ILE:HG13	13	0.25
(1,1205)	2:569:B:PRO:HA	2:568:B:PRO:HG2	6	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1194)	2:689:B:LYS:HA	2:610:B:LYS:HE3	14	0.25
(1,1060)	2:666:B:THR:HG22	1:40:A:LEU:HA	12	0.25
(1,1057)	2:650:B:PRO:HG2	2:666:B:THR:HG23	7	0.25
(1,1006)	2:652:B:PHE:HA	1:41:A:VAL:HA	14	0.25
(1,950)	2:572:B:PRO:HB2	2:573:B:PRO:HD3	4	0.25
(1,686)	2:600:B:ILE:HG13	2:600:B:ILE:HG21	1	0.25
(1,671)	2:596:B:THR:HG21	2:596:B:THR:HA	7	0.25
(1,503)	2:677:B:LEU:HB2	2:677:B:LEU:HD13	11	0.25
(1,427)	2:654:B:PHE:HB2	2:656:B:GLN:HE22	12	0.25
(1,426)	2:654:B:PHE:HB3	2:656:B:GLN:HE22	11	0.25
(1,253)	2:617:B:GLU:HG2	2:633:B:ALA:HB3	6	0.25
(1,132)	2:591:B:VAL:HG21	2:577:B:LYS:HA	7	0.25
(1,124)	2:596:B:THR:HG22	2:684:B:ILE:HD11	3	0.25
(1,95)	2:589:B:LYS:HE3	2:583:B:LEU:HD13	6	0.25
(1,83)	2:588:B:LEU:HD12	2:588:B:LEU:HD22	9	0.25
(1,2860)	2:659:B:SER:H	2:675:B:SER:HA	6	0.24
(1,2678)	1:34:A:VAL:HB	1:34:A:VAL:HG21	3	0.24
(1,2678)	1:34:A:VAL:HB	1:34:A:VAL:HG21	7	0.24
(1,2678)	1:34:A:VAL:HB	1:34:A:VAL:HG13	11	0.24
(1,2678)	1:34:A:VAL:HB	1:34:A:VAL:HG12	14	0.24
(1,2654)	2:674:B:CYS:HB2	2:676:B:LYS:HD3	3	0.24
(1,2320)	2:617:B:GLU:HG3	2:679:B:VAL:HG22	7	0.24
(1,2320)	2:617:B:GLU:HG3	2:679:B:VAL:HG22	9	0.24
(1,2029)	2:662:B:CYS:H	2:660:B:SER:HB2	9	0.24
(1,1982)	2:655:B:GLY:H	2:596:B:THR:HG21	8	0.24
(1,1980)	2:655:B:GLY:H	2:654:B:PHE:HB2	5	0.24
(1,1979)	2:655:B:GLY:H	2:654:B:PHE:HA	2	0.24
(1,1835)	2:627:B:VAL:H	2:646:B:LEU:HA	6	0.24
(1,1835)	2:627:B:VAL:H	2:646:B:LEU:HA	8	0.24
(1,1835)	2:627:B:VAL:H	2:646:B:LEU:HA	10	0.24
(1,1628)	2:600:B:ILE:H	2:600:B:ILE:HG12	5	0.24
(1,1540)	2:590:B:LYS:H	2:590:B:LYS:HE2	10	0.24
(1,1533)	2:589:B:LYS:H	2:589:B:LYS:HB3	4	0.24
(1,1525)	2:588:B:LEU:H	2:587:B:GLU:HB3	3	0.24
(1,1525)	2:588:B:LEU:H	2:587:B:GLU:HB3	13	0.24
(1,1449)	2:577:B:LYS:H	2:672:B:LEU:HB3	8	0.24
(1,1430)	2:575:B:PHE:H	2:576:B:MET:H	4	0.24
(1,1130)	2:580:B:ILE:HG23	2:580:B:ILE:HG12	1	0.24
(1,1130)	2:580:B:ILE:HG22	2:580:B:ILE:HG12	2	0.24
(1,1130)	2:580:B:ILE:HG23	2:580:B:ILE:HG12	3	0.24
(1,1130)	2:580:B:ILE:HG21	2:580:B:ILE:HG12	7	0.24
(1,1130)	2:580:B:ILE:HG22	2:580:B:ILE:HG12	14	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1060)	2:666:B:THR:HG21	1:40:A:LEU:HA	11	0.24
(1,950)	2:572:B:PRO:HB2	2:573:B:PRO:HD3	6	0.24
(1,887)	2:630:B:ILE:HG22	2:643:B:VAL:HG13	5	0.24
(1,777)	2:612:B:ASP:HB3	1:44:A:LEU:HD11	10	0.24
(1,671)	2:596:B:THR:HG23	2:596:B:THR:HA	6	0.24
(1,503)	2:677:B:LEU:HB2	2:677:B:LEU:HD11	1	0.24
(1,503)	2:677:B:LEU:HB2	2:677:B:LEU:HD13	14	0.24
(1,383)	2:646:B:LEU:H	2:645:B:VAL:HB	12	0.24
(1,149)	2:596:B:THR:H	2:595:B:LYS:HB2	9	0.24
(1,132)	2:591:B:VAL:HG23	2:577:B:LYS:HA	2	0.24
(1,124)	2:596:B:THR:HG22	2:684:B:ILE:HD13	2	0.24
(1,98)	2:672:B:LEU:HD11	2:591:B:VAL:HG21	15	0.24
(2,2)	2:595:B:LYS:HD2	2:658:B:TRP:HB3	1	0.23
(1,2678)	1:34:A:VAL:HB	1:34:A:VAL:HG11	2	0.23
(1,2678)	1:34:A:VAL:HB	1:34:A:VAL:HG13	9	0.23
(1,2678)	1:34:A:VAL:HB	1:34:A:VAL:HG11	12	0.23
(1,2596)	2:574:B:TYR:HB3	2:581:B:ILE:HD11	9	0.23
(1,2407)	2:618:B:ARG:HB3	2:631:B:GLN:HG2	1	0.23
(1,2289)	2:575:B:PHE:HE2	1:39:A:SER:HB3	1	0.23
(1,2176)	2:684:B:ILE:H	2:684:B:ILE:HG12	10	0.23
(1,2176)	2:684:B:ILE:H	2:684:B:ILE:HG12	13	0.23
(1,2107)	2:674:B:CYS:H	2:674:B:CYS:HB3	1	0.23
(1,1980)	2:655:B:GLY:H	2:654:B:PHE:HB2	15	0.23
(1,1953)	2:649:B:TYR:H	2:649:B:TYR:HB3	12	0.23
(1,1953)	2:649:B:TYR:H	2:649:B:TYR:HB3	13	0.23
(1,1835)	2:627:B:VAL:H	2:646:B:LEU:HA	13	0.23
(1,1540)	2:590:B:LYS:H	2:590:B:LYS:HE2	5	0.23
(1,1525)	2:588:B:LEU:H	2:587:B:GLU:HB3	11	0.23
(1,1425)	2:571:B:LEU:H	2:571:B:LEU:HB2	9	0.23
(1,1295)	2:589:B:LYS:HB2	2:590:B:LYS:H	10	0.23
(1,1211)	2:630:B:ILE:HA	2:619:B:ILE:HG13	1	0.23
(1,1130)	2:580:B:ILE:HG22	2:580:B:ILE:HG12	5	0.23
(1,1086)	2:609:B:LEU:HD21	1:37:A:TRP:HZ3	13	0.23
(1,1060)	2:666:B:THR:HG22	1:40:A:LEU:HA	1	0.23
(1,1060)	2:666:B:THR:HG23	1:40:A:LEU:HA	7	0.23
(1,950)	2:572:B:PRO:HB2	2:573:B:PRO:HD3	11	0.23
(1,931)	2:639:B:ALA:HB1	2:634:B:VAL:HG22	2	0.23
(1,671)	2:596:B:THR:HG23	2:596:B:THR:HA	12	0.23
(1,426)	2:654:B:PHE:HB3	2:656:B:GLN:HE22	14	0.23
(1,422)	2:654:B:PHE:HB2	2:682:B:VAL:HG13	4	0.23
(1,276)	2:619:B:ILE:HG22	2:628:B:ALA:HB2	7	0.23
(1,276)	2:619:B:ILE:HG23	2:628:B:ALA:HB1	14	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,149)	2:596:B:THR:H	2:595:B:LYS:HB2	3	0.23
(1,132)	2:591:B:VAL:HG23	2:577:B:LYS:HA	11	0.23
(1,83)	2:588:B:LEU:HD11	2:588:B:LEU:HD23	7	0.23
(1,2678)	1:34:A:VAL:HB	1:34:A:VAL:HG13	6	0.22
(1,2654)	2:674:B:CYS:HB2	2:676:B:LYS:HD3	2	0.22
(1,2597)	2:649:B:TYR:HB3	2:645:B:VAL:HG11	3	0.22
(1,2529)	2:613:B:SER:HB2	2:682:B:VAL:HG12	6	0.22
(1,2488)	2:590:B:LYS:HB3	2:592:B:GLU:HA	14	0.22
(1,2465)	2:686:B:LEU:HD22	1:37:A:TRP:HE3	5	0.22
(1,2263)	2:614:B:SER:HB2	1:47:A:SER:HB3	5	0.22
(1,2210)	2:579:B:SER:HA	1:39:A:SER:HG	6	0.22
(1,2203)	2:609:B:LEU:HD12	1:37:A:TRP:HZ3	14	0.22
(1,2176)	2:684:B:ILE:H	2:684:B:ILE:HG12	5	0.22
(1,2107)	2:674:B:CYS:H	2:674:B:CYS:HB3	15	0.22
(1,2019)	2:660:B:SER:H	2:663:B:PRO:HB2	3	0.22
(1,2019)	2:660:B:SER:H	2:663:B:PRO:HB2	6	0.22
(1,1982)	2:655:B:GLY:H	2:596:B:THR:HG21	1	0.22
(1,1980)	2:655:B:GLY:H	2:654:B:PHE:HB2	10	0.22
(1,1931)	2:679:B:VAL:H	2:678:B:SER:HB2	10	0.22
(1,1725)	2:616:B:VAL:H	2:616:B:VAL:HG21	6	0.22
(1,1533)	2:589:B:LYS:H	2:589:B:LYS:HB3	6	0.22
(1,1312)	2:654:B:PHE:HB3	2:684:B:ILE:HG12	7	0.22
(1,1211)	2:630:B:ILE:HA	2:619:B:ILE:HG13	8	0.22
(1,1194)	2:689:B:LYS:HA	2:610:B:LYS:HE3	12	0.22
(1,1130)	2:580:B:ILE:HG23	2:580:B:ILE:HG12	9	0.22
(1,1130)	2:580:B:ILE:HG22	2:580:B:ILE:HG12	15	0.22
(1,1060)	2:666:B:THR:HG21	1:40:A:LEU:HA	15	0.22
(1,1006)	2:652:B:PHE:HA	1:41:A:VAL:HA	1	0.22
(1,797)	2:660:B:SER:HB2	1:40:A:LEU:HA	9	0.22
(1,671)	2:596:B:THR:HG22	2:596:B:THR:HA	10	0.22
(1,503)	2:677:B:LEU:HB2	2:677:B:LEU:HD13	8	0.22
(1,404)	2:648:B:GLU:HG3	2:669:B:LEU:HD13	9	0.22
(1,211)	2:611:B:ILE:H	2:610:B:LYS:HB2	8	0.22
(1,83)	2:588:B:LEU:HD12	2:588:B:LEU:HD22	13	0.22
(1,69)	2:587:B:GLU:HG3	2:587:B:GLU:HA	9	0.22
(1,2678)	1:34:A:VAL:HB	1:34:A:VAL:HG23	4	0.21
(1,2678)	1:34:A:VAL:HB	1:34:A:VAL:HG13	10	0.21
(1,2678)	1:34:A:VAL:HB	1:34:A:VAL:HG21	13	0.21
(1,2678)	1:34:A:VAL:HB	1:34:A:VAL:HG11	15	0.21
(1,2599)	2:645:B:VAL:HG13	2:629:B:VAL:HA	11	0.21
(1,2490)	2:656:B:GLN:HB2	2:682:B:VAL:HA	5	0.21
(1,2488)	2:590:B:LYS:HB3	2:592:B:GLU:HA	3	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2465)	2:686:B:LEU:HD21	1:37:A:TRP:HE3	7	0.21
(1,2465)	2:677:B:LEU:HD13	2:651:B:PHE:HD1	10	0.21
(1,2463)	2:678:B:SER:H	2:677:B:LEU:HG	11	0.21
(1,2313)	2:583:B:LEU:HD11	2:589:B:LYS:HE2	5	0.21
(1,2289)	2:575:B:PHE:HE2	1:39:A:SER:HB3	15	0.21
(1,2176)	2:684:B:ILE:H	2:684:B:ILE:HG12	2	0.21
(1,2176)	2:684:B:ILE:H	2:684:B:ILE:HG12	15	0.21
(1,2107)	2:674:B:CYS:H	2:674:B:CYS:HB3	6	0.21
(1,2019)	2:660:B:SER:H	2:663:B:PRO:HB2	7	0.21
(1,1980)	2:655:B:GLY:H	2:654:B:PHE:HB2	7	0.21
(1,1870)	2:636:B:GLU:H	2:636:B:GLU:HG2	11	0.21
(1,1782)	2:622:B:SER:H	2:621:B:ASP:HB2	13	0.21
(1,1541)	2:590:B:LYS:H	2:589:B:LYS:HE2	15	0.21
(1,1533)	2:589:B:LYS:H	2:589:B:LYS:HB3	3	0.21
(1,1533)	2:589:B:LYS:H	2:589:B:LYS:HB3	14	0.21
(1,1525)	2:588:B:LEU:H	2:587:B:GLU:HB3	4	0.21
(1,1437)	2:576:B:MET:H	2:576:B:MET:HG3	7	0.21
(1,1430)	2:575:B:PHE:H	2:576:B:MET:H	1	0.21
(1,1211)	2:630:B:ILE:HA	2:619:B:ILE:HG13	9	0.21
(1,1194)	2:689:B:LYS:HA	2:610:B:LYS:HE3	9	0.21
(1,1130)	2:580:B:ILE:HG21	2:580:B:ILE:HG12	11	0.21
(1,1130)	2:580:B:ILE:HG22	2:580:B:ILE:HG12	13	0.21
(1,950)	2:572:B:PRO:HB2	2:573:B:PRO:HD3	7	0.21
(1,950)	2:572:B:PRO:HB2	2:573:B:PRO:HD3	9	0.21
(1,712)	2:603:B:ALA:HA	2:606:B:SER:HA	5	0.21
(1,671)	2:596:B:THR:HG22	2:596:B:THR:HA	5	0.21
(1,671)	2:596:B:THR:HG23	2:596:B:THR:HA	15	0.21
(1,503)	2:677:B:LEU:HB2	2:677:B:LEU:HD11	2	0.21
(1,503)	2:677:B:LEU:HB2	2:677:B:LEU:HD11	3	0.21
(1,503)	2:677:B:LEU:HB2	2:677:B:LEU:HD13	10	0.21
(1,503)	2:677:B:LEU:HB2	2:677:B:LEU:HD11	12	0.21
(1,503)	2:677:B:LEU:HB2	2:677:B:LEU:HD11	13	0.21
(1,416)	2:653:B:VAL:HB	2:656:B:GLN:HB3	3	0.21
(1,132)	2:591:B:VAL:HG23	2:577:B:LYS:HA	1	0.21
(1,132)	2:591:B:VAL:HG22	2:577:B:LYS:HA	3	0.21
(1,132)	2:591:B:VAL:HG21	2:577:B:LYS:HA	5	0.21
(1,83)	2:588:B:LEU:HD12	2:588:B:LEU:HD21	3	0.21
(1,83)	2:588:B:LEU:HD11	2:588:B:LEU:HD21	8	0.21
(1,27)	2:577:B:LYS:HE3	2:577:B:LYS:HG3	3	0.21
(1,2903)	2:678:B:SER:H	2:676:B:LYS:HG3	10	0.2
(1,2860)	2:659:B:SER:H	2:675:B:SER:HA	1	0.2
(1,2860)	2:659:B:SER:H	2:675:B:SER:HA	10	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2860)	2:659:B:SER:H	2:675:B:SER:HA	13	0.2
(1,2698)	2:576:B:MET:H	2:575:B:PHE:HB2	13	0.2
(1,2678)	1:34:A:VAL:HB	1:34:A:VAL:HG11	8	0.2
(1,2665)	2:591:B:VAL:HG12	2:658:B:TRP:HH2	7	0.2
(1,2665)	2:591:B:VAL:HG12	2:594:B:LEU:H	8	0.2
(1,2535)	2:660:B:SER:HB2	2:662:B:CYS:HA	1	0.2
(1,2465)	2:686:B:LEU:HD21	1:37:A:TRP:HE3	13	0.2
(1,2407)	2:618:B:ARG:HB3	2:631:B:GLN:HG2	9	0.2
(1,2392)	2:653:B:VAL:HB	2:656:B:GLN:HG2	12	0.2
(1,2378)	2:620:B:GLU:HG3	2:629:B:VAL:HG12	8	0.2
(1,2107)	2:674:B:CYS:H	2:674:B:CYS:HB3	9	0.2
(1,1967)	2:653:B:VAL:H	1:41:A:VAL:HA	14	0.2
(1,1953)	2:649:B:TYR:H	2:649:B:TYR:HB3	1	0.2
(1,1953)	2:649:B:TYR:H	2:649:B:TYR:HB3	7	0.2
(1,1931)	2:679:B:VAL:H	2:678:B:SER:HB2	14	0.2
(1,1891)	2:639:B:ALA:H	2:637:B:HIS:HB3	5	0.2
(1,1725)	2:616:B:VAL:H	2:616:B:VAL:HG21	3	0.2
(1,1698)	2:610:B:LYS:H	2:609:B:LEU:HD13	3	0.2
(1,1449)	2:577:B:LYS:H	2:672:B:LEU:HB3	7	0.2
(1,1337)	1:40:A:LEU:HD13	1:40:A:LEU:HD21	15	0.2
(1,1312)	2:654:B:PHE:HB3	2:684:B:ILE:HG12	10	0.2
(1,1295)	2:589:B:LYS:HB2	2:590:B:LYS:H	6	0.2
(1,1211)	2:630:B:ILE:HA	2:619:B:ILE:HG13	14	0.2
(1,1060)	2:666:B:THR:HG22	1:40:A:LEU:HA	9	0.2
(1,1006)	2:652:B:PHE:HA	1:41:A:VAL:HA	2	0.2
(1,1006)	2:652:B:PHE:HA	1:41:A:VAL:HA	12	0.2
(1,950)	2:572:B:PRO:HB2	2:573:B:PRO:HD3	1	0.2
(1,887)	2:630:B:ILE:HG23	2:643:B:VAL:HG11	2	0.2
(1,887)	2:630:B:ILE:HG21	2:643:B:VAL:HG11	7	0.2
(1,671)	2:596:B:THR:HG23	2:596:B:THR:HA	13	0.2
(1,503)	2:677:B:LEU:HB2	2:677:B:LEU:HD11	9	0.2
(1,383)	2:646:B:LEU:H	2:645:B:VAL:HB	1	0.2
(1,232)	2:611:B:ILE:HG21	2:684:B:ILE:HD12	12	0.2
(1,124)	2:596:B:THR:HG21	2:684:B:ILE:HD13	10	0.2
(1,83)	2:588:B:LEU:HD11	2:588:B:LEU:HD23	4	0.2
(1,83)	2:588:B:LEU:HD12	2:588:B:LEU:HD23	14	0.2
(1,2702)	2:578:B:GLY:H	2:590:B:LYS:HB2	8	0.19
(1,2698)	2:576:B:MET:H	2:575:B:PHE:HB2	6	0.19
(1,2698)	2:576:B:MET:H	2:575:B:PHE:HB2	7	0.19
(1,2665)	2:591:B:VAL:HG12	2:658:B:TRP:HH2	10	0.19
(1,2637)	2:679:B:VAL:HG11	2:679:B:VAL:HB	4	0.19
(1,2529)	2:613:B:SER:HB2	2:682:B:VAL:HG12	11	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2451)	2:674:B:CYS:HB2	2:673:B:PRO:HB2	13	0.19
(1,2320)	2:617:B:GLU:HG3	2:679:B:VAL:HG22	6	0.19
(1,1980)	2:655:B:GLY:H	2:654:B:PHE:HB2	6	0.19
(1,1980)	2:655:B:GLY:H	2:654:B:PHE:HB2	9	0.19
(1,1953)	2:649:B:TYR:H	2:649:B:TYR:HB3	3	0.19
(1,1953)	2:649:B:TYR:H	2:649:B:TYR:HB3	14	0.19
(1,1931)	2:679:B:VAL:H	2:678:B:SER:HB2	8	0.19
(1,1835)	2:627:B:VAL:H	2:646:B:LEU:HA	2	0.19
(1,1835)	2:627:B:VAL:H	2:646:B:LEU:HA	11	0.19
(1,1725)	2:616:B:VAL:H	2:616:B:VAL:HG22	4	0.19
(1,1697)	2:610:B:LYS:H	2:610:B:LYS:HG2	11	0.19
(1,1638)	2:601:B:GLN:H	2:601:B:GLN:HG2	7	0.19
(1,1557)	2:592:B:GLU:H	2:590:B:LYS:HB2	2	0.19
(1,1525)	2:588:B:LEU:H	2:587:B:GLU:HB3	8	0.19
(1,1465)	2:580:B:ILE:H	2:579:B:SER:HB3	15	0.19
(1,1312)	2:654:B:PHE:HB3	2:684:B:ILE:HG12	12	0.19
(1,1130)	2:580:B:ILE:HG22	2:580:B:ILE:HG12	4	0.19
(1,1006)	2:652:B:PHE:HA	1:41:A:VAL:HA	6	0.19
(1,797)	2:660:B:SER:HB2	1:40:A:LEU:HA	6	0.19
(1,712)	2:603:B:ALA:HA	2:606:B:SER:HA	2	0.19
(1,124)	2:596:B:THR:HG23	2:684:B:ILE:HD12	4	0.19
(1,83)	2:588:B:LEU:HD13	2:588:B:LEU:HD21	12	0.19
(1,27)	2:577:B:LYS:HE3	2:577:B:LYS:HG3	9	0.19
(2,7)	2:578:B:GLY:HA3	2:590:B:LYS:HG3	3	0.18
(2,7)	2:578:B:GLY:HA3	2:590:B:LYS:HG3	6	0.18
(2,7)	2:578:B:GLY:HA3	2:590:B:LYS:HG3	7	0.18
(1,2935)	2:583:B:LEU:HD21	1:39:A:SER:HB3	14	0.18
(1,2702)	2:578:B:GLY:H	2:577:B:LYS:HD2	4	0.18
(1,2702)	2:578:B:GLY:H	2:577:B:LYS:HD2	11	0.18
(1,2702)	2:578:B:GLY:H	2:577:B:LYS:HD2	15	0.18
(1,2698)	2:576:B:MET:H	2:575:B:PHE:HB2	15	0.18
(1,2678)	1:34:A:VAL:HB	1:34:A:VAL:HG13	1	0.18
(1,2656)	2:619:B:ILE:HG21	2:630:B:ILE:HA	13	0.18
(1,2647)	2:687:B:THR:HG22	2:610:B:LYS:HD3	3	0.18
(1,2529)	2:613:B:SER:HB2	2:682:B:VAL:HG11	3	0.18
(1,2488)	2:590:B:LYS:HB3	2:592:B:GLU:HA	2	0.18
(1,2199)	2:689:B:LYS:H	2:689:B:LYS:HG3	14	0.18
(1,1980)	2:655:B:GLY:H	2:654:B:PHE:HB2	12	0.18
(1,1953)	2:649:B:TYR:H	2:649:B:TYR:HB3	5	0.18
(1,1953)	2:649:B:TYR:H	2:649:B:TYR:HB3	6	0.18
(1,1953)	2:649:B:TYR:H	2:649:B:TYR:HB3	15	0.18
(1,1835)	2:627:B:VAL:H	2:646:B:LEU:HA	12	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1725)	2:616:B:VAL:H	2:616:B:VAL:HG22	1	0.18
(1,1725)	2:616:B:VAL:H	2:616:B:VAL:HG22	15	0.18
(1,1697)	2:610:B:LYS:H	2:610:B:LYS:HG2	8	0.18
(1,1638)	2:601:B:GLN:H	2:601:B:GLN:HG2	13	0.18
(1,1540)	2:590:B:LYS:H	2:590:B:LYS:HE3	1	0.18
(1,1465)	2:580:B:ILE:H	2:579:B:SER:HB3	1	0.18
(1,1424)	2:571:B:LEU:H	2:570:B:THR:HA	2	0.18
(1,1335)	1:44:A:LEU:HD11	1:44:A:LEU:HD21	4	0.18
(1,1298)	2:615:B:THR:HA	2:682:B:VAL:HB	2	0.18
(1,1295)	2:589:B:LYS:HB2	2:590:B:LYS:H	1	0.18
(1,1240)	2:600:B:ILE:HG12	2:597:B:GLU:HA	8	0.18
(1,1218)	2:659:B:SER:HB3	2:677:B:LEU:HD23	4	0.18
(1,1194)	2:689:B:LYS:HA	2:610:B:LYS:HE2	6	0.18
(1,1006)	2:652:B:PHE:HA	1:41:A:VAL:HA	13	0.18
(1,1006)	2:652:B:PHE:HA	1:41:A:VAL:HA	15	0.18
(1,887)	2:630:B:ILE:HG23	2:643:B:VAL:HG11	9	0.18
(1,887)	2:630:B:ILE:HG22	2:643:B:VAL:HG11	11	0.18
(1,712)	2:603:B:ALA:HA	2:606:B:SER:HA	1	0.18
(1,712)	2:603:B:ALA:HA	2:606:B:SER:HA	11	0.18
(1,591)	2:580:B:ILE:HD11	2:590:B:LYS:HE3	11	0.18
(1,578)	2:577:B:LYS:HD3	2:671:B:ASP:HB2	10	0.18
(1,503)	2:677:B:LEU:HB2	2:677:B:LEU:HD12	6	0.18
(1,427)	2:654:B:PHE:HB2	2:656:B:GLN:HE22	9	0.18
(1,427)	2:654:B:PHE:HB2	2:656:B:GLN:HE22	10	0.18
(1,365)	2:665:B:ARG:HD3	2:647:B:VAL:HG22	8	0.18
(1,365)	2:665:B:ARG:HD3	2:647:B:VAL:HG23	15	0.18
(1,351)	2:679:B:VAL:HG13	2:679:B:VAL:HA	12	0.18
(1,232)	2:611:B:ILE:HG21	2:684:B:ILE:HD12	8	0.18
(1,132)	2:591:B:VAL:HG23	2:577:B:LYS:HA	6	0.18
(1,124)	2:596:B:THR:HG23	2:684:B:ILE:HD12	14	0.18
(1,83)	2:588:B:LEU:HD12	2:588:B:LEU:HD22	10	0.18
(1,83)	2:588:B:LEU:HD12	2:588:B:LEU:HD23	11	0.18
(2,7)	2:578:B:GLY:HA3	2:590:B:LYS:HG3	10	0.17
(2,7)	2:578:B:GLY:HA3	2:590:B:LYS:HG3	11	0.17
(2,2)	2:595:B:LYS:HD2	2:658:B:TRP:HB3	4	0.17
(1,2698)	2:576:B:MET:H	2:575:B:PHE:HB2	2	0.17
(1,2698)	2:576:B:MET:H	2:575:B:PHE:HB2	3	0.17
(1,2698)	2:576:B:MET:H	2:575:B:PHE:HB2	8	0.17
(1,2681)	1:34:A:VAL:HG11	1:35:A:PHE:H	5	0.17
(1,2681)	1:34:A:VAL:HG13	1:35:A:PHE:H	10	0.17
(1,2678)	1:34:A:VAL:HB	1:34:A:VAL:HG11	5	0.17
(1,2488)	2:590:B:LYS:HB3	2:592:B:GLU:HA	15	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2482)	2:582:B:GLN:HB2	2:580:B:ILE:HG21	4	0.17
(1,2465)	2:677:B:LEU:HD11	2:651:B:PHE:HD1	9	0.17
(1,2411)	2:646:B:LEU:H	2:645:B:VAL:HG21	6	0.17
(1,2313)	2:583:B:LEU:HD11	2:589:B:LYS:HE2	14	0.17
(1,2210)	2:579:B:SER:HA	1:39:A:SER:HG	12	0.17
(1,1967)	2:653:B:VAL:H	1:41:A:VAL:HA	2	0.17
(1,1953)	2:649:B:TYR:H	2:649:B:TYR:HB3	2	0.17
(1,1953)	2:649:B:TYR:H	2:649:B:TYR:HB3	10	0.17
(1,1789)	2:624:B:SER:H	2:624:B:SER:HB3	3	0.17
(1,1725)	2:616:B:VAL:H	2:616:B:VAL:HG21	11	0.17
(1,1638)	2:601:B:GLN:H	2:601:B:GLN:HG2	10	0.17
(1,1527)	2:588:B:LEU:H	2:588:B:LEU:HD11	15	0.17
(1,1422)	2:570:B:THR:H	2:570:B:THR:HG21	2	0.17
(1,1337)	1:40:A:LEU:HD13	1:40:A:LEU:HD23	11	0.17
(1,1335)	1:44:A:LEU:HD11	1:44:A:LEU:HD21	1	0.17
(1,1298)	2:615:B:THR:HA	2:682:B:VAL:HB	9	0.17
(1,1130)	2:580:B:ILE:HG22	2:580:B:ILE:HG12	8	0.17
(1,1013)	2:681:B:ASP:HB3	2:653:B:VAL:HG23	7	0.17
(1,1006)	2:652:B:PHE:HA	1:41:A:VAL:HA	10	0.17
(1,988)	2:647:B:VAL:HB	2:662:B:CYS:HB2	4	0.17
(1,950)	2:572:B:PRO:HB2	2:573:B:PRO:HD3	10	0.17
(1,910)	2:672:B:LEU:HD11	2:592:B:GLU:HB2	11	0.17
(1,641)	2:683:B:CYS:HB3	2:651:B:PHE:HB2	3	0.17
(1,552)	2:686:B:LEU:HD13	2:611:B:ILE:HA	8	0.17
(1,427)	2:654:B:PHE:HB2	2:656:B:GLN:HE22	6	0.17
(1,427)	2:654:B:PHE:HB2	2:656:B:GLN:HE22	7	0.17
(1,427)	2:654:B:PHE:HB2	2:656:B:GLN:HE22	15	0.17
(1,383)	2:646:B:LEU:H	2:645:B:VAL:HB	7	0.17
(1,351)	2:679:B:VAL:HG13	2:679:B:VAL:HA	7	0.17
(1,351)	2:679:B:VAL:HG12	2:679:B:VAL:HA	11	0.17
(1,132)	2:591:B:VAL:HG22	2:577:B:LYS:HA	12	0.17
(1,130)	2:672:B:LEU:HD22	2:591:B:VAL:HG21	15	0.17
(1,124)	2:596:B:THR:HG21	2:684:B:ILE:HD11	8	0.17
(2,7)	2:578:B:GLY:HA3	2:590:B:LYS:HG3	5	0.16
(2,7)	2:578:B:GLY:HA3	2:590:B:LYS:HG3	8	0.16
(1,2935)	2:583:B:LEU:HD23	1:39:A:SER:HB3	7	0.16
(1,2698)	2:576:B:MET:H	2:575:B:PHE:HB2	9	0.16
(1,2535)	2:660:B:SER:HB2	2:662:B:CYS:HA	6	0.16
(1,2488)	2:590:B:LYS:HB3	2:592:B:GLU:HA	12	0.16
(1,2313)	2:583:B:LEU:HD11	2:589:B:LYS:HE2	2	0.16
(1,2210)	2:579:B:SER:HA	1:39:A:SER:HG	1	0.16
(1,2107)	2:674:B:CYS:H	2:674:B:CYS:HB3	11	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2001)	2:658:B:TRP:HE1	2:594:B:LEU:HB2	10	0.16
(1,1725)	2:616:B:VAL:H	2:616:B:VAL:HG21	7	0.16
(1,1725)	2:616:B:VAL:H	2:616:B:VAL:HG23	8	0.16
(1,1725)	2:616:B:VAL:H	2:616:B:VAL:HG23	10	0.16
(1,1725)	2:616:B:VAL:H	2:616:B:VAL:HG22	12	0.16
(1,1725)	2:616:B:VAL:H	2:616:B:VAL:HG22	14	0.16
(1,1557)	2:592:B:GLU:H	2:590:B:LYS:HB2	9	0.16
(1,1541)	2:590:B:LYS:H	2:589:B:LYS:HE2	13	0.16
(1,1527)	2:588:B:LEU:H	2:588:B:LEU:HD13	5	0.16
(1,1527)	2:588:B:LEU:H	2:588:B:LEU:HD11	14	0.16
(1,1437)	2:576:B:MET:H	2:576:B:MET:HG3	3	0.16
(1,1437)	2:576:B:MET:H	2:576:B:MET:HG3	15	0.16
(1,1337)	1:40:A:LEU:HD12	1:40:A:LEU:HD23	9	0.16
(1,1335)	1:44:A:LEU:HD13	1:44:A:LEU:HD22	10	0.16
(1,1298)	2:615:B:THR:HA	2:682:B:VAL:HB	1	0.16
(1,1298)	2:615:B:THR:HA	2:682:B:VAL:HB	5	0.16
(1,1240)	2:600:B:ILE:HG12	2:597:B:GLU:HA	2	0.16
(1,1185)	2:687:B:THR:HA	1:43:A:PHE:HD2	7	0.16
(1,1094)	2:672:B:LEU:HD21	2:672:B:LEU:HB2	9	0.16
(1,1060)	2:666:B:THR:HG23	1:40:A:LEU:HA	13	0.16
(1,931)	2:639:B:ALA:HB1	2:634:B:VAL:HG22	14	0.16
(1,641)	2:683:B:CYS:HB3	2:651:B:PHE:HB2	1	0.16
(1,416)	2:653:B:VAL:HB	2:656:B:GLN:HB3	2	0.16
(1,383)	2:646:B:LEU:H	2:645:B:VAL:HB	14	0.16
(1,365)	2:665:B:ARG:HD3	2:647:B:VAL:HG21	14	0.16
(1,253)	2:617:B:GLU:HG2	2:633:B:ALA:HB3	7	0.16
(1,232)	2:611:B:ILE:HG21	2:684:B:ILE:HD11	15	0.16
(1,149)	2:596:B:THR:H	2:595:B:LYS:HB2	2	0.16
(1,83)	2:588:B:LEU:HD13	2:588:B:LEU:HD22	1	0.16
(1,83)	2:588:B:LEU:HD11	2:588:B:LEU:HD23	5	0.16
(2,7)	2:578:B:GLY:HA3	2:590:B:LYS:HG3	4	0.15
(1,2903)	2:678:B:SER:H	2:676:B:LYS:HG3	7	0.15
(1,2860)	2:659:B:SER:H	2:675:B:SER:HA	9	0.15
(1,2698)	2:576:B:MET:H	2:576:B:MET:HE3	11	0.15
(1,2665)	2:591:B:VAL:HG11	2:658:B:TRP:HH2	5	0.15
(1,2637)	2:679:B:VAL:HG12	2:679:B:VAL:HB	1	0.15
(1,2535)	2:660:B:SER:HB2	2:662:B:CYS:HA	12	0.15
(1,2465)	2:677:B:LEU:HD13	2:651:B:PHE:HD1	11	0.15
(1,2463)	2:678:B:SER:H	2:677:B:LEU:HG	1	0.15
(1,2463)	2:678:B:SER:H	2:677:B:LEU:HG	3	0.15
(1,2318)	2:665:B:ARG:HB2	2:669:B:LEU:HD11	4	0.15
(1,2210)	2:579:B:SER:HA	1:39:A:SER:HG	4	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2203)	2:609:B:LEU:HD13	1:37:A:TRP:HZ3	15	0.15
(1,2019)	2:660:B:SER:H	2:663:B:PRO:HB2	13	0.15
(1,1723)	2:616:B:VAL:H	2:615:B:THR:HG22	3	0.15
(1,1697)	2:610:B:LYS:H	2:610:B:LYS:HG2	12	0.15
(1,1527)	2:588:B:LEU:H	2:588:B:LEU:HD11	10	0.15
(1,1465)	2:580:B:ILE:H	2:579:B:SER:HB3	2	0.15
(1,1449)	2:577:B:LYS:H	2:672:B:LEU:HB3	2	0.15
(1,1295)	2:589:B:LYS:HB2	2:590:B:LYS:H	2	0.15
(1,1295)	2:589:B:LYS:HB2	2:590:B:LYS:H	9	0.15
(1,1218)	2:659:B:SER:HB3	2:677:B:LEU:HD21	15	0.15
(1,1060)	2:666:B:THR:HG23	1:40:A:LEU:HA	5	0.15
(1,1057)	2:650:B:PRO:HG2	2:666:B:THR:HG23	13	0.15
(1,950)	2:572:B:PRO:HB2	2:573:B:PRO:HD3	15	0.15
(1,663)	2:589:B:LYS:HB3	2:594:B:LEU:HD21	5	0.15
(1,576)	2:577:B:LYS:HD2	2:671:B:ASP:HB2	15	0.15
(1,574)	2:576:B:MET:HB2	2:575:B:PHE:HD1	8	0.15
(1,393)	2:646:B:LEU:HB2	2:646:B:LEU:HD22	13	0.15
(1,393)	2:646:B:LEU:HB2	2:646:B:LEU:HD23	15	0.15
(1,351)	2:679:B:VAL:HG12	2:679:B:VAL:HA	5	0.15
(1,351)	2:679:B:VAL:HG11	2:679:B:VAL:HA	6	0.15
(1,351)	2:679:B:VAL:HG13	2:679:B:VAL:HA	10	0.15
(1,351)	2:679:B:VAL:HG13	2:679:B:VAL:HA	13	0.15
(1,83)	2:588:B:LEU:HD13	2:588:B:LEU:HD23	2	0.15
(1,83)	2:588:B:LEU:HD11	2:588:B:LEU:HD22	6	0.15
(1,27)	2:577:B:LYS:HE3	2:577:B:LYS:HG3	12	0.15
(2,7)	2:578:B:GLY:HA3	2:590:B:LYS:HG3	2	0.14
(2,7)	2:578:B:GLY:HA3	2:590:B:LYS:HG3	14	0.14
(1,2935)	2:583:B:LEU:HD22	1:39:A:SER:HB3	8	0.14
(1,2860)	2:659:B:SER:H	2:675:B:SER:HA	4	0.14
(1,2860)	2:659:B:SER:H	2:675:B:SER:HA	14	0.14
(1,2647)	2:687:B:THR:HG22	2:610:B:LYS:HB3	2	0.14
(1,2637)	2:679:B:VAL:HG12	2:679:B:VAL:HB	2	0.14
(1,2637)	2:679:B:VAL:HG12	2:679:B:VAL:HB	3	0.14
(1,2637)	2:679:B:VAL:HG12	2:679:B:VAL:HB	8	0.14
(1,2637)	2:679:B:VAL:HG12	2:679:B:VAL:HB	9	0.14
(1,2637)	2:679:B:VAL:HG13	2:679:B:VAL:HB	14	0.14
(1,2609)	2:660:B:SER:HA	2:677:B:LEU:HB3	15	0.14
(1,2535)	2:660:B:SER:HB2	2:662:B:CYS:HA	14	0.14
(1,2465)	2:686:B:LEU:HD23	1:37:A:TRP:HE3	15	0.14
(1,2324)	2:589:B:LYS:HE2	2:589:B:LYS:HB3	9	0.14
(1,2208)	2:674:B:CYS:HB3	1:40:A:LEU:HB2	14	0.14
(1,2203)	2:609:B:LEU:HD12	1:37:A:TRP:HZ3	5	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2155)	2:681:B:ASP:H	2:616:B:VAL:HG23	5	0.14
(1,2107)	2:674:B:CYS:H	2:674:B:CYS:HB3	4	0.14
(1,2029)	2:662:B:CYS:H	2:660:B:SER:HB2	12	0.14
(1,1967)	2:653:B:VAL:H	1:41:A:VAL:HA	1	0.14
(1,1931)	2:679:B:VAL:H	2:678:B:SER:HB2	4	0.14
(1,1901)	2:640:B:GLN:H	2:640:B:GLN:HG2	9	0.14
(1,1789)	2:624:B:SER:H	2:624:B:SER:HB3	14	0.14
(1,1725)	2:616:B:VAL:H	2:616:B:VAL:HG21	2	0.14
(1,1725)	2:616:B:VAL:H	2:616:B:VAL:HG23	5	0.14
(1,1725)	2:616:B:VAL:H	2:616:B:VAL:HG23	9	0.14
(1,1725)	2:616:B:VAL:H	2:616:B:VAL:HG22	13	0.14
(1,1638)	2:601:B:GLN:H	2:601:B:GLN:HG2	5	0.14
(1,1557)	2:592:B:GLU:H	2:590:B:LYS:HB2	12	0.14
(1,1544)	2:590:B:LYS:H	2:590:B:LYS:HG2	15	0.14
(1,1525)	2:588:B:LEU:H	2:587:B:GLU:HB3	10	0.14
(1,1437)	2:576:B:MET:H	2:576:B:MET:HG3	14	0.14
(1,1337)	1:40:A:LEU:HD12	1:40:A:LEU:HD22	3	0.14
(1,1337)	1:40:A:LEU:HD12	1:40:A:LEU:HD21	8	0.14
(1,1337)	1:40:A:LEU:HD13	1:40:A:LEU:HD21	10	0.14
(1,1337)	1:40:A:LEU:HD13	1:40:A:LEU:HD23	12	0.14
(1,1337)	1:40:A:LEU:HD13	1:40:A:LEU:HD22	13	0.14
(1,1295)	2:589:B:LYS:HB2	2:590:B:LYS:H	4	0.14
(1,1208)	2:610:B:LYS:HB3	2:610:B:LYS:HE2	12	0.14
(1,1090)	2:670:B:PHE:HB2	2:575:B:PHE:HZ	7	0.14
(1,1060)	2:666:B:THR:HG21	1:40:A:LEU:HA	2	0.14
(1,1057)	2:650:B:PRO:HG2	2:666:B:THR:HG23	2	0.14
(1,591)	2:580:B:ILE:HD13	2:590:B:LYS:HE3	5	0.14
(1,393)	2:646:B:LEU:HB2	2:646:B:LEU:HD23	2	0.14
(1,393)	2:646:B:LEU:HB2	2:646:B:LEU:HD23	4	0.14
(1,393)	2:646:B:LEU:HB2	2:646:B:LEU:HD22	5	0.14
(1,351)	2:679:B:VAL:HG12	2:679:B:VAL:HA	8	0.14
(1,351)	2:679:B:VAL:HG12	2:679:B:VAL:HA	9	0.14
(1,351)	2:679:B:VAL:HG11	2:679:B:VAL:HA	15	0.14
(1,62)	2:586:B:GLY:HA3	2:587:B:GLU:HG3	7	0.14
(2,7)	2:578:B:GLY:HA3	2:590:B:LYS:HG3	1	0.13
(1,2954)	2:594:B:LEU:HD23	1:34:A:VAL:HG23	11	0.13
(1,2860)	2:659:B:SER:H	2:675:B:SER:HA	3	0.13
(1,2860)	2:659:B:SER:H	2:675:B:SER:HA	15	0.13
(1,2702)	2:578:B:GLY:H	2:590:B:LYS:HB2	10	0.13
(1,2647)	2:687:B:THR:HG22	2:610:B:LYS:HD3	13	0.13
(1,2637)	2:679:B:VAL:HG11	2:679:B:VAL:HB	6	0.13
(1,2637)	2:679:B:VAL:HG12	2:679:B:VAL:HB	11	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2637)	2:679:B:VAL:HG13	2:679:B:VAL:HB	12	0.13
(1,2637)	2:679:B:VAL:HG13	2:679:B:VAL:HB	13	0.13
(1,2596)	2:574:B:TYR:HB3	2:581:B:ILE:HD11	10	0.13
(1,2515)	2:611:B:ILE:HG21	2:603:B:ALA:HB1	11	0.13
(1,2463)	2:678:B:SER:H	2:677:B:LEU:HG	9	0.13
(1,2411)	2:646:B:LEU:H	2:645:B:VAL:HG23	10	0.13
(1,2313)	2:583:B:LEU:HD13	2:589:B:LYS:HE2	12	0.13
(1,2155)	2:681:B:ASP:H	2:616:B:VAL:HG23	12	0.13
(1,2155)	2:681:B:ASP:H	2:616:B:VAL:HG22	14	0.13
(1,2018)	2:660:B:SER:H	2:674:B:CYS:HB2	11	0.13
(1,1789)	2:624:B:SER:H	2:624:B:SER:HB3	10	0.13
(1,1789)	2:624:B:SER:H	2:624:B:SER:HB3	12	0.13
(1,1723)	2:616:B:VAL:H	2:615:B:THR:HG21	1	0.13
(1,1723)	2:616:B:VAL:H	2:615:B:THR:HG21	11	0.13
(1,1638)	2:601:B:GLN:H	2:601:B:GLN:HG2	15	0.13
(1,1557)	2:592:B:GLU:H	2:590:B:LYS:HB2	14	0.13
(1,1527)	2:588:B:LEU:H	2:588:B:LEU:HD12	2	0.13
(1,1437)	2:576:B:MET:H	2:576:B:MET:HG3	4	0.13
(1,1402)	1:40:A:LEU:HD13	1:39:A:SER:H	12	0.13
(1,1352)	1:47:A:SER:HA	1:48:A:GLN:HG3	14	0.13
(1,1337)	1:40:A:LEU:HD11	1:40:A:LEU:HD22	2	0.13
(1,1337)	1:40:A:LEU:HD13	1:40:A:LEU:HD21	5	0.13
(1,1335)	1:44:A:LEU:HD11	1:44:A:LEU:HD23	3	0.13
(1,1240)	2:600:B:ILE:HG12	2:597:B:GLU:HA	10	0.13
(1,1090)	2:670:B:PHE:HB2	2:575:B:PHE:HZ	5	0.13
(1,1060)	2:666:B:THR:HG23	1:40:A:LEU:HA	8	0.13
(1,931)	2:639:B:ALA:HB2	2:634:B:VAL:HG21	3	0.13
(1,663)	2:589:B:LYS:HB3	2:594:B:LEU:HD21	2	0.13
(1,591)	2:580:B:ILE:HD12	2:590:B:LYS:HE3	1	0.13
(1,578)	2:577:B:LYS:HD3	2:671:B:ASP:HB2	14	0.13
(1,427)	2:654:B:PHE:HB2	2:656:B:GLN:HE22	13	0.13
(1,393)	2:646:B:LEU:HB2	2:646:B:LEU:HD21	6	0.13
(1,393)	2:646:B:LEU:HB2	2:646:B:LEU:HD21	9	0.13
(1,351)	2:679:B:VAL:HG12	2:679:B:VAL:HA	2	0.13
(1,319)	2:628:B:ALA:HB3	2:647:B:VAL:HG13	9	0.13
(1,232)	2:611:B:ILE:HG23	2:684:B:ILE:HD13	14	0.13
(1,124)	2:596:B:THR:HG22	2:684:B:ILE:HD13	15	0.13
(1,66)	2:587:B:GLU:HG2	2:587:B:GLU:HA	11	0.13
(1,62)	2:586:B:GLY:HA3	2:587:B:GLU:HG3	12	0.13
(1,21)	2:571:B:LEU:HD21	2:571:B:LEU:HB2	3	0.13
(2,7)	2:578:B:GLY:HA3	2:590:B:LYS:HG3	15	0.12
(2,6)	2:590:B:LYS:HD2	2:589:B:LYS:HA	4	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2702)	2:578:B:GLY:H	2:577:B:LYS:HD2	1	0.12
(1,2702)	2:578:B:GLY:H	2:577:B:LYS:HD2	13	0.12
(1,2698)	2:576:B:MET:H	2:576:B:MET:HE1	10	0.12
(1,2637)	2:679:B:VAL:HG12	2:679:B:VAL:HB	5	0.12
(1,2637)	2:679:B:VAL:HG21	2:679:B:VAL:HB	7	0.12
(1,2637)	2:679:B:VAL:HG13	2:679:B:VAL:HB	10	0.12
(1,2637)	2:679:B:VAL:HG11	2:679:B:VAL:HB	15	0.12
(1,2599)	2:645:B:VAL:HG11	2:629:B:VAL:HA	15	0.12
(1,2535)	2:660:B:SER:HB2	2:662:B:CYS:HA	13	0.12
(1,2488)	2:590:B:LYS:HB3	2:592:B:GLU:HA	13	0.12
(1,2478)	2:590:B:LYS:HD3	2:578:B:GLY:HA2	9	0.12
(1,2407)	2:618:B:ARG:HB3	2:631:B:GLN:HG2	15	0.12
(1,2203)	2:609:B:LEU:HD11	1:37:A:TRP:HZ3	2	0.12
(1,2203)	2:609:B:LEU:HD12	1:37:A:TRP:HZ3	8	0.12
(1,2155)	2:681:B:ASP:H	2:616:B:VAL:HG23	8	0.12
(1,2107)	2:674:B:CYS:H	2:674:B:CYS:HB3	2	0.12
(1,2107)	2:674:B:CYS:H	2:674:B:CYS:HB3	8	0.12
(1,2018)	2:660:B:SER:H	2:674:B:CYS:HB2	1	0.12
(1,2018)	2:660:B:SER:H	2:674:B:CYS:HB2	6	0.12
(1,2018)	2:660:B:SER:H	2:674:B:CYS:HB2	9	0.12
(1,1953)	2:649:B:TYR:H	2:649:B:TYR:HB3	11	0.12
(1,1789)	2:624:B:SER:H	2:624:B:SER:HB3	9	0.12
(1,1789)	2:624:B:SER:H	2:624:B:SER:HB3	13	0.12
(1,1527)	2:588:B:LEU:H	2:588:B:LEU:HD13	6	0.12
(1,1422)	2:570:B:THR:H	2:570:B:THR:HG21	7	0.12
(1,1337)	1:40:A:LEU:HD11	1:40:A:LEU:HD21	6	0.12
(1,1337)	1:40:A:LEU:HD13	1:40:A:LEU:HD23	7	0.12
(1,1337)	1:40:A:LEU:HD13	1:40:A:LEU:HD22	14	0.12
(1,1335)	1:44:A:LEU:HD12	1:44:A:LEU:HD22	12	0.12
(1,1295)	2:589:B:LYS:HB2	2:590:B:LYS:H	8	0.12
(1,1211)	2:630:B:ILE:HA	2:619:B:ILE:HG13	7	0.12
(1,1090)	2:670:B:PHE:HB2	2:575:B:PHE:HZ	2	0.12
(1,887)	2:630:B:ILE:HG22	2:643:B:VAL:HG12	8	0.12
(1,663)	2:589:B:LYS:HB3	2:594:B:LEU:HD21	11	0.12
(1,642)	2:683:B:CYS:HB2	2:651:B:PHE:HB2	12	0.12
(1,441)	2:594:B:LEU:HG	2:589:B:LYS:HA	3	0.12
(1,441)	2:594:B:LEU:HG	2:589:B:LYS:HA	5	0.12
(1,416)	2:653:B:VAL:HB	2:656:B:GLN:HB3	1	0.12
(1,393)	2:646:B:LEU:HB2	2:646:B:LEU:HD23	8	0.12
(1,351)	2:679:B:VAL:HG12	2:679:B:VAL:HA	1	0.12
(1,351)	2:679:B:VAL:HG12	2:679:B:VAL:HA	3	0.12
(1,253)	2:617:B:GLU:HG2	2:633:B:ALA:HB2	1	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,232)	2:611:B:ILE:HG21	2:684:B:ILE:HD11	10	0.12
(1,211)	2:611:B:ILE:H	2:610:B:LYS:HB2	11	0.12
(1,2903)	2:678:B:SER:H	2:676:B:LYS:HG3	12	0.11
(1,2903)	2:678:B:SER:H	2:676:B:LYS:HG3	14	0.11
(1,2860)	2:659:B:SER:H	2:675:B:SER:HA	8	0.11
(1,2698)	2:576:B:MET:H	2:576:B:MET:HE1	4	0.11
(1,2675)	2:571:B:LEU:HD21	2:572:B:PRO:HG2	15	0.11
(1,2656)	2:619:B:ILE:HG22	2:630:B:ILE:HA	10	0.11
(1,2647)	2:687:B:THR:HG22	2:689:B:LYS:HB2	1	0.11
(1,2535)	2:660:B:SER:HB2	2:662:B:CYS:HA	3	0.11
(1,2465)	2:677:B:LEU:HD11	2:651:B:PHE:HD1	3	0.11
(1,2407)	2:618:B:ARG:HB3	2:631:B:GLN:HG2	13	0.11
(1,2029)	2:662:B:CYS:H	2:660:B:SER:HB2	14	0.11
(1,1901)	2:640:B:GLN:H	2:640:B:GLN:HG2	10	0.11
(1,1789)	2:624:B:SER:H	2:624:B:SER:HB3	1	0.11
(1,1789)	2:624:B:SER:H	2:624:B:SER:HB3	7	0.11
(1,1570)	2:593:B:ASP:H	2:592:B:GLU:HG3	15	0.11
(1,1557)	2:592:B:GLU:H	2:590:B:LYS:HB2	13	0.11
(1,1527)	2:588:B:LEU:H	2:588:B:LEU:HD12	1	0.11
(1,1527)	2:588:B:LEU:H	2:588:B:LEU:HD11	9	0.11
(1,1425)	2:571:B:LEU:H	2:571:B:LEU:HB2	1	0.11
(1,1422)	2:570:B:THR:H	2:570:B:THR:HG23	11	0.11
(1,1370)	1:44:A:LEU:HA	1:44:A:LEU:HD23	4	0.11
(1,1337)	1:40:A:LEU:HD13	1:40:A:LEU:HD23	4	0.11
(1,1335)	1:44:A:LEU:HD11	1:44:A:LEU:HD22	2	0.11
(1,1335)	1:44:A:LEU:HD12	1:44:A:LEU:HD21	11	0.11
(1,1295)	2:589:B:LYS:HB2	2:590:B:LYS:H	5	0.11
(1,1240)	2:600:B:ILE:HG12	2:597:B:GLU:HA	9	0.11
(1,1090)	2:670:B:PHE:HB2	2:575:B:PHE:HZ	6	0.11
(1,1006)	2:652:B:PHE:HA	1:41:A:VAL:HA	9	0.11
(1,1006)	2:652:B:PHE:HA	1:41:A:VAL:HA	11	0.11
(1,608)	2:589:B:LYS:HE2	2:589:B:LYS:HG3	3	0.11
(1,608)	2:589:B:LYS:HE2	2:589:B:LYS:HG3	4	0.11
(1,608)	2:589:B:LYS:HE2	2:589:B:LYS:HG3	9	0.11
(1,574)	2:576:B:MET:HB2	2:575:B:PHE:HD2	1	0.11
(1,574)	2:576:B:MET:HB2	2:575:B:PHE:HD1	10	0.11
(1,559)	2:688:B:LEU:H	2:688:B:LEU:HG	1	0.11
(1,427)	2:654:B:PHE:HB2	2:656:B:GLN:HE22	3	0.11
(1,404)	2:648:B:GLU:HG3	2:669:B:LEU:HD12	11	0.11
(1,393)	2:646:B:LEU:HB2	2:646:B:LEU:HD21	11	0.11
(1,351)	2:679:B:VAL:HG13	2:679:B:VAL:HA	14	0.11
(1,303)	2:627:B:VAL:HB	2:624:B:SER:HB3	7	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,303)	2:627:B:VAL:HB	2:624:B:SER:HB3	9	0.11
(1,211)	2:611:B:ILE:H	2:610:B:LYS:HB2	10	0.11
(1,83)	2:588:B:LEU:HD12	2:588:B:LEU:HD21	15	0.11
(1,66)	2:587:B:GLU:HG2	2:587:B:GLU:HA	3	0.11
(1,21)	2:571:B:LEU:HD21	2:571:B:LEU:HB2	12	0.11
(1,2860)	2:659:B:SER:H	2:675:B:SER:HA	2	0.1
(1,2656)	2:619:B:ILE:HG21	2:630:B:ILE:HA	9	0.1
(1,2465)	2:677:B:LEU:HD12	2:651:B:PHE:HD2	2	0.1
(1,2313)	2:583:B:LEU:HD11	2:589:B:LYS:HE2	1	0.1
(1,2108)	2:674:B:CYS:H	2:673:B:PRO:HB2	15	0.1
(1,1977)	2:654:B:PHE:H	2:682:B:VAL:HG22	14	0.1
(1,1901)	2:640:B:GLN:H	2:640:B:GLN:HG2	1	0.1
(1,1638)	2:601:B:GLN:H	2:601:B:GLN:HG2	12	0.1
(1,1437)	2:576:B:MET:H	2:576:B:MET:HG3	1	0.1
(1,1337)	1:40:A:LEU:HD13	1:40:A:LEU:HD21	1	0.1
(1,1090)	2:670:B:PHE:HB2	2:575:B:PHE:HZ	3	0.1
(1,1090)	2:670:B:PHE:HB2	2:575:B:PHE:HZ	8	0.1
(1,1090)	2:670:B:PHE:HB2	2:575:B:PHE:HZ	10	0.1
(1,1060)	2:666:B:THR:HG23	1:40:A:LEU:HA	3	0.1
(1,441)	2:594:B:LEU:HG	2:589:B:LYS:HA	9	0.1
(1,426)	2:654:B:PHE:HB3	2:656:B:GLN:HE22	2	0.1
(1,393)	2:646:B:LEU:HB2	2:646:B:LEU:HD21	7	0.1
(1,66)	2:587:B:GLU:HG2	2:587:B:GLU:HA	8	0.1
(1,50)	2:583:B:LEU:HD11	2:583:B:LEU:HD23	15	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found