Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 06:27 PM EDT

PDB ID	:	2MPF
BMRB ID	:	19977
Title	:	Solution structure human HCN2 CNBD in the cAMP-unbound state
Authors	:	Saponaro, A.; Pauleta, S.R.; Cantini, F.; Matzapetakis, M.; Hammann, C.; Banci, L.; Thiel, G.; Santoro, B.; Moroni, A.
Deposited on	:	2014-05-16

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

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

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

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

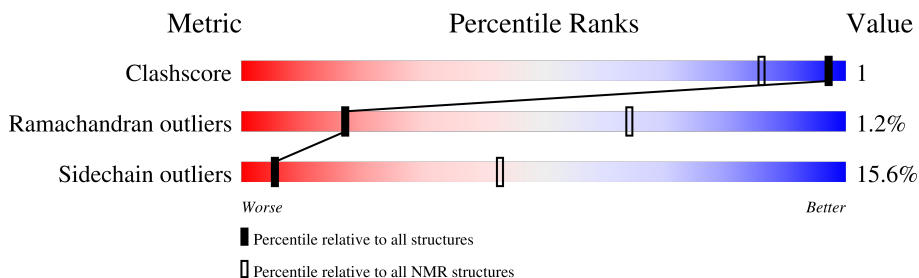|		
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance ⓘ

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

The overall completeness of chemical shifts assignment is 87%.

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	Percentile Ranks	Value
Clashscore		1
Ramachandran outliers		1.2%
Sidechain outliers		15.6%

Worse *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all NMR structures

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

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

Mol	Chain	Length	Quality of chain
1	A	158	58% 18% 11% 12%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *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:535-A:655 (121)	1.33	5

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

3 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 2252 atoms, of which 1139 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	139	2252	709	1139	195	200	9	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	515	GLY	-	expression tag	UNP Q9UL51
A	516	PRO	-	expression tag	UNP Q9UL51
A	517	SER	-	expression tag	UNP Q9UL51
A	518	SER	-	expression tag	UNP Q9UL51
A	519	PRO	-	expression tag	UNP Q9UL51
A	520	MET	-	expression tag	UNP Q9UL51

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: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2
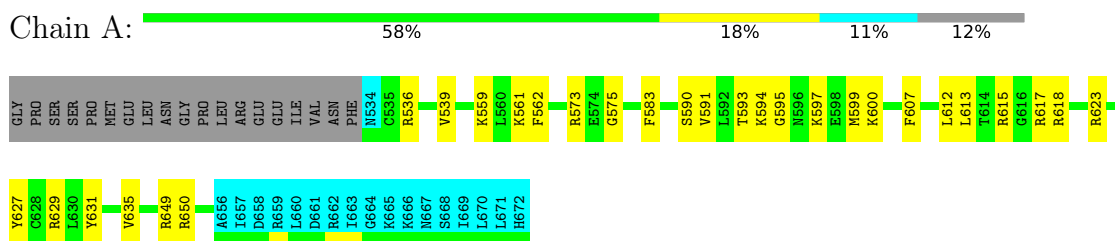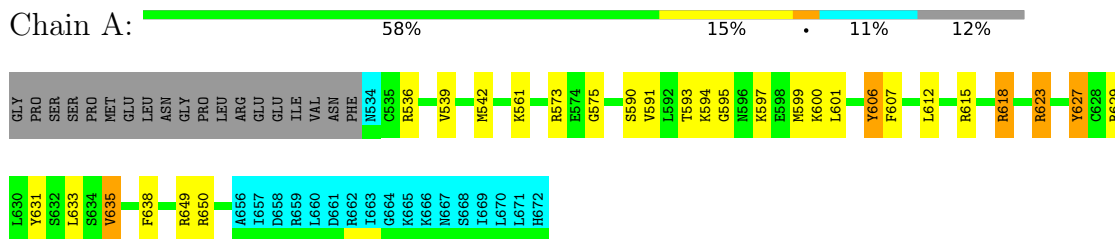

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2

4.2.2 Score per residue for model 2

• Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2

Chain A:

4.2.3 Score per residue for model 3

• Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2

Chain A:

4.2.4 Score per residue for model 4

• Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2

Chain A:

4.2.5 Score per residue for model 5 (medoid)

• Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2

Chain A:

4.2.6 Score per residue for model 6

• Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2

Chain A:

4.2.7 Score per residue for model 7

• Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2

Chain A:
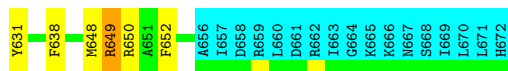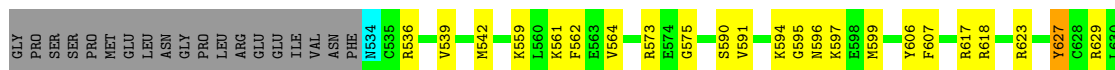

4.2.8 Score per residue for model 8

• Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2

Chain A:

4.2.9 Score per residue for model 9

• Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2

Chain A:

4.2.10 Score per residue for model 10

• Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2
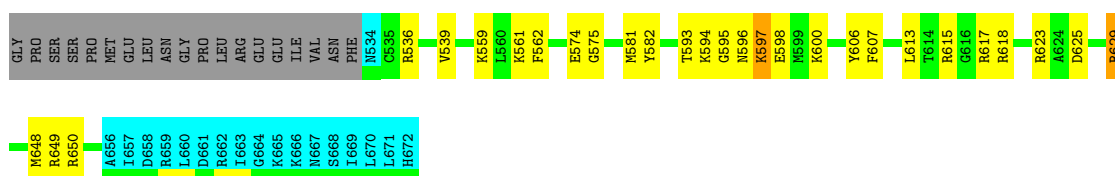
Chain A:

4.2.11 Score per residue for model 11

• Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2

Chain A:

4.2.12 Score per residue for model 12

• Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2
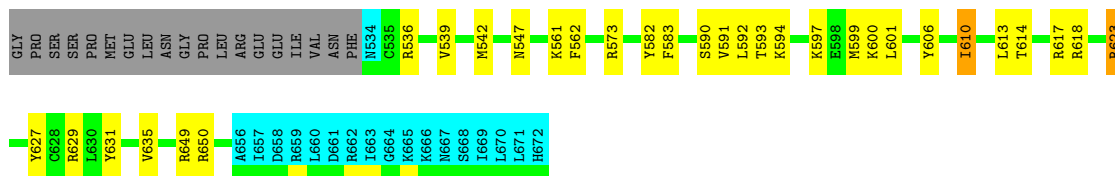
Chain A:

4.2.13 Score per residue for model 13

• Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2
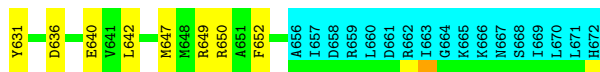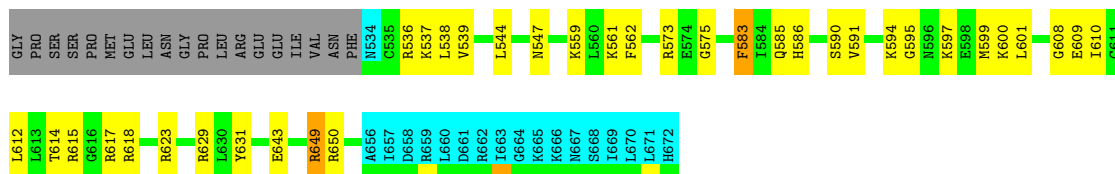
Chain A:

4.2.14 Score per residue for model 14

• Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2
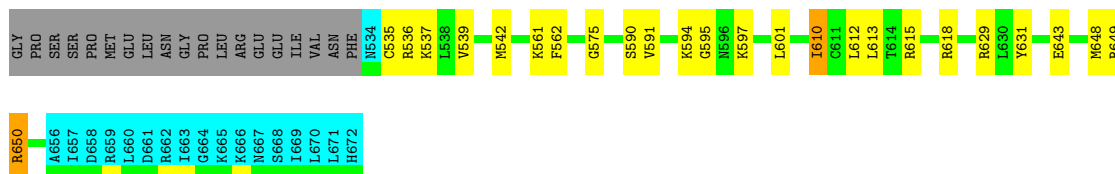
Chain A:

4.2.15 Score per residue for model 15

• Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2
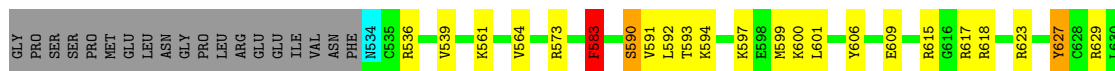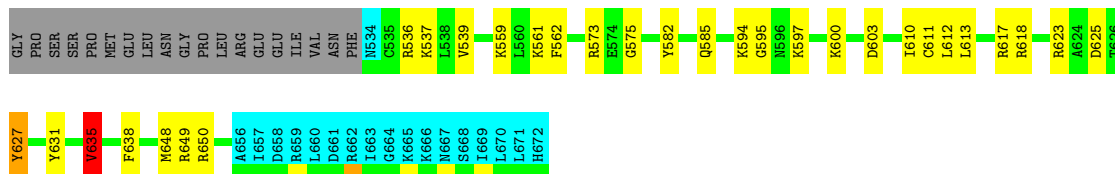
Chain A:

4.2.16 Score per residue for model 16

• Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2
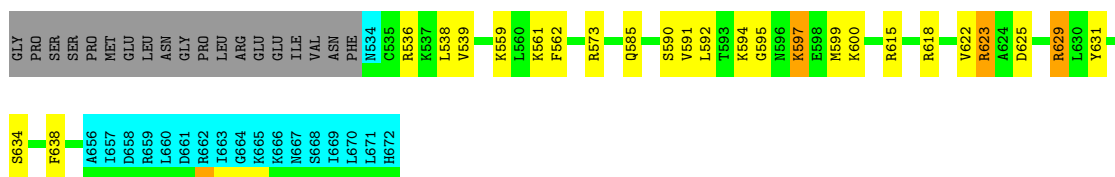
Chain A:

4.2.17 Score per residue for model 17

• Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2
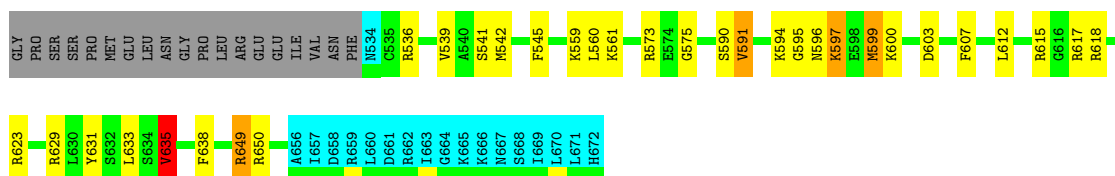
4.2.18 Score per residue for model 18

• Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2
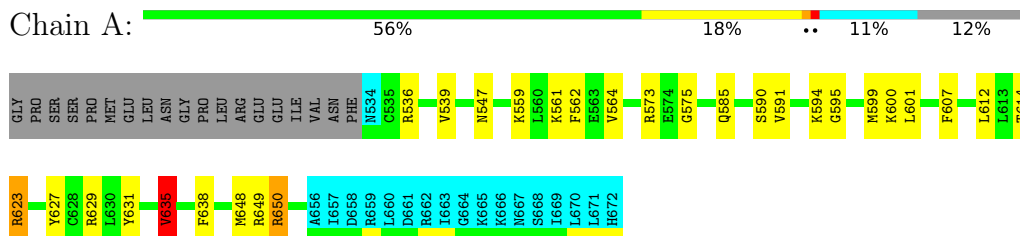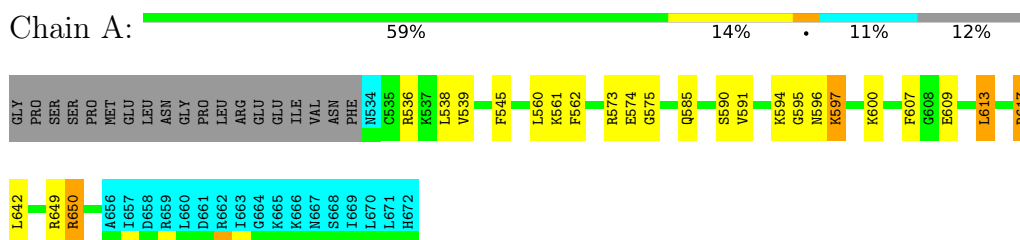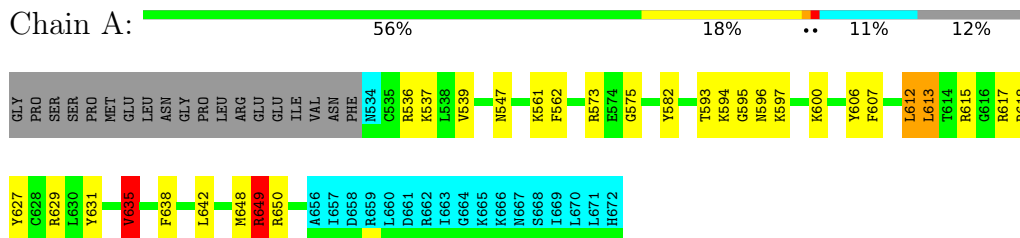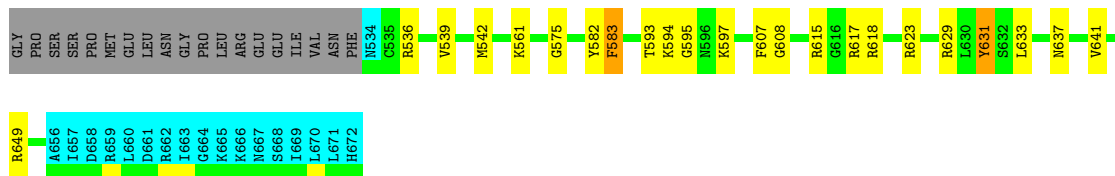

4.2.19 Score per residue for model 19

• Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2
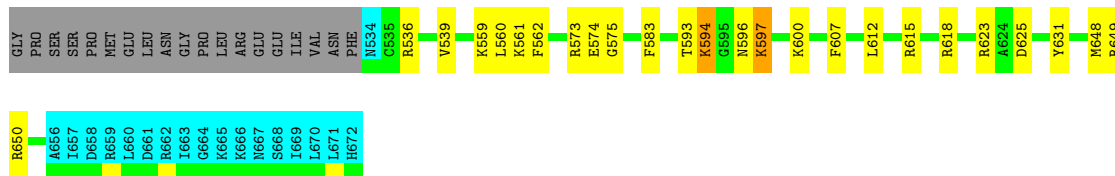
4.2.20 Score per residue for model 20

• Molecule 1: Potassium/sodium hyperpolarization-activated cyclic nucleotide-gated channel 2

Chain A:

61%   14% • 11%   12%

5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *torsion angle dynamics, molecular dynamics.*

Of the 500 calculated structures, 20 were deposited, based on the following criterion: *target function.*

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

Software name	Classification	Version
CYANA	structure solution	2.1
Amber	refinement	12
CANDID	structure solution	
CYANA	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1886
Number of shifts mapped to atoms	1673
Number of unparsed shifts	0
Number of shifts with mapping errors	213
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.75±0.01	0±0/987 (0.0± 0.0%)	1.24±0.04	10±2/1328 (0.7± 0.1%)
All	All	0.75	0/19740 (0.0%)	1.24	194/26560 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	3.5±1.6
All	All	0	69

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	617	ARG	NE-CZ-NH1	10.89	125.75	120.30	3	16
1	A	536	ARG	NE-CZ-NH1	9.94	125.27	120.30	9	20
1	A	573	ARG	NE-CZ-NH1	9.12	124.86	120.30	15	13
1	A	649	ARG	NE-CZ-NH1	9.08	124.84	120.30	5	17
1	A	618	ARG	NE-CZ-NH1	9.02	124.81	120.30	4	17
1	A	623	ARG	NE-CZ-NH1	8.93	124.76	120.30	1	17
1	A	629	ARG	NE-CZ-NH1	8.85	124.72	120.30	1	18
1	A	615	ARG	NE-CZ-NH1	8.78	124.69	120.30	6	15
1	A	650	ARG	NE-CZ-NH1	8.68	124.64	120.30	15	16
1	A	591	VAL	CG1-CB-CG2	-7.95	98.19	110.90	17	14
1	A	583	PHE	CB-CG-CD2	-7.89	115.27	120.80	18	5
1	A	627	TYR	CB-CG-CD2	-7.78	116.33	121.00	15	2
1	A	635	VAL	CG1-CB-CG2	-7.74	98.51	110.90	5	6
1	A	583	PHE	CB-CG-CD1	7.46	126.02	120.80	18	3
1	A	631	TYR	CB-CG-CD2	-6.48	117.11	121.00	20	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models Worst	Total
1	A	606	TYR	CB-CG-CD2	-6.43	117.14	121.00	12	1
1	A	631	TYR	CB-CG-CD1	5.79	124.48	121.00	20	1
1	A	652	PHE	CB-CG-CD2	-5.79	116.75	120.80	2	1
1	A	622	VAL	CA-CB-CG1	5.58	119.27	110.90	3	2
1	A	627	TYR	CB-CG-CD1	5.51	124.31	121.00	15	1
1	A	638	PHE	CB-CG-CD2	-5.37	117.04	120.80	3	1
1	A	629	ARG	NE-CZ-NH2	-5.30	117.65	120.30	4	2
1	A	536	ARG	NE-CZ-NH2	-5.20	117.70	120.30	17	1
1	A	618	ARG	NE-CZ-NH2	-5.18	117.71	120.30	2	1
1	A	647	MET	CG-SD-CE	-5.14	91.98	100.20	4	1
1	A	617	ARG	NE-CZ-NH2	-5.09	117.75	120.30	3	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	595	GLY	Peptide	16
1	A	590	SER	Peptide	14
1	A	599	MET	Peptide	11
1	A	606	TYR	Sidechain	4
1	A	545	PHE	Sidechain	4
1	A	582	TYR	Sidechain	2
1	A	645	TYR	Sidechain	2
1	A	649	ARG	Sidechain	2
1	A	607	PHE	Peptide	2
1	A	610	ILE	Peptide	2
1	A	597	LYS	Peptide	2
1	A	596	ASN	Peptide	1
1	A	572	ILE	Peptide	1
1	A	631	TYR	Sidechain	1
1	A	613	LEU	Peptide	1
1	A	593	THR	Peptide	1
1	A	608	GLY	Peptide	1
1	A	592	LEU	Peptide	1
1	A	629	ARG	Sidechain	1

6.2　Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	968	981	981	1±1
All	All	19360	19620	19620	22

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:612:LEU:HD23	1:A:635:VAL:HG22	0.62	1.71	17	6
1:A:637:ASN:O	1:A:641:VAL:HG12	0.57	2.00	18	2
1:A:564:VAL:HG11	1:A:627:TYR:CE1	0.48	2.42	9	5
1:A:613:LEU:HD13	1:A:613:LEU:H	0.45	1.72	8	1
1:A:596:ASN:CA	1:A:597:LYS:HE3	0.45	2.42	7	3
1:A:596:ASN:HA	1:A:597:LYS:HE3	0.43	1.88	10	1
1:A:591:VAL:HG12	1:A:599:MET:C	0.43	2.33	17	1
1:A:591:VAL:HG12	1:A:599:MET:O	0.43	2.14	17	1
1:A:583:PHE:CE1	1:A:631:TYR:CE2	0.41	3.08	4	1
1:A:560:LEU:HD23	1:A:561:LYS:N	0.41	2.30	17	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	121/158 (77%)	115±1 (95±1%)	4±1 (3±1%)	2±1 (1±1%)	17	64
All	All	2420/3160 (77%)	2307 (95%)	83 (3%)	30 (1%)	17	64

All 8 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	575	GLY	15
1	A	610	ILE	5
1	A	612	LEU	4
1	A	609	GLU	2
1	A	535	CYS	1
1	A	611	CYS	1
1	A	608	GLY	1
1	A	594	LYS	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	106/139 (76%)	90±3 (84±3%)	16±3 (16±3%)	5	43
All	All	2120/2780 (76%)	1790 (84%)	330 (16%)	5	43

All 57 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	539	VAL	20
1	A	561	LYS	19
1	A	594	LYS	19
1	A	597	LYS	19
1	A	600	LYS	16
1	A	631	TYR	15
1	A	562	PHE	14
1	A	559	LYS	12
1	A	607	PHE	11
1	A	593	THR	10
1	A	613	LEU	10
1	A	638	PHE	9
1	A	648	MET	8
1	A	583	PHE	8
1	A	601	LEU	7
1	A	623	ARG	7
1	A	627	TYR	7
1	A	649	ARG	7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	585	GLN	7
1	A	635	VAL	7
1	A	542	MET	6
1	A	633	LEU	5
1	A	547	ASN	5
1	A	582	TYR	5
1	A	650	ARG	5
1	A	625	ASP	5
1	A	573	ARG	4
1	A	642	LEU	4
1	A	574	GLU	4
1	A	537	LYS	4
1	A	544	LEU	3
1	A	609	GLU	3
1	A	614	THR	3
1	A	538	LEU	3
1	A	560	LEU	3
1	A	596	ASN	3
1	A	643	GLU	3
1	A	603	ASP	3
1	A	606	TYR	2
1	A	536	ARG	2
1	A	612	LEU	2
1	A	592	LEU	2
1	A	640	GLU	2
1	A	579	LYS	2
1	A	598	GLU	2
1	A	629	ARG	2
1	A	618	ARG	1
1	A	590	SER	1
1	A	636	ASP	1
1	A	652	PHE	1
1	A	617	ARG	1
1	A	581	MET	1
1	A	580	LYS	1
1	A	586	HIS	1
1	A	634	SER	1
1	A	541	SER	1
1	A	615	ARG	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation ⓘ

The completeness of assignment taking into account all chemical shift lists is 87% for the well-defined parts and 85% 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	1886
Number of shifts mapped to atoms	1673
Number of unparsed shifts	0
Number of shifts with mapping errors	213
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

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

- No matching atom found in the structure. All 213 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	516	PRO	CA	62.224	0.3	1
1	A	516	PRO	CB	34.52	0.3	1
1	A	516	PRO	CG	24.622	0.3	1
1	A	516	PRO	CD	50.251	0.3	1
1	A	516	PRO	HA	4.511	0.020	1
1	A	516	PRO	HB2	2.303	0.020	2
1	A	516	PRO	HB3	2.103	0.020	2
1	A	516	PRO	HG2	1.879	0.020	2
1	A	516	PRO	HG3	1.771	0.020	2
1	A	516	PRO	HD2	3.484	0.020	2
1	A	516	PRO	HD3	3.44	0.020	2
1	A	517	SER	C	174.078	0.3	1
1	A	517	SER	CA	58.273	0.3	1
1	A	517	SER	CB	63.721	0.3	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	517	SER	HA	4.416	0.020	1
1	A	517	SER	HB2	3.8	0.020	1
1	A	517	SER	HB3	3.8	0.020	1
1	A	518	SER	CA	56.265	0.3	1
1	A	518	SER	CB	63.262	0.3	1
1	A	518	SER	H	8.221	0.020	1
1	A	518	SER	HA	3.796	0.020	1
1	A	518	SER	HB2	3.798	0.020	1
1	A	518	SER	HB3	3.798	0.020	1
1	A	518	SER	N	118.569	0.3	1
1	A	519	PRO	C	177.009	0.3	1
1	A	519	PRO	CA	63.448	0.3	1
1	A	519	PRO	CB	31.854	0.3	1
1	A	519	PRO	CG	27.245	0.3	1
1	A	519	PRO	CD	50.595	0.3	1
1	A	519	PRO	HA	4.335	0.020	1
1	A	519	PRO	HB2	2.24	0.020	2
1	A	519	PRO	HB3	1.858	0.020	2
1	A	519	PRO	HG2	1.947	0.020	1
1	A	519	PRO	HG3	1.947	0.020	1
1	A	519	PRO	HD2	3.747	0.020	2
1	A	519	PRO	HD3	3.656	0.020	2
1	A	520	MET	C	176.293	0.3	1
1	A	520	MET	CA	55.805	0.3	1
1	A	520	MET	CB	32.709	0.3	1
1	A	520	MET	CG	31.878	0.3	1
1	A	520	MET	H	8.258	0.020	1
1	A	520	MET	HA	4.321	0.020	1
1	A	520	MET	HB2	1.985	0.020	2
1	A	520	MET	HB3	1.912	0.020	2
1	A	520	MET	HG2	2.513	0.020	2
1	A	520	MET	HG3	2.466	0.020	2
1	A	520	MET	N	119.429	0.3	1
1	A	521	GLU	C	176.319	0.3	1
1	A	521	GLU	CA	56.479	0.3	1
1	A	521	GLU	CB	30.1	0.3	1
1	A	521	GLU	CG	36.13	0.3	1
1	A	521	GLU	H	8.21	0.020	1
1	A	521	GLU	HA	4.198	0.020	1
1	A	521	GLU	HB2	1.944	0.020	2
1	A	521	GLU	HB3	1.858	0.020	2

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	521	GLU	HG2	2.152	0.020	1
1	A	521	GLU	HG3	2.152	0.020	1
1	A	521	GLU	N	121.524	0.3	1
1	A	522	LEU	C	176.887	0.3	1
1	A	522	LEU	CA	55.161	0.3	1
1	A	522	LEU	CB	42.16	0.3	1
1	A	522	LEU	CG	26.779	0.3	1
1	A	522	LEU	CD1	24.692	0.3	1
1	A	522	LEU	CD2	23.423	0.3	1
1	A	522	LEU	H	8.112	0.020	1
1	A	522	LEU	HA	4.253	0.020	1
1	A	522	LEU	HB2	1.502	0.020	1
1	A	522	LEU	HB3	1.502	0.020	1
1	A	522	LEU	HG	1.528	0.020	1
1	A	522	LEU	HD11	0.832	0.020	1
1	A	522	LEU	HD12	0.832	0.020	1
1	A	522	LEU	HD13	0.832	0.020	1
1	A	522	LEU	HD21	0.772	0.020	1
1	A	522	LEU	HD22	0.772	0.020	1
1	A	522	LEU	HD23	0.772	0.020	1
1	A	522	LEU	N	122.766	0.3	1
1	A	523	ASN	C	175.081	0.3	1
1	A	523	ASN	CA	53.023	0.3	1
1	A	523	ASN	CB	39.104	0.3	1
1	A	523	ASN	CG	176.659	0.3	1
1	A	523	ASN	H	8.286	0.020	1
1	A	523	ASN	HA	4.691	0.020	1
1	A	523	ASN	HB2	2.768	0.020	2
1	A	523	ASN	HB3	2.664	0.020	2
1	A	523	ASN	HD21	7.514	0.020	1
1	A	523	ASN	HD22	6.845	0.020	1
1	A	523	ASN	N	118.606	0.3	1
1	A	523	ASN	ND2	112.953	0.3	1
1	A	524	GLY	CA	44.931	0.3	1
1	A	524	GLY	H	8.061	0.020	1
1	A	524	GLY	HA2	3.987	0.020	1
1	A	524	GLY	HA3	3.987	0.020	1
1	A	524	GLY	N	108.964	0.3	1
1	A	525	PRO	C	177.141	0.3	1
1	A	525	PRO	CA	63.096	0.3	1
1	A	525	PRO	CB	32.16	0.3	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	525	PRO	CG	26.909	0.3	1
1	A	525	PRO	CD	49.638	0.3	1
1	A	525	PRO	HA	4.443	0.020	1
1	A	525	PRO	HB2	2.243	0.020	2
1	A	525	PRO	HB3	2.183	0.020	2
1	A	525	PRO	HG2	1.948	0.020	2
1	A	525	PRO	HG3	1.899	0.020	2
1	A	525	PRO	HD2	3.514	0.020	1
1	A	525	PRO	HD3	3.514	0.020	1
1	A	526	LEU	C	177.423	0.3	1
1	A	526	LEU	CA	55.254	0.3	1
1	A	526	LEU	CB	42.118	0.3	1
1	A	526	LEU	CG	26.818	0.3	1
1	A	526	LEU	CD1	24.733	0.3	1
1	A	526	LEU	CD2	23.518	0.3	1
1	A	526	LEU	H	8.203	0.020	1
1	A	526	LEU	HA	4.247	0.020	1
1	A	526	LEU	HB2	1.557	0.020	2
1	A	526	LEU	HB3	1.498	0.020	2
1	A	526	LEU	HG	1.531	0.020	1
1	A	526	LEU	HD11	0.832	0.020	1
1	A	526	LEU	HD12	0.832	0.020	1
1	A	526	LEU	HD13	0.832	0.020	1
1	A	526	LEU	HD21	0.775	0.020	1
1	A	526	LEU	HD22	0.775	0.020	1
1	A	526	LEU	HD23	0.775	0.020	1
1	A	526	LEU	N	121.258	0.3	1
1	A	527	ARG	C	176.456	0.3	1
1	A	527	ARG	CA	56.555	0.3	1
1	A	527	ARG	CB	30.478	0.3	1
1	A	527	ARG	CG	26.943	0.3	1
1	A	527	ARG	CD	43.109	0.3	1
1	A	527	ARG	H	8.116	0.020	1
1	A	527	ARG	HA	4.165	0.020	1
1	A	527	ARG	HB2	1.753	0.020	2
1	A	527	ARG	HB3	1.713	0.020	2
1	A	527	ARG	HG2	1.556	0.020	1
1	A	527	ARG	HG3	1.556	0.020	1
1	A	527	ARG	HD2	3.116	0.020	1
1	A	527	ARG	HD3	3.116	0.020	1
1	A	527	ARG	N	121.455	0.3	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	528	GLU	C	176.574	0.3	1
1	A	528	GLU	CA	57.209	0.3	1
1	A	528	GLU	CB	29.972	0.3	1
1	A	528	GLU	CG	36.194	0.3	1
1	A	528	GLU	H	8.338	0.020	1
1	A	528	GLU	HA	4.092	0.020	1
1	A	528	GLU	HB2	1.943	0.020	2
1	A	528	GLU	HB3	1.859	0.020	2
1	A	528	GLU	HG2	2.154	0.020	1
1	A	528	GLU	HG3	2.154	0.020	1
1	A	528	GLU	N	121.28	0.3	1
1	A	529	GLU	C	176.85	0.3	1
1	A	529	GLU	CA	57.056	0.3	1
1	A	529	GLU	CB	29.838	0.3	1
1	A	529	GLU	CG	36.171	0.3	1
1	A	529	GLU	H	8.366	0.020	1
1	A	529	GLU	HA	4.097	0.020	1
1	A	529	GLU	HB2	1.941	0.020	2
1	A	529	GLU	HB3	1.866	0.020	2
1	A	529	GLU	HG2	2.154	0.020	1
1	A	529	GLU	HG3	2.154	0.020	1
1	A	529	GLU	N	120.988	0.3	1
1	A	530	ILE	C	176.611	0.3	1
1	A	530	ILE	CA	61.653	0.3	1
1	A	530	ILE	CB	38.119	0.3	1
1	A	530	ILE	CG1	27.436	0.3	1
1	A	530	ILE	CG2	17.405	0.3	1
1	A	530	ILE	CD1	12.603	0.3	1
1	A	530	ILE	H	7.941	0.020	1
1	A	530	ILE	HA	4.004	0.020	1
1	A	530	ILE	HB	1.803	0.020	1
1	A	530	ILE	HG12	1.375	0.020	2
1	A	530	ILE	HG13	1.093	0.020	2
1	A	530	ILE	HG21	0.789	0.020	1
1	A	530	ILE	HG22	0.789	0.020	1
1	A	530	ILE	HG23	0.789	0.020	1
1	A	530	ILE	HD11	0.719	0.020	1
1	A	530	ILE	HD12	0.719	0.020	1
1	A	530	ILE	HD13	0.719	0.020	1
1	A	530	ILE	N	121.269	0.3	1
1	A	531	VAL	C	176.308	0.3	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	531	VAL	CA	63.257	0.3	1
1	A	531	VAL	CB	32.11	0.3	1
1	A	531	VAL	CG1	20.932	0.3	1
1	A	531	VAL	H	7.952	0.020	1
1	A	531	VAL	HA	3.862	0.020	1
1	A	531	VAL	HB	1.92	0.020	1
1	A	531	VAL	HG11	0.767	0.020	1
1	A	531	VAL	HG12	0.767	0.020	1
1	A	531	VAL	HG13	0.767	0.020	1
1	A	531	VAL	HG21	0.767	0.020	1
1	A	531	VAL	HG22	0.767	0.020	1
1	A	531	VAL	HG23	0.767	0.020	1
1	A	531	VAL	N	122.87	0.3	1
1	A	532	ASN	C	175.26	0.3	1
1	A	532	ASN	CA	53.718	0.3	1
1	A	532	ASN	CB	38.469	0.3	1
1	A	532	ASN	H	8.267	0.020	1
1	A	532	ASN	HA	4.502	0.020	1
1	A	532	ASN	HB2	2.682	0.020	1
1	A	532	ASN	HB3	2.682	0.020	1
1	A	532	ASN	HD21	7.516	0.020	1
1	A	532	ASN	HD22	6.786	0.020	1
1	A	532	ASN	N	120.311	0.3	1
1	A	532	ASN	ND2	112.632	0.3	1
1	A	533	PHE	CA	59.097	0.3	1
1	A	533	PHE	CB	39.05	0.3	1
1	A	533	PHE	H	8.055	0.020	1
1	A	533	PHE	HA	4.289	0.020	1
1	A	533	PHE	HB2	3.105	0.020	2
1	A	533	PHE	HB3	2.973	0.020	2
1	A	533	PHE	HD1	7.247	0.020	1
1	A	533	PHE	HD2	7.247	0.020	1
1	A	533	PHE	HE1	7.181	0.020	1
1	A	533	PHE	HE2	7.181	0.020	1
1	A	533	PHE	N	120.952	0.3	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	152	0.07 ± 0.22	None needed (< 0.5 ppm)
$^{13}C_\beta$	142	0.11 ± 0.10	None needed (< 0.5 ppm)
$^{13}C'$	131	0.16 ± 0.14	None needed (< 0.5 ppm)
^{15}N	139	0.49 ± 0.52	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 87%, i.e. 1479 atoms were assigned a chemical shift out of a possible 1698. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	576/605 (95%)	240/246 (98%)	224/242 (93%)	112/117 (96%)
Sidechain	839/952 (88%)	570/620 (92%)	261/290 (90%)	8/42 (19%)
Aromatic	64/141 (45%)	63/68 (93%)	1/72 (1%)	0/1 (0%)
Overall	1479/1698 (87%)	873/934 (93%)	486/604 (80%)	120/160 (75%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 1673 atoms were assigned a chemical shift out of a possible 1968. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	645/696 (93%)	269/283 (95%)	251/278 (90%)	125/135 (93%)
Sidechain	963/1124 (86%)	655/731 (90%)	300/341 (88%)	8/52 (15%)
Aromatic	65/148 (44%)	64/72 (89%)	1/74 (1%)	0/2 (0%)
Overall	1673/1968 (85%)	988/1086 (91%)	552/693 (80%)	133/189 (70%)

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	582	TYR	HB3	0.61	$0.93 - 4.76$	-5.8
1	A	571	ILE	HG13	-1.10	$-0.82 - 3.23$	-5.7

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from

the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:
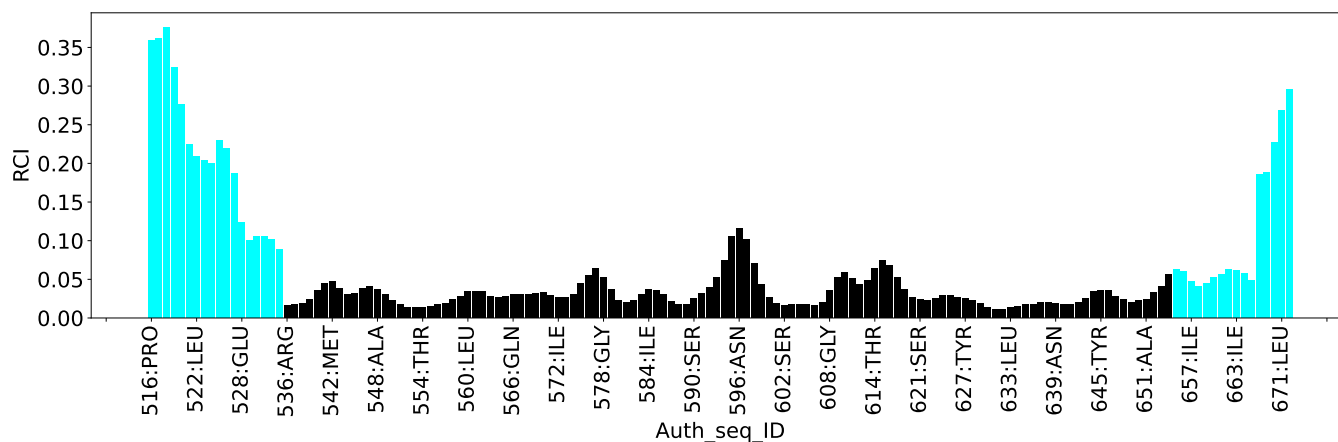
8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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

Description	Value
Total distance restraints	1687
Intra-residue ($|i-j|=0$)	406
Sequential ($|i-j|=1$)	534
Medium range ($|i-j|>1$ and $|i-j|<5$)	262
Long range ($|i-j|\geq 5$)	449
Inter-chain	0
Hydrogen bond restraints	36
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	103
Number of restraints per residue	10.7
Number of long range restraints per residue[1]	3.1

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

8.2 Residual restraint violations (i)

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

8.2.1 Average number of distance violations per model (i)

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	5.5	0.2
0.2-0.5 (Medium)	6.8	0.5
>0.5 (Large)	9.6	2.12

8.2.2   Average number of dihedral-angle violations per model ⓘ

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

9   Distance violation analysis ⓘ

9.1   Summary of distance violations ⓘ

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

Restraints type	Count	$\%^1$	Violated[3]			Consistently Violated[4]		
			Count	$\%^2$	$\%^1$	Count	$\%^2$	$\%^1$
Intra-residue (|i-j|=0)	406	24.1	17	4.2	1.0	0	0.0	0.0
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	327	19.4	9	2.8	0.5	0	0.0	0.0
Sidechain-Sidechain	78	4.6	8	10.3	0.5	0	0.0	0.0
Sequential (|i-j|=1)	534	31.7	18	3.4	1.1	0	0.0	0.0
Backbone-Backbone	158	9.4	1	0.6	0.1	0	0.0	0.0
Backbone-Sidechain	325	19.3	11	3.4	0.7	0	0.0	0.0
Sidechain-Sidechain	51	3.0	6	11.8	0.4	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	262	15.5	10	3.8	0.6	0	0.0	0.0
Backbone-Backbone	86	5.1	1	1.2	0.1	0	0.0	0.0
Backbone-Sidechain	116	6.9	3	2.6	0.2	0	0.0	0.0
Sidechain-Sidechain	60	3.6	6	10.0	0.4	0	0.0	0.0
Long range (|i-j|≥5)	449	26.6	33	7.3	2.0	0	0.0	0.0
Backbone-Backbone	90	5.3	2	2.2	0.1	0	0.0	0.0
Backbone-Sidechain	188	11.1	13	6.9	0.8	0	0.0	0.0
Sidechain-Sidechain	171	10.1	18	10.5	1.1	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	36	2.1	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	1687	100.0	78	4.6	4.6	0	0.0	0.0
Backbone-Backbone	371	22.0	4	1.1	0.2	0	0.0	0.0
Backbone-Sidechain	956	56.7	36	3.8	2.1	0	0.0	0.0
Sidechain-Sidechain	360	21.3	38	10.6	2.3	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations ⓘ
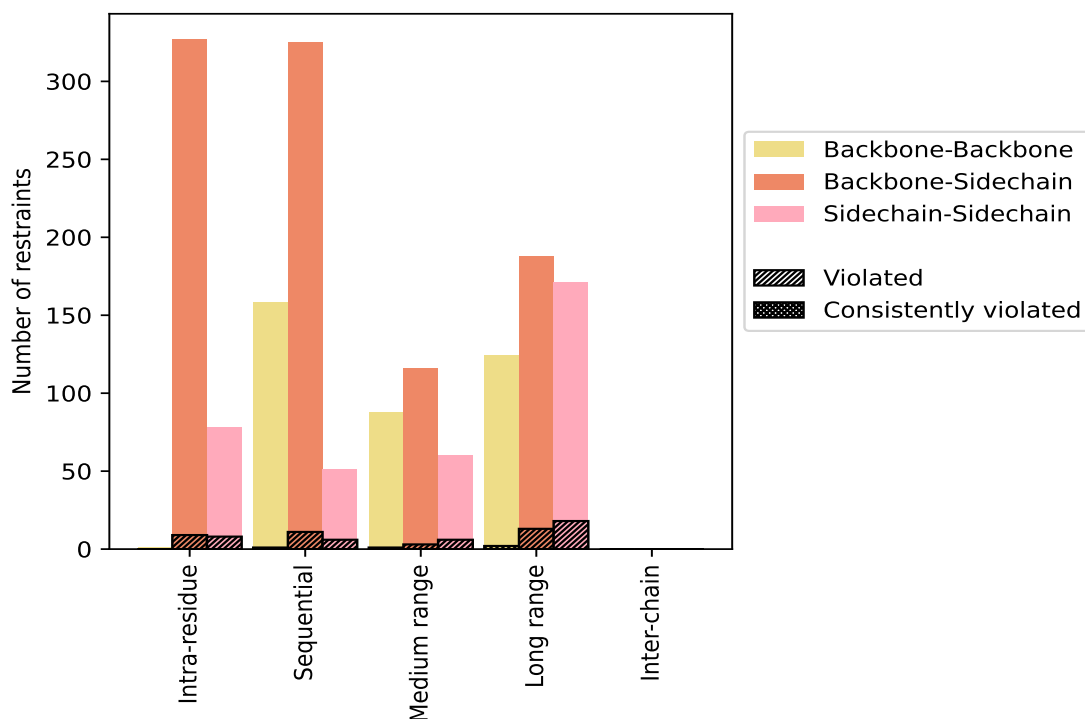
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model ⓘ

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	5	5	7	8	0	25	0.48	1.65	0.45	0.23
2	1	2	6	10	0	19	0.62	1.35	0.4	0.59
3	3	5	4	8	0	20	0.62	2.09	0.56	0.43
4	3	7	6	10	0	26	0.63	1.82	0.52	0.5
5	2	6	6	10	0	24	0.69	1.73	0.5	0.5
6	3	3	5	12	0	23	0.6	2.08	0.51	0.44
7	4	3	6	9	0	22	0.58	2.12	0.5	0.41
8	3	6	3	10	0	22	0.55	1.5	0.36	0.49
9	2	3	5	18	0	28	0.45	1.53	0.35	0.33
10	0	4	5	7	0	16	0.6	1.29	0.37	0.56
11	2	4	6	16	0	28	0.65	1.82	0.51	0.46

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				
12	1	5	6	21	0	33	0.71	1.75	0.47	0.71
13	4	3	5	8	0	20	0.64	2.11	0.53	0.5
14	6	3	5	11	0	25	0.45	1.52	0.39	0.29
15	2	5	3	7	0	17	0.6	1.52	0.37	0.54
16	4	3	5	12	0	24	0.45	1.45	0.39	0.26
17	2	6	6	10	0	24	0.53	1.84	0.45	0.38
18	1	1	4	9	0	15	0.69	1.8	0.48	0.47
19	3	3	4	4	0	14	0.44	1.42	0.38	0.34
20	2	2	4	3	0	11	0.57	1.51	0.41	0.46

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

9.2.1　Bar graph : Distance Violation statistics for each model ⓘ
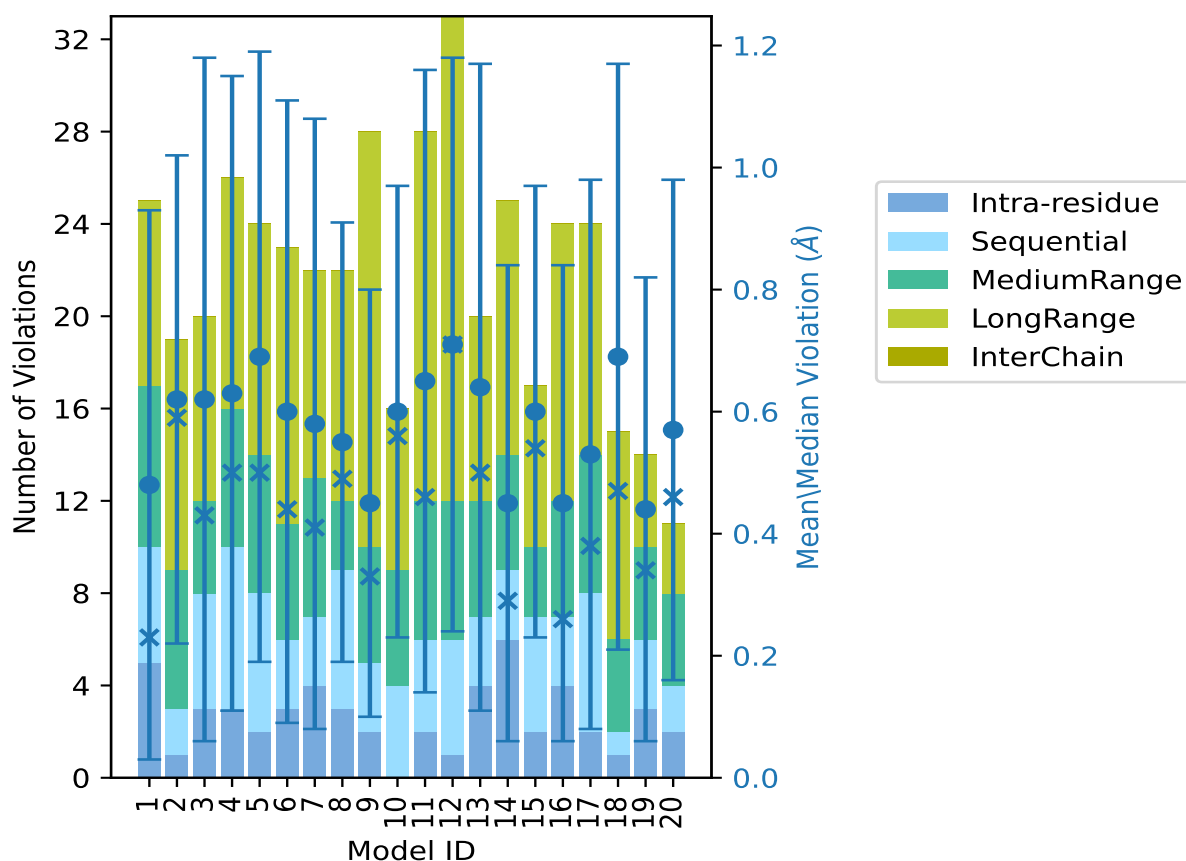
The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

9.3   Distance violation statistics for the ensemble ⓘ

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, 1573(IR:389, SQ:516, MR:252, LR:416, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
9	7	2	6	0	24	1	5.0
3	3	0	4	0	10	2	10.0
1	1	0	4	0	6	3	15.0
1	1	1	2	0	5	4	20.0
0	0	1	1	0	2	5	25.0
0	3	0	1	0	4	6	30.0
0	0	1	1	0	2	7	35.0
1	0	0	2	0	3	8	40.0
0	0	0	4	0	4	9	45.0
0	1	0	2	0	3	10	50.0
1	0	0	0	0	1	11	55.0
1	1	0	2	0	4	12	60.0
0	0	0	2	0	2	13	65.0
0	0	1	1	0	2	14	70.0
0	0	0	1	0	1	15	75.0
0	0	2	0	0	2	16	80.0
0	0	0	0	0	0	17	85.0
0	0	1	0	0	1	18	90.0
0	1	1	0	0	2	19	95.0
0	0	0	0	0	0	20	100.0

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

9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ
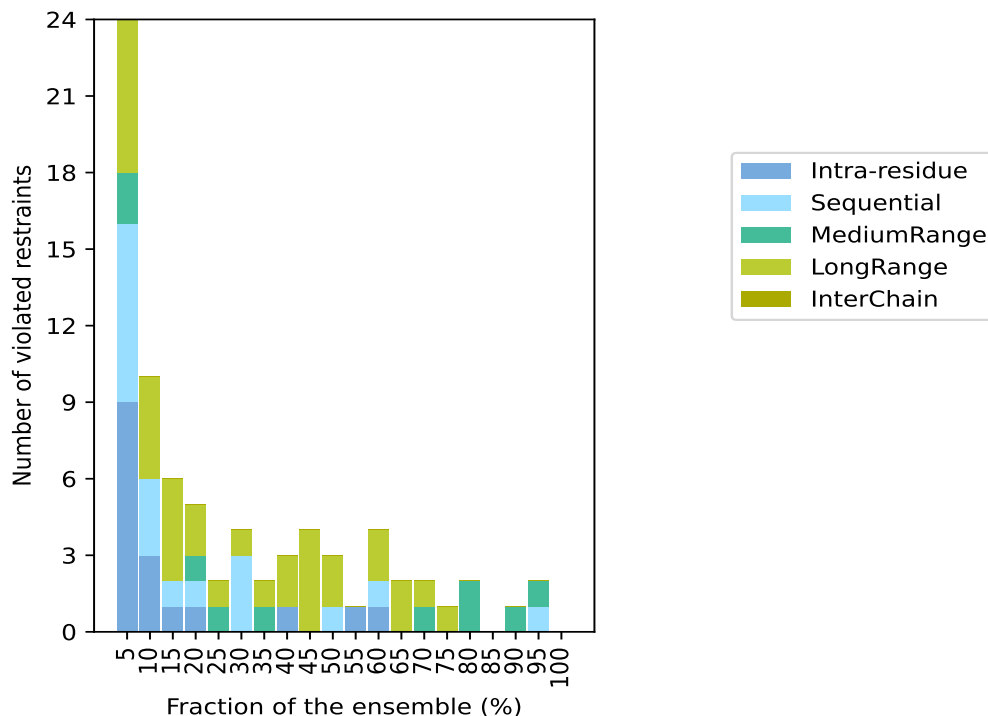
9.4 Most violated distance restraints in the ensemble ⓘ

9.4.1 Histogram : Distribution of mean distance violations ⓘ

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble
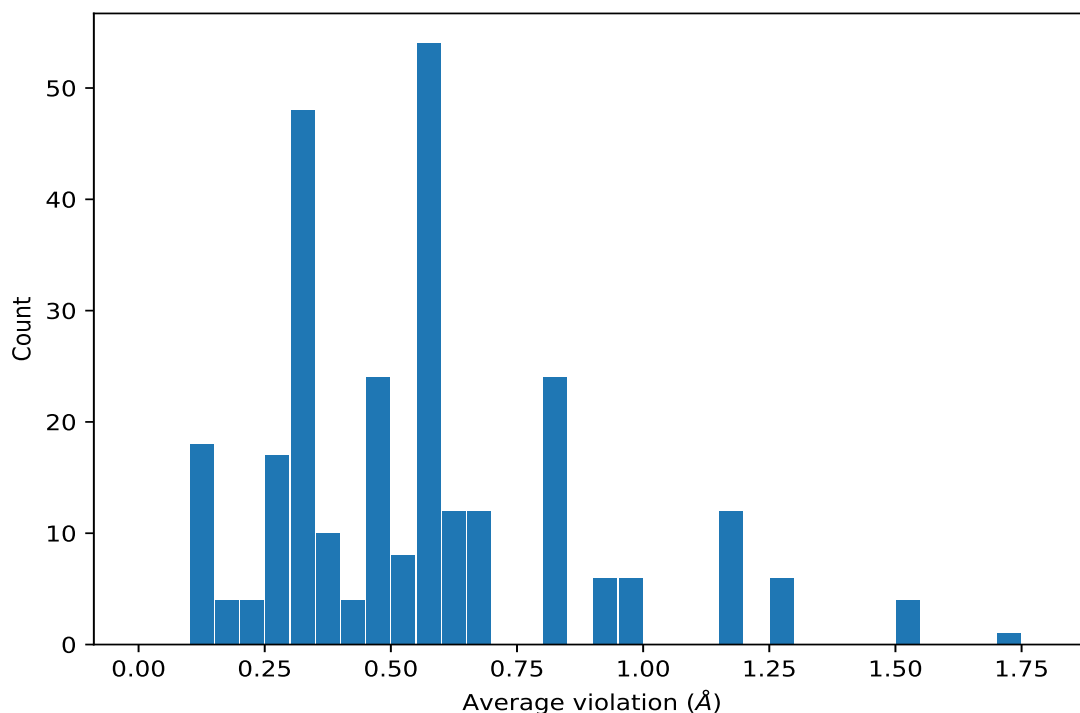
9.4.2   Table: Most violated distance restraints   ⓘ

The following table provides the mean and the standard deviation of 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)
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD1	19	0.98	0.45	0.95
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD2	19	0.98	0.45	0.95
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD1	19	0.98	0.45	0.95
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD2	19	0.98	0.45	0.95
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD1	19	0.98	0.45	0.95
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD2	19	0.98	0.45	0.95
(1,1039)	1:A:592:LEU:HD11	1:A:593:THR:H	19	0.67	0.22	0.72
(1,1039)	1:A:592:LEU:HD12	1:A:593:THR:H	19	0.67	0.22	0.72
(1,1039)	1:A:592:LEU:HD13	1:A:593:THR:H	19	0.67	0.22	0.72
(1,1039)	1:A:592:LEU:HD21	1:A:593:THR:H	19	0.67	0.22	0.72
(1,1039)	1:A:592:LEU:HD22	1:A:593:THR:H	19	0.67	0.22	0.72
(1,1039)	1:A:592:LEU:HD23	1:A:593:THR:H	19	0.67	0.22	0.72
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD11	18	1.18	0.54	1.38
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD12	18	1.18	0.54	1.38
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD13	18	1.18	0.54	1.38
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD21	18	1.18	0.54	1.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD22	18	1.18	0.54	1.38
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD23	18	1.18	0.54	1.38
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG21	16	1.17	0.52	1.28
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG22	16	1.17	0.52	1.28
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG23	16	1.17	0.52	1.28
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG21	16	1.17	0.52	1.28
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG22	16	1.17	0.52	1.28
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG23	16	1.17	0.52	1.28
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD2	16	0.85	0.37	0.91
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD3	16	0.85	0.37	0.91
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD2	16	0.85	0.37	0.91
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD3	16	0.85	0.37	0.91
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD2	16	0.85	0.37	0.91
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD3	16	0.85	0.37	0.91
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD11	15	0.67	0.14	0.71
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD12	15	0.67	0.14	0.71
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD13	15	0.67	0.14	0.71
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD21	15	0.67	0.14	0.71
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD22	15	0.67	0.14	0.71
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD23	15	0.67	0.14	0.71
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD11	14	1.26	0.32	1.37
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD12	14	1.26	0.32	1.37
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD13	14	1.26	0.32	1.37
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD21	14	1.26	0.32	1.37
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD22	14	1.26	0.32	1.37
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD23	14	1.26	0.32	1.37
(1,1022)	1:A:591:VAL:HG21	1:A:600:LYS:HA	14	0.16	0.01	0.16
(1,1022)	1:A:591:VAL:HG22	1:A:600:LYS:HA	14	0.16	0.01	0.16
(1,1022)	1:A:591:VAL:HG23	1:A:600:LYS:HA	14	0.16	0.01	0.16
(1,145)	1:A:538:LEU:HD11	1:A:605:SER:H	13	0.62	0.37	0.53
(1,145)	1:A:538:LEU:HD12	1:A:605:SER:H	13	0.62	0.37	0.53
(1,145)	1:A:538:LEU:HD13	1:A:605:SER:H	13	0.62	0.37	0.53
(1,145)	1:A:538:LEU:HD21	1:A:605:SER:H	13	0.62	0.37	0.53
(1,145)	1:A:538:LEU:HD22	1:A:605:SER:H	13	0.62	0.37	0.53
(1,145)	1:A:538:LEU:HD23	1:A:605:SER:H	13	0.62	0.37	0.53
(1,986)	1:A:590:SER:HA	1:A:600:LYS:H	13	0.14	0.02	0.14
(1,701)	1:A:574:GLU:HG2	1:A:579:LYS:HD2	12	1.53	0.47	1.38
(1,701)	1:A:574:GLU:HG2	1:A:579:LYS:HD3	12	1.53	0.47	1.38
(1,701)	1:A:574:GLU:HG3	1:A:579:LYS:HD2	12	1.53	0.47	1.38
(1,701)	1:A:574:GLU:HG3	1:A:579:LYS:HD3	12	1.53	0.47	1.38
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB1	12	0.82	0.15	0.8
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB2	12	0.82	0.15	0.8

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB3	12	0.82	0.15	0.8
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB1	12	0.82	0.15	0.8
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB2	12	0.82	0.15	0.8
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB3	12	0.82	0.15	0.8
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD11	12	0.55	0.26	0.5
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD12	12	0.55	0.26	0.5
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD13	12	0.55	0.26	0.5
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD21	12	0.55	0.26	0.5
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD22	12	0.55	0.26	0.5
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD23	12	0.55	0.26	0.5
(1,1100)	1:A:597:LYS:HG2	1:A:597:LYS:HE2	12	0.4	0.1	0.44
(1,1100)	1:A:597:LYS:HG2	1:A:597:LYS:HE3	12	0.4	0.1	0.44
(1,1100)	1:A:597:LYS:HG3	1:A:597:LYS:HE2	12	0.4	0.1	0.44
(1,1100)	1:A:597:LYS:HG3	1:A:597:LYS:HE3	12	0.4	0.1	0.44
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD11	11	0.34	0.08	0.32
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD12	11	0.34	0.08	0.32
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD13	11	0.34	0.08	0.32
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD21	11	0.34	0.08	0.32
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD22	11	0.34	0.08	0.32
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD23	11	0.34	0.08	0.32
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD11	10	0.8	0.41	0.67
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD12	10	0.8	0.41	0.67
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD13	10	0.8	0.41	0.67
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD21	10	0.8	0.41	0.67
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD22	10	0.8	0.41	0.67
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD23	10	0.8	0.41	0.67
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD11	10	0.8	0.41	0.67
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD12	10	0.8	0.41	0.67
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD13	10	0.8	0.41	0.67
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD21	10	0.8	0.41	0.67
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD22	10	0.8	0.41	0.67
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD23	10	0.8	0.41	0.67
(1,235)	1:A:544:LEU:HD11	1:A:652:PHE:HD1	10	0.56	0.27	0.54
(1,235)	1:A:544:LEU:HD11	1:A:652:PHE:HD2	10	0.56	0.27	0.54
(1,235)	1:A:544:LEU:HD12	1:A:652:PHE:HD1	10	0.56	0.27	0.54
(1,235)	1:A:544:LEU:HD12	1:A:652:PHE:HD2	10	0.56	0.27	0.54
(1,235)	1:A:544:LEU:HD13	1:A:652:PHE:HD1	10	0.56	0.27	0.54
(1,235)	1:A:544:LEU:HD13	1:A:652:PHE:HD2	10	0.56	0.27	0.54
(1,1044)	1:A:592:LEU:HD11	1:A:623:ARG:H	10	0.45	0.18	0.5
(1,1044)	1:A:592:LEU:HD12	1:A:623:ARG:H	10	0.45	0.18	0.5
(1,1044)	1:A:592:LEU:HD13	1:A:623:ARG:H	10	0.45	0.18	0.5
(1,1044)	1:A:592:LEU:HD21	1:A:623:ARG:H	10	0.45	0.18	0.5

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1044)	1:A:592:LEU:HD22	1:A:623:ARG:H	10	0.45	0.18	0.5
(1,1044)	1:A:592:LEU:HD23	1:A:623:ARG:H	10	0.45	0.18	0.5
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD11	9	0.6	0.35	0.73
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD12	9	0.6	0.35	0.73
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD13	9	0.6	0.35	0.73
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD11	9	0.6	0.35	0.73
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD12	9	0.6	0.35	0.73
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD13	9	0.6	0.35	0.73
(1,1041)	1:A:592:LEU:HD11	1:A:598:GLU:HG2	9	0.33	0.14	0.3
(1,1041)	1:A:592:LEU:HD12	1:A:598:GLU:HG2	9	0.33	0.14	0.3
(1,1041)	1:A:592:LEU:HD13	1:A:598:GLU:HG2	9	0.33	0.14	0.3
(1,1041)	1:A:592:LEU:HD21	1:A:598:GLU:HG2	9	0.33	0.14	0.3
(1,1041)	1:A:592:LEU:HD22	1:A:598:GLU:HG2	9	0.33	0.14	0.3
(1,1041)	1:A:592:LEU:HD23	1:A:598:GLU:HG2	9	0.33	0.14	0.3
(1,405)	1:A:556:MET:HE1	1:A:638:PHE:HD1	9	0.3	0.08	0.25
(1,405)	1:A:556:MET:HE1	1:A:638:PHE:HD2	9	0.3	0.08	0.25
(1,405)	1:A:556:MET:HE2	1:A:638:PHE:HD1	9	0.3	0.08	0.25
(1,405)	1:A:556:MET:HE2	1:A:638:PHE:HD2	9	0.3	0.08	0.25
(1,405)	1:A:556:MET:HE3	1:A:638:PHE:HD1	9	0.3	0.08	0.25
(1,405)	1:A:556:MET:HE3	1:A:638:PHE:HD2	9	0.3	0.08	0.25
(1,1019)	1:A:591:VAL:HG21	1:A:599:MET:HA	9	0.13	0.02	0.13
(1,1019)	1:A:591:VAL:HG22	1:A:599:MET:HA	9	0.13	0.02	0.13
(1,1019)	1:A:591:VAL:HG23	1:A:599:MET:HA	9	0.13	0.02	0.13
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD11	8	0.45	0.17	0.47
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD12	8	0.45	0.17	0.47
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD13	8	0.45	0.17	0.47
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD21	8	0.45	0.17	0.47
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD22	8	0.45	0.17	0.47
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD23	8	0.45	0.17	0.47
(1,842)	1:A:584:ILE:HD11	1:A:607:PHE:HD1	8	0.45	0.12	0.42
(1,842)	1:A:584:ILE:HD11	1:A:607:PHE:HD2	8	0.45	0.12	0.42
(1,842)	1:A:584:ILE:HD12	1:A:607:PHE:HD1	8	0.45	0.12	0.42
(1,842)	1:A:584:ILE:HD12	1:A:607:PHE:HD2	8	0.45	0.12	0.42
(1,842)	1:A:584:ILE:HD13	1:A:607:PHE:HD1	8	0.45	0.12	0.42
(1,842)	1:A:584:ILE:HD13	1:A:607:PHE:HD2	8	0.45	0.12	0.42
(1,500)	1:A:562:PHE:HE1	1:A:629:ARG:HG2	8	0.37	0.11	0.36
(1,500)	1:A:562:PHE:HE1	1:A:629:ARG:HG3	8	0.37	0.11	0.36
(1,500)	1:A:562:PHE:HE2	1:A:629:ARG:HG2	8	0.37	0.11	0.36
(1,500)	1:A:562:PHE:HE2	1:A:629:ARG:HG3	8	0.37	0.11	0.36
(1,577)	1:A:566:GLN:HG2	1:A:627:TYR:HD1	7	0.29	0.12	0.24
(1,577)	1:A:566:GLN:HG2	1:A:627:TYR:HD2	7	0.29	0.12	0.24
(1,577)	1:A:566:GLN:HG3	1:A:627:TYR:HD1	7	0.29	0.12	0.24

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,577)	1:A:566:GLN:HG3	1:A:627:TYR:HD2	7	0.29	0.12	0.24
(1,1264)	1:A:626:THR:H	1:A:628:CYS:HB2	7	0.14	0.01	0.14
(1,699)	1:A:574:GLU:HG2	1:A:575:GLY:HA2	6	0.51	0.08	0.49
(1,699)	1:A:574:GLU:HG2	1:A:575:GLY:HA3	6	0.51	0.08	0.49
(1,699)	1:A:574:GLU:HG3	1:A:575:GLY:HA2	6	0.51	0.08	0.49
(1,699)	1:A:574:GLU:HG3	1:A:575:GLY:HA3	6	0.51	0.08	0.49
(1,1072)	1:A:594:LYS:HD2	1:A:595:GLY:HA2	6	0.51	0.2	0.5
(1,1072)	1:A:594:LYS:HD2	1:A:595:GLY:HA3	6	0.51	0.2	0.5
(1,1072)	1:A:594:LYS:HD3	1:A:595:GLY:HA2	6	0.51	0.2	0.5
(1,1072)	1:A:594:LYS:HD3	1:A:595:GLY:HA3	6	0.51	0.2	0.5
(1,137)	1:A:538:LEU:HD11	1:A:584:ILE:H	6	0.47	0.23	0.38
(1,137)	1:A:538:LEU:HD12	1:A:584:ILE:H	6	0.47	0.23	0.38
(1,137)	1:A:538:LEU:HD13	1:A:584:ILE:H	6	0.47	0.23	0.38
(1,137)	1:A:538:LEU:HD21	1:A:584:ILE:H	6	0.47	0.23	0.38
(1,137)	1:A:538:LEU:HD22	1:A:584:ILE:H	6	0.47	0.23	0.38
(1,137)	1:A:538:LEU:HD23	1:A:584:ILE:H	6	0.47	0.23	0.38
(1,1327)	1:A:635:VAL:HG21	1:A:636:ASP:HA	6	0.15	0.01	0.15
(1,1327)	1:A:635:VAL:HG22	1:A:636:ASP:HA	6	0.15	0.01	0.15
(1,1327)	1:A:635:VAL:HG23	1:A:636:ASP:HA	6	0.15	0.01	0.15
(1,1045)	1:A:592:LEU:HD11	1:A:623:ARG:HD2	5	0.34	0.15	0.34
(1,1045)	1:A:592:LEU:HD12	1:A:623:ARG:HD2	5	0.34	0.15	0.34
(1,1045)	1:A:592:LEU:HD13	1:A:623:ARG:HD2	5	0.34	0.15	0.34
(1,1045)	1:A:592:LEU:HD21	1:A:623:ARG:HD2	5	0.34	0.15	0.34
(1,1045)	1:A:592:LEU:HD22	1:A:623:ARG:HD2	5	0.34	0.15	0.34
(1,1045)	1:A:592:LEU:HD23	1:A:623:ARG:HD2	5	0.34	0.15	0.34
(1,1045)	1:A:592:LEU:HD11	1:A:623:ARG:HD3	5	0.34	0.15	0.34
(1,1045)	1:A:592:LEU:HD12	1:A:623:ARG:HD3	5	0.34	0.15	0.34
(1,1045)	1:A:592:LEU:HD13	1:A:623:ARG:HD3	5	0.34	0.15	0.34
(1,1045)	1:A:592:LEU:HD21	1:A:623:ARG:HD3	5	0.34	0.15	0.34
(1,1045)	1:A:592:LEU:HD22	1:A:623:ARG:HD3	5	0.34	0.15	0.34
(1,1045)	1:A:592:LEU:HD23	1:A:623:ARG:HD3	5	0.34	0.15	0.34
(1,1015)	1:A:591:VAL:HG11	1:A:593:THR:H	5	0.12	0.01	0.12
(1,1015)	1:A:591:VAL:HG12	1:A:593:THR:H	5	0.12	0.01	0.12
(1,1015)	1:A:591:VAL:HG13	1:A:593:THR:H	5	0.12	0.01	0.12
(1,141)	1:A:538:LEU:HD11	1:A:585:GLN:HB2	4	0.58	0.28	0.55
(1,141)	1:A:538:LEU:HD11	1:A:585:GLN:HB3	4	0.58	0.28	0.55
(1,141)	1:A:538:LEU:HD12	1:A:585:GLN:HB2	4	0.58	0.28	0.55
(1,141)	1:A:538:LEU:HD12	1:A:585:GLN:HB3	4	0.58	0.28	0.55
(1,141)	1:A:538:LEU:HD13	1:A:585:GLN:HB2	4	0.58	0.28	0.55
(1,141)	1:A:538:LEU:HD13	1:A:585:GLN:HB3	4	0.58	0.28	0.55
(1,141)	1:A:538:LEU:HD21	1:A:585:GLN:HB2	4	0.58	0.28	0.55
(1,141)	1:A:538:LEU:HD21	1:A:585:GLN:HB3	4	0.58	0.28	0.55

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,141)	1:A:538:LEU:HD22	1:A:585:GLN:HB2	4	0.58	0.28	0.55
(1,141)	1:A:538:LEU:HD22	1:A:585:GLN:HB3	4	0.58	0.28	0.55
(1,141)	1:A:538:LEU:HD23	1:A:585:GLN:HB2	4	0.58	0.28	0.55
(1,141)	1:A:538:LEU:HD23	1:A:585:GLN:HB3	4	0.58	0.28	0.55
(1,209)	1:A:542:MET:HE1	1:A:545:PHE:HD1	4	0.55	0.35	0.43
(1,209)	1:A:542:MET:HE1	1:A:545:PHE:HD2	4	0.55	0.35	0.43
(1,209)	1:A:542:MET:HE2	1:A:545:PHE:HD1	4	0.55	0.35	0.43
(1,209)	1:A:542:MET:HE2	1:A:545:PHE:HD2	4	0.55	0.35	0.43
(1,209)	1:A:542:MET:HE3	1:A:545:PHE:HD1	4	0.55	0.35	0.43
(1,209)	1:A:542:MET:HE3	1:A:545:PHE:HD2	4	0.55	0.35	0.43
(1,932)	1:A:588:VAL:HG11	1:A:602:SER:HB3	4	0.32	0.04	0.31
(1,932)	1:A:588:VAL:HG12	1:A:602:SER:HB3	4	0.32	0.04	0.31
(1,932)	1:A:588:VAL:HG13	1:A:602:SER:HB3	4	0.32	0.04	0.31
(1,932)	1:A:588:VAL:HG21	1:A:602:SER:HB3	4	0.32	0.04	0.31
(1,932)	1:A:588:VAL:HG22	1:A:602:SER:HB3	4	0.32	0.04	0.31
(1,932)	1:A:588:VAL:HG23	1:A:602:SER:HB3	4	0.32	0.04	0.31
(1,205)	1:A:542:MET:HE1	1:A:543:PRO:HG2	4	0.3	0.2	0.22
(1,205)	1:A:542:MET:HE1	1:A:543:PRO:HG3	4	0.3	0.2	0.22
(1,205)	1:A:542:MET:HE2	1:A:543:PRO:HG2	4	0.3	0.2	0.22
(1,205)	1:A:542:MET:HE2	1:A:543:PRO:HG3	4	0.3	0.2	0.22
(1,205)	1:A:542:MET:HE3	1:A:543:PRO:HG2	4	0.3	0.2	0.22
(1,205)	1:A:542:MET:HE3	1:A:543:PRO:HG3	4	0.3	0.2	0.22
(1,1506)	1:A:650:ARG:HB2	1:A:650:ARG:HD2	4	0.2	0.05	0.2
(1,1506)	1:A:650:ARG:HB2	1:A:650:ARG:HD3	4	0.2	0.05	0.2
(1,1506)	1:A:650:ARG:HB3	1:A:650:ARG:HD2	4	0.2	0.05	0.2
(1,1506)	1:A:650:ARG:HB3	1:A:650:ARG:HD3	4	0.2	0.05	0.2
(1,142)	1:A:538:LEU:HD11	1:A:586:HIS:H	3	0.62	0.31	0.55
(1,142)	1:A:538:LEU:HD12	1:A:586:HIS:H	3	0.62	0.31	0.55
(1,142)	1:A:538:LEU:HD13	1:A:586:HIS:H	3	0.62	0.31	0.55
(1,142)	1:A:538:LEU:HD21	1:A:586:HIS:H	3	0.62	0.31	0.55
(1,142)	1:A:538:LEU:HD22	1:A:586:HIS:H	3	0.62	0.31	0.55
(1,142)	1:A:538:LEU:HD23	1:A:586:HIS:H	3	0.62	0.31	0.55
(1,138)	1:A:538:LEU:HD11	1:A:585:GLN:H	3	0.58	0.21	0.49
(1,138)	1:A:538:LEU:HD12	1:A:585:GLN:H	3	0.58	0.21	0.49
(1,138)	1:A:538:LEU:HD13	1:A:585:GLN:H	3	0.58	0.21	0.49
(1,138)	1:A:538:LEU:HD21	1:A:585:GLN:H	3	0.58	0.21	0.49
(1,138)	1:A:538:LEU:HD22	1:A:585:GLN:H	3	0.58	0.21	0.49
(1,138)	1:A:538:LEU:HD23	1:A:585:GLN:H	3	0.58	0.21	0.49
(1,139)	1:A:538:LEU:HD11	1:A:585:GLN:HA	3	0.57	0.33	0.56
(1,139)	1:A:538:LEU:HD12	1:A:585:GLN:HA	3	0.57	0.33	0.56
(1,139)	1:A:538:LEU:HD13	1:A:585:GLN:HA	3	0.57	0.33	0.56
(1,139)	1:A:538:LEU:HD21	1:A:585:GLN:HA	3	0.57	0.33	0.56

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,139)	1:A:538:LEU:HD22	1:A:585:GLN:HA	3	0.57	0.33	0.56
(1,139)	1:A:538:LEU:HD23	1:A:585:GLN:HA	3	0.57	0.33	0.56
(1,1043)	1:A:592:LEU:HD11	1:A:599:MET:H	3	0.39	0.3	0.24
(1,1043)	1:A:592:LEU:HD12	1:A:599:MET:H	3	0.39	0.3	0.24
(1,1043)	1:A:592:LEU:HD13	1:A:599:MET:H	3	0.39	0.3	0.24
(1,1043)	1:A:592:LEU:HD21	1:A:599:MET:H	3	0.39	0.3	0.24
(1,1043)	1:A:592:LEU:HD22	1:A:599:MET:H	3	0.39	0.3	0.24
(1,1043)	1:A:592:LEU:HD23	1:A:599:MET:H	3	0.39	0.3	0.24
(1,1427)	1:A:643:GLU:H	1:A:643:GLU:HB2	3	0.13	0.01	0.14
(1,1127)	1:A:600:LYS:HD3	1:A:601:LEU:H	3	0.12	0.01	0.11
(1,1336)	1:A:636:ASP:HB2	1:A:637:ASN:HD22	2	1.74	0.01	1.74
(1,1476)	1:A:647:MET:HE1	1:A:648:MET:HG2	2	0.94	0.05	0.94
(1,1476)	1:A:647:MET:HE1	1:A:648:MET:HG3	2	0.94	0.05	0.94
(1,1476)	1:A:647:MET:HE2	1:A:648:MET:HG2	2	0.94	0.05	0.94
(1,1476)	1:A:647:MET:HE2	1:A:648:MET:HG3	2	0.94	0.05	0.94
(1,1476)	1:A:647:MET:HE3	1:A:648:MET:HG2	2	0.94	0.05	0.94
(1,1476)	1:A:647:MET:HE3	1:A:648:MET:HG3	2	0.94	0.05	0.94
(1,211)	1:A:542:MET:HE1	1:A:606:TYR:HD1	2	0.56	0.2	0.56
(1,211)	1:A:542:MET:HE1	1:A:606:TYR:HD2	2	0.56	0.2	0.56
(1,211)	1:A:542:MET:HE2	1:A:606:TYR:HD1	2	0.56	0.2	0.56
(1,211)	1:A:542:MET:HE2	1:A:606:TYR:HD2	2	0.56	0.2	0.56
(1,211)	1:A:542:MET:HE3	1:A:606:TYR:HD1	2	0.56	0.2	0.56
(1,211)	1:A:542:MET:HE3	1:A:606:TYR:HD2	2	0.56	0.2	0.56
(1,968)	1:A:589:VAL:HG21	1:A:607:PHE:HD1	2	0.33	0.01	0.33
(1,968)	1:A:589:VAL:HG21	1:A:607:PHE:HD2	2	0.33	0.01	0.33
(1,968)	1:A:589:VAL:HG22	1:A:607:PHE:HD1	2	0.33	0.01	0.33
(1,968)	1:A:589:VAL:HG22	1:A:607:PHE:HD2	2	0.33	0.01	0.33
(1,968)	1:A:589:VAL:HG23	1:A:607:PHE:HD1	2	0.33	0.01	0.33
(1,968)	1:A:589:VAL:HG23	1:A:607:PHE:HD2	2	0.33	0.01	0.33
(1,1042)	1:A:592:LEU:HD11	1:A:598:GLU:HB2	2	0.33	0.13	0.33
(1,1042)	1:A:592:LEU:HD11	1:A:598:GLU:HB3	2	0.33	0.13	0.33
(1,1042)	1:A:592:LEU:HD12	1:A:598:GLU:HB2	2	0.33	0.13	0.33
(1,1042)	1:A:592:LEU:HD12	1:A:598:GLU:HB3	2	0.33	0.13	0.33
(1,1042)	1:A:592:LEU:HD13	1:A:598:GLU:HB2	2	0.33	0.13	0.33
(1,1042)	1:A:592:LEU:HD13	1:A:598:GLU:HB3	2	0.33	0.13	0.33
(1,1042)	1:A:592:LEU:HD21	1:A:598:GLU:HB2	2	0.33	0.13	0.33
(1,1042)	1:A:592:LEU:HD21	1:A:598:GLU:HB3	2	0.33	0.13	0.33
(1,1042)	1:A:592:LEU:HD22	1:A:598:GLU:HB2	2	0.33	0.13	0.33
(1,1042)	1:A:592:LEU:HD22	1:A:598:GLU:HB3	2	0.33	0.13	0.33
(1,1042)	1:A:592:LEU:HD23	1:A:598:GLU:HB2	2	0.33	0.13	0.33
(1,1042)	1:A:592:LEU:HD23	1:A:598:GLU:HB3	2	0.33	0.13	0.33
(1,1612)	1:A:663:ILE:HA	1:A:663:ILE:HG12	2	0.26	0.01	0.26

Continued from previous page...

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1429)	1:A:643:GLU:HB2	1:A:643:GLU:HG2	2	0.16	0.04	0.16
(1,696)	1:A:574:GLU:HA	1:A:579:LYS:HD2	2	0.12	0.01	0.12
(1,696)	1:A:574:GLU:HA	1:A:579:LYS:HD3	2	0.12	0.01	0.12
(1,1074)	1:A:595:GLY:HA2	1:A:596:ASN:HB3	2	0.11	0.0	0.11
(1,1074)	1:A:595:GLY:HA3	1:A:596:ASN:HB3	2	0.11	0.0	0.11
(1,1588)	1:A:659:ARG:H	1:A:659:ARG:HB2	2	0.11	0.0	0.11

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

9.5 All violated distance restraints ⓘ

9.5.1 Histogram : Distribution of distance violations ⓘ

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.
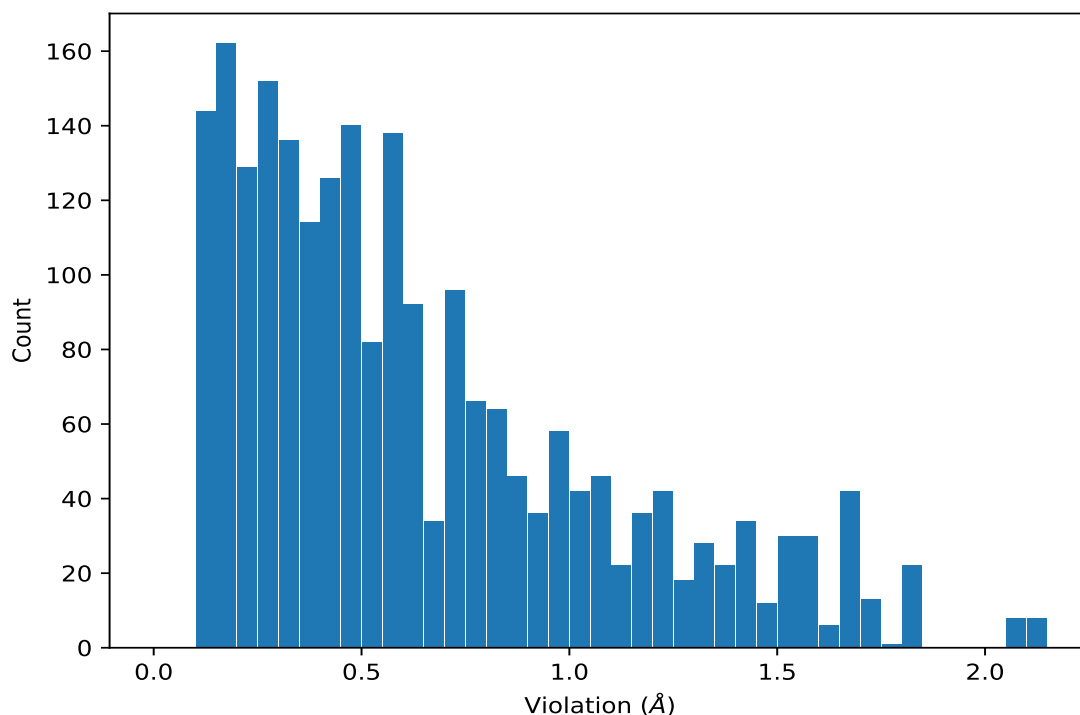
9.5.2 Table : All distance violations ⓘ

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)
(1,701)	1:A:574:GLU:HG2	1:A:579:LYS:HD2	7	2.12
(1,701)	1:A:574:GLU:HG2	1:A:579:LYS:HD3	7	2.12
(1,701)	1:A:574:GLU:HG3	1:A:579:LYS:HD2	7	2.12
(1,701)	1:A:574:GLU:HG3	1:A:579:LYS:HD3	7	2.12
(1,701)	1:A:574:GLU:HG2	1:A:579:LYS:HD2	13	2.11
(1,701)	1:A:574:GLU:HG2	1:A:579:LYS:HD3	13	2.11
(1,701)	1:A:574:GLU:HG3	1:A:579:LYS:HD2	13	2.11
(1,701)	1:A:574:GLU:HG3	1:A:579:LYS:HD3	13	2.11
(1,701)	1:A:574:GLU:HG2	1:A:579:LYS:HD2	3	2.09
(1,701)	1:A:574:GLU:HG2	1:A:579:LYS:HD3	3	2.09
(1,701)	1:A:574:GLU:HG3	1:A:579:LYS:HD2	3	2.09
(1,701)	1:A:574:GLU:HG3	1:A:579:LYS:HD3	3	2.09
(1,701)	1:A:574:GLU:HG2	1:A:579:LYS:HD2	6	2.08
(1,701)	1:A:574:GLU:HG2	1:A:579:LYS:HD3	6	2.08
(1,701)	1:A:574:GLU:HG3	1:A:579:LYS:HD2	6	2.08
(1,701)	1:A:574:GLU:HG3	1:A:579:LYS:HD3	6	2.08
(1,701)	1:A:574:GLU:HG2	1:A:579:LYS:HD2	17	1.84
(1,701)	1:A:574:GLU:HG2	1:A:579:LYS:HD3	17	1.84
(1,701)	1:A:574:GLU:HG3	1:A:579:LYS:HD2	17	1.84
(1,701)	1:A:574:GLU:HG3	1:A:579:LYS:HD3	17	1.84
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD11	11	1.82
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD12	11	1.82
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD13	11	1.82
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD21	11	1.82
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD22	11	1.82
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD23	11	1.82
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD1	4	1.82
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD2	4	1.82
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD1	4	1.82
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD2	4	1.82
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD1	4	1.82
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD2	4	1.82
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG21	18	1.8
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG22	18	1.8
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG23	18	1.8
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG21	18	1.8
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG22	18	1.8
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG23	18	1.8
(1,1336)	1:A:636:ASP:HB2	1:A:637:ASN:HD22	12	1.75
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG21	12	1.73
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG22	12	1.73
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG23	12	1.73
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG21	12	1.73

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG22	12	1.73
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG23	12	1.73
(1,1336)	1:A:636:ASP:HB2	1:A:637:ASN:HD22	5	1.73
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG21	4	1.72
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG22	4	1.72
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG23	4	1.72
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG21	4	1.72
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG22	4	1.72
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG23	4	1.72
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD11	11	1.67
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD12	11	1.67
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD13	11	1.67
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD21	11	1.67
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD22	11	1.67
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD23	11	1.67
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD11	13	1.67
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD12	13	1.67
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD13	13	1.67
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD21	13	1.67
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD22	13	1.67
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD23	13	1.67
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD11	3	1.66
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD12	3	1.66
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD13	3	1.66
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD21	3	1.66
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD22	3	1.66
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD23	3	1.66
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD11	4	1.66
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD12	4	1.66
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD13	4	1.66
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD21	4	1.66
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD22	4	1.66
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD23	4	1.66
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG21	1	1.65
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG22	1	1.65
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG23	1	1.65
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG21	1	1.65
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG22	1	1.65
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG23	1	1.65
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD11	5	1.65
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD12	5	1.65
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD13	5	1.65

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD21	5	1.65
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD22	5	1.65
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD23	5	1.65
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD11	5	1.65
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD12	5	1.65
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD13	5	1.65
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD21	5	1.65
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD22	5	1.65
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD23	5	1.65
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG21	5	1.64
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG22	5	1.64
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG23	5	1.64
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG21	5	1.64
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG22	5	1.64
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG23	5	1.64
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD11	7	1.59
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD12	7	1.59
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD13	7	1.59
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD21	7	1.59
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD22	7	1.59
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD23	7	1.59
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD11	12	1.59
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD12	12	1.59
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD13	12	1.59
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD21	12	1.59
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD22	12	1.59
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD23	12	1.59
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD11	6	1.58
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD12	6	1.58
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD13	6	1.58
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD21	6	1.58
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD22	6	1.58
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD23	6	1.58
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD1	18	1.58
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD2	18	1.58
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD1	18	1.58
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD2	18	1.58
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD1	18	1.58
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD2	18	1.58
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD1	11	1.57
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD2	11	1.57
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD1	11	1.57

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD2	11	1.57
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD1	11	1.57
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD2	11	1.57
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD11	9	1.53
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD12	9	1.53
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD13	9	1.53
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD21	9	1.53
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD22	9	1.53
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD23	9	1.53
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG21	15	1.52
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG22	15	1.52
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG23	15	1.52
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG21	15	1.52
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG22	15	1.52
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG23	15	1.52
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD1	14	1.52
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD2	14	1.52
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD1	14	1.52
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD2	14	1.52
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD1	14	1.52
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD2	14	1.52
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG21	20	1.51
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG22	20	1.51
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG23	20	1.51
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG21	20	1.51
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG22	20	1.51
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG23	20	1.51
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD1	8	1.5
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD2	8	1.5
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD1	8	1.5
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD2	8	1.5
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD1	8	1.5
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD2	8	1.5
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD11	13	1.47
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD12	13	1.47
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD13	13	1.47
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD21	13	1.47
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD22	13	1.47
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD23	13	1.47
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD11	16	1.45
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD12	16	1.45
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD13	16	1.45

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD21	16	1.45
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD22	16	1.45
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD23	16	1.45
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD11	12	1.44
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD12	12	1.44
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD13	12	1.44
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD21	12	1.44
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD22	12	1.44
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD23	12	1.44
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD11	16	1.43
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD12	16	1.43
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD13	16	1.43
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD21	16	1.43
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD22	16	1.43
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD23	16	1.43
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD11	1	1.43
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD12	1	1.43
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD13	1	1.43
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD21	1	1.43
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD22	1	1.43
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD23	1	1.43
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD11	3	1.43
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD12	3	1.43
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD13	3	1.43
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD21	3	1.43
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD22	3	1.43
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD23	3	1.43
(1,701)	1:A:574:GLU:HG2	1:A:579:LYS:HD2	19	1.42
(1,701)	1:A:574:GLU:HG2	1:A:579:LYS:HD3	19	1.42
(1,701)	1:A:574:GLU:HG3	1:A:579:LYS:HD2	19	1.42
(1,701)	1:A:574:GLU:HG3	1:A:579:LYS:HD3	19	1.42
(1,145)	1:A:538:LEU:HD11	1:A:605:SER:H	11	1.42
(1,145)	1:A:538:LEU:HD12	1:A:605:SER:H	11	1.42
(1,145)	1:A:538:LEU:HD13	1:A:605:SER:H	11	1.42
(1,145)	1:A:538:LEU:HD21	1:A:605:SER:H	11	1.42
(1,145)	1:A:538:LEU:HD22	1:A:605:SER:H	11	1.42
(1,145)	1:A:538:LEU:HD23	1:A:605:SER:H	11	1.42
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD11	6	1.37
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD12	6	1.37
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD13	6	1.37
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD21	6	1.37
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD22	6	1.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD23	6	1.37
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD11	7	1.37
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD12	7	1.37
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD13	7	1.37
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD21	7	1.37
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD22	7	1.37
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD23	7	1.37
(1,701)	1:A:574:GLU:HG2	1:A:579:LYS:HD2	2	1.35
(1,701)	1:A:574:GLU:HG2	1:A:579:LYS:HD3	2	1.35
(1,701)	1:A:574:GLU:HG3	1:A:579:LYS:HD2	2	1.35
(1,701)	1:A:574:GLU:HG3	1:A:579:LYS:HD3	2	1.35
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD2	4	1.35
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD3	4	1.35
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD2	4	1.35
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD3	4	1.35
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD2	4	1.35
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD3	4	1.35
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD11	1	1.34
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD12	1	1.34
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD13	1	1.34
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD21	1	1.34
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD22	1	1.34
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD23	1	1.34
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD11	5	1.34
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD12	5	1.34
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD13	5	1.34
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD21	5	1.34
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD22	5	1.34
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD23	5	1.34
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD2	15	1.34
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD3	15	1.34
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD2	15	1.34
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD3	15	1.34
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD2	15	1.34
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD3	15	1.34
(1,701)	1:A:574:GLU:HG2	1:A:579:LYS:HD2	11	1.33
(1,701)	1:A:574:GLU:HG2	1:A:579:LYS:HD3	11	1.33
(1,701)	1:A:574:GLU:HG3	1:A:579:LYS:HD2	11	1.33
(1,701)	1:A:574:GLU:HG3	1:A:579:LYS:HD3	11	1.33
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG21	2	1.32
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG22	2	1.32
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG23	2	1.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG21	2	1.32
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG22	2	1.32
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG23	2	1.32
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD1	10	1.29
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD2	10	1.29
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD1	10	1.29
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD2	10	1.29
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD1	10	1.29
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD2	10	1.29
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD11	9	1.25
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD12	9	1.25
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD13	9	1.25
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD21	9	1.25
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD22	9	1.25
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD23	9	1.25
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD2	8	1.25
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD3	8	1.25
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD2	8	1.25
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD3	8	1.25
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD2	8	1.25
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD3	8	1.25
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD11	14	1.24
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD12	14	1.24
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD13	14	1.24
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD21	14	1.24
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD22	14	1.24
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD23	14	1.24
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG21	17	1.24
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG22	17	1.24
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG23	17	1.24
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG21	17	1.24
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG22	17	1.24
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG23	17	1.24
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD2	17	1.23
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD3	17	1.23
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD2	17	1.23
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD3	17	1.23
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD2	17	1.23
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD3	17	1.23
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD11	5	1.22
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD12	5	1.22
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD13	5	1.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD21	5	1.22
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD22	5	1.22
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD23	5	1.22
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG21	10	1.21
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG22	10	1.21
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG23	10	1.21
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG21	10	1.21
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG22	10	1.21
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG23	10	1.21
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD1	19	1.21
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD2	19	1.21
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD1	19	1.21
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD2	19	1.21
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD1	19	1.21
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD2	19	1.21
(1,1039)	1:A:592:LEU:HD11	1:A:593:THR:H	11	1.21
(1,1039)	1:A:592:LEU:HD12	1:A:593:THR:H	11	1.21
(1,1039)	1:A:592:LEU:HD13	1:A:593:THR:H	11	1.21
(1,1039)	1:A:592:LEU:HD21	1:A:593:THR:H	11	1.21
(1,1039)	1:A:592:LEU:HD22	1:A:593:THR:H	11	1.21
(1,1039)	1:A:592:LEU:HD23	1:A:593:THR:H	11	1.21
(1,145)	1:A:538:LEU:HD11	1:A:605:SER:H	17	1.18
(1,145)	1:A:538:LEU:HD12	1:A:605:SER:H	17	1.18
(1,145)	1:A:538:LEU:HD13	1:A:605:SER:H	17	1.18
(1,145)	1:A:538:LEU:HD21	1:A:605:SER:H	17	1.18
(1,145)	1:A:538:LEU:HD22	1:A:605:SER:H	17	1.18
(1,145)	1:A:538:LEU:HD23	1:A:605:SER:H	17	1.18
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD11	14	1.16
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD12	14	1.16
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD13	14	1.16
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD21	14	1.16
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD22	14	1.16
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD23	14	1.16
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD11	6	1.16
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD12	6	1.16
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD13	6	1.16
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD21	6	1.16
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD22	6	1.16
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD23	6	1.16
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD11	6	1.16
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD12	6	1.16
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD13	6	1.16

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD21	6	1.16
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD22	6	1.16
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD23	6	1.16
(1,235)	1:A:544:LEU:HD11	1:A:652:PHE:HD1	12	1.15
(1,235)	1:A:544:LEU:HD11	1:A:652:PHE:HD2	12	1.15
(1,235)	1:A:544:LEU:HD12	1:A:652:PHE:HD1	12	1.15
(1,235)	1:A:544:LEU:HD12	1:A:652:PHE:HD2	12	1.15
(1,235)	1:A:544:LEU:HD13	1:A:652:PHE:HD1	12	1.15
(1,235)	1:A:544:LEU:HD13	1:A:652:PHE:HD2	12	1.15
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD2	18	1.15
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD3	18	1.15
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD2	18	1.15
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD3	18	1.15
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD2	18	1.15
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD3	18	1.15
(1,701)	1:A:574:GLU:HG2	1:A:579:LYS:HD2	18	1.14
(1,701)	1:A:574:GLU:HG2	1:A:579:LYS:HD3	18	1.14
(1,701)	1:A:574:GLU:HG3	1:A:579:LYS:HD2	18	1.14
(1,701)	1:A:574:GLU:HG3	1:A:579:LYS:HD3	18	1.14
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD2	6	1.14
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD3	6	1.14
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD2	6	1.14
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD3	6	1.14
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD2	6	1.14
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD3	6	1.14
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG21	8	1.14
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG22	8	1.14
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG23	8	1.14
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG21	8	1.14
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG22	8	1.14
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG23	8	1.14
(1,209)	1:A:542:MET:HE1	1:A:545:PHE:HD1	3	1.11
(1,209)	1:A:542:MET:HE1	1:A:545:PHE:HD2	3	1.11
(1,209)	1:A:542:MET:HE2	1:A:545:PHE:HD1	3	1.11
(1,209)	1:A:542:MET:HE2	1:A:545:PHE:HD2	3	1.11
(1,209)	1:A:542:MET:HE3	1:A:545:PHE:HD1	3	1.11
(1,209)	1:A:542:MET:HE3	1:A:545:PHE:HD2	3	1.11
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD11	2	1.09
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD12	2	1.09
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD13	2	1.09
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD21	2	1.09
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD22	2	1.09

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD23	2	1.09
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD11	16	1.08
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD12	16	1.08
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD13	16	1.08
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD11	16	1.08
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD12	16	1.08
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD13	16	1.08
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD11	3	1.07
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD12	3	1.07
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD13	3	1.07
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD21	3	1.07
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD22	3	1.07
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD23	3	1.07
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD11	3	1.07
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD12	3	1.07
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD13	3	1.07
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD21	3	1.07
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD22	3	1.07
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD23	3	1.07
(1,701)	1:A:574:GLU:HG2	1:A:579:LYS:HD2	4	1.06
(1,701)	1:A:574:GLU:HG2	1:A:579:LYS:HD3	4	1.06
(1,701)	1:A:574:GLU:HG3	1:A:579:LYS:HD2	4	1.06
(1,701)	1:A:574:GLU:HG3	1:A:579:LYS:HD3	4	1.06
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD1	13	1.06
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD2	13	1.06
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD1	13	1.06
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD2	13	1.06
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD1	13	1.06
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD2	13	1.06
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD11	12	1.06
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD12	12	1.06
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD13	12	1.06
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD21	12	1.06
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD22	12	1.06
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD23	12	1.06
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD11	12	1.06
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD12	12	1.06
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD13	12	1.06
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD21	12	1.06
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD22	12	1.06
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD23	12	1.06
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD2	1	1.04

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD3	1	1.04
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD2	1	1.04
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD3	1	1.04
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD2	1	1.04
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD3	1	1.04
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD2	20	1.04
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD3	20	1.04
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD2	20	1.04
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD3	20	1.04
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD2	20	1.04
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD3	20	1.04
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB1	8	1.03
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB2	8	1.03
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB3	8	1.03
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB1	8	1.03
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB2	8	1.03
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB3	8	1.03
(1,142)	1:A:538:LEU:HD11	1:A:586:HIS:H	12	1.03
(1,142)	1:A:538:LEU:HD12	1:A:586:HIS:H	12	1.03
(1,142)	1:A:538:LEU:HD13	1:A:586:HIS:H	12	1.03
(1,142)	1:A:538:LEU:HD21	1:A:586:HIS:H	12	1.03
(1,142)	1:A:538:LEU:HD22	1:A:586:HIS:H	12	1.03
(1,142)	1:A:538:LEU:HD23	1:A:586:HIS:H	12	1.03
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD11	17	1.02
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD12	17	1.02
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD13	17	1.02
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD21	17	1.02
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD22	17	1.02
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD23	17	1.02
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB1	5	1.02
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB2	5	1.02
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB3	5	1.02
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB1	5	1.02
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB2	5	1.02
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB3	5	1.02
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD11	5	1.01
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD12	5	1.01
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD13	5	1.01
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD11	5	1.01
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD12	5	1.01
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD13	5	1.01
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB1	12	0.99

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB2	12	0.99
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB3	12	0.99
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB1	12	0.99
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB2	12	0.99
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB3	12	0.99
(1,1476)	1:A:647:MET:HE1	1:A:648:MET:HG2	4	0.99
(1,1476)	1:A:647:MET:HE1	1:A:648:MET:HG3	4	0.99
(1,1476)	1:A:647:MET:HE2	1:A:648:MET:HG2	4	0.99
(1,1476)	1:A:647:MET:HE2	1:A:648:MET:HG3	4	0.99
(1,1476)	1:A:647:MET:HE3	1:A:648:MET:HG2	4	0.99
(1,1476)	1:A:647:MET:HE3	1:A:648:MET:HG3	4	0.99
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB1	2	0.97
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB2	2	0.97
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB3	2	0.97
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB1	2	0.97
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB2	2	0.97
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB3	2	0.97
(1,141)	1:A:538:LEU:HD11	1:A:585:GLN:HB2	12	0.97
(1,141)	1:A:538:LEU:HD11	1:A:585:GLN:HB3	12	0.97
(1,141)	1:A:538:LEU:HD12	1:A:585:GLN:HB2	12	0.97
(1,141)	1:A:538:LEU:HD12	1:A:585:GLN:HB3	12	0.97
(1,141)	1:A:538:LEU:HD13	1:A:585:GLN:HB2	12	0.97
(1,141)	1:A:538:LEU:HD13	1:A:585:GLN:HB3	12	0.97
(1,141)	1:A:538:LEU:HD21	1:A:585:GLN:HB2	12	0.97
(1,141)	1:A:538:LEU:HD21	1:A:585:GLN:HB3	12	0.97
(1,141)	1:A:538:LEU:HD22	1:A:585:GLN:HB2	12	0.97
(1,141)	1:A:538:LEU:HD22	1:A:585:GLN:HB3	12	0.97
(1,141)	1:A:538:LEU:HD23	1:A:585:GLN:HB2	12	0.97
(1,141)	1:A:538:LEU:HD23	1:A:585:GLN:HB3	12	0.97
(1,139)	1:A:538:LEU:HD11	1:A:585:GLN:HA	12	0.97
(1,139)	1:A:538:LEU:HD12	1:A:585:GLN:HA	12	0.97
(1,139)	1:A:538:LEU:HD13	1:A:585:GLN:HA	12	0.97
(1,139)	1:A:538:LEU:HD21	1:A:585:GLN:HA	12	0.97
(1,139)	1:A:538:LEU:HD22	1:A:585:GLN:HA	12	0.97
(1,139)	1:A:538:LEU:HD23	1:A:585:GLN:HA	12	0.97
(1,701)	1:A:574:GLU:HG2	1:A:579:LYS:HD2	10	0.96
(1,701)	1:A:574:GLU:HG2	1:A:579:LYS:HD3	10	0.96
(1,701)	1:A:574:GLU:HG3	1:A:579:LYS:HD2	10	0.96
(1,701)	1:A:574:GLU:HG3	1:A:579:LYS:HD3	10	0.96
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD1	3	0.96
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD2	3	0.96
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD1	3	0.96

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD2	3	0.96
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD1	3	0.96
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD2	3	0.96
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD1	15	0.95
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD2	15	0.95
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD1	15	0.95
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD2	15	0.95
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD1	15	0.95
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD2	15	0.95
(1,1039)	1:A:592:LEU:HD11	1:A:593:THR:H	4	0.95
(1,1039)	1:A:592:LEU:HD12	1:A:593:THR:H	4	0.95
(1,1039)	1:A:592:LEU:HD13	1:A:593:THR:H	4	0.95
(1,1039)	1:A:592:LEU:HD21	1:A:593:THR:H	4	0.95
(1,1039)	1:A:592:LEU:HD22	1:A:593:THR:H	4	0.95
(1,1039)	1:A:592:LEU:HD23	1:A:593:THR:H	4	0.95
(1,137)	1:A:538:LEU:HD11	1:A:584:ILE:H	11	0.94
(1,137)	1:A:538:LEU:HD12	1:A:584:ILE:H	11	0.94
(1,137)	1:A:538:LEU:HD13	1:A:584:ILE:H	11	0.94
(1,137)	1:A:538:LEU:HD21	1:A:584:ILE:H	11	0.94
(1,137)	1:A:538:LEU:HD22	1:A:584:ILE:H	11	0.94
(1,137)	1:A:538:LEU:HD23	1:A:584:ILE:H	11	0.94
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD11	7	0.93
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD12	7	0.93
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD13	7	0.93
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD21	7	0.93
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD22	7	0.93
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD23	7	0.93
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD1	2	0.92
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD2	2	0.92
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD1	2	0.92
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD2	2	0.92
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD1	2	0.92
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD2	2	0.92
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD11	9	0.91
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD12	9	0.91
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD13	9	0.91
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD21	9	0.91
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD22	9	0.91
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD23	9	0.91
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD11	10	0.9
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD12	10	0.9
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD13	10	0.9

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD21	10	0.9
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD22	10	0.9
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD23	10	0.9
(1,145)	1:A:538:LEU:HD11	1:A:605:SER:H	12	0.9
(1,145)	1:A:538:LEU:HD12	1:A:605:SER:H	12	0.9
(1,145)	1:A:538:LEU:HD13	1:A:605:SER:H	12	0.9
(1,145)	1:A:538:LEU:HD21	1:A:605:SER:H	12	0.9
(1,145)	1:A:538:LEU:HD22	1:A:605:SER:H	12	0.9
(1,145)	1:A:538:LEU:HD23	1:A:605:SER:H	12	0.9
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB1	1	0.89
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB2	1	0.89
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB3	1	0.89
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB1	1	0.89
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB2	1	0.89
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB3	1	0.89
(1,1476)	1:A:647:MET:HE1	1:A:648:MET:HG2	12	0.89
(1,1476)	1:A:647:MET:HE1	1:A:648:MET:HG3	12	0.89
(1,1476)	1:A:647:MET:HE2	1:A:648:MET:HG2	12	0.89
(1,1476)	1:A:647:MET:HE2	1:A:648:MET:HG3	12	0.89
(1,1476)	1:A:647:MET:HE3	1:A:648:MET:HG2	12	0.89
(1,1476)	1:A:647:MET:HE3	1:A:648:MET:HG3	12	0.89
(1,145)	1:A:538:LEU:HD11	1:A:605:SER:H	4	0.89
(1,145)	1:A:538:LEU:HD12	1:A:605:SER:H	4	0.89
(1,145)	1:A:538:LEU:HD13	1:A:605:SER:H	4	0.89
(1,145)	1:A:538:LEU:HD21	1:A:605:SER:H	4	0.89
(1,145)	1:A:538:LEU:HD22	1:A:605:SER:H	4	0.89
(1,145)	1:A:538:LEU:HD23	1:A:605:SER:H	4	0.89
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD11	12	0.88
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD12	12	0.88
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD13	12	0.88
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD11	12	0.88
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD12	12	0.88
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD13	12	0.88
(1,235)	1:A:544:LEU:HD11	1:A:652:PHE:HD1	7	0.86
(1,235)	1:A:544:LEU:HD11	1:A:652:PHE:HD2	7	0.86
(1,235)	1:A:544:LEU:HD12	1:A:652:PHE:HD1	7	0.86
(1,235)	1:A:544:LEU:HD12	1:A:652:PHE:HD2	7	0.86
(1,235)	1:A:544:LEU:HD13	1:A:652:PHE:HD1	7	0.86
(1,235)	1:A:544:LEU:HD13	1:A:652:PHE:HD2	7	0.86
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB1	10	0.86
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB2	10	0.86
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB3	10	0.86

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB1	10	0.86
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB2	10	0.86
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB3	10	0.86
(1,138)	1:A:538:LEU:HD11	1:A:585:GLN:H	12	0.86
(1,138)	1:A:538:LEU:HD12	1:A:585:GLN:H	12	0.86
(1,138)	1:A:538:LEU:HD13	1:A:585:GLN:H	12	0.86
(1,138)	1:A:538:LEU:HD21	1:A:585:GLN:H	12	0.86
(1,138)	1:A:538:LEU:HD22	1:A:585:GLN:H	12	0.86
(1,138)	1:A:538:LEU:HD23	1:A:585:GLN:H	12	0.86
(1,701)	1:A:574:GLU:HG2	1:A:579:LYS:HD2	20	0.85
(1,701)	1:A:574:GLU:HG2	1:A:579:LYS:HD3	20	0.85
(1,701)	1:A:574:GLU:HG3	1:A:579:LYS:HD2	20	0.85
(1,701)	1:A:574:GLU:HG3	1:A:579:LYS:HD3	20	0.85
(1,1072)	1:A:594:LYS:HD2	1:A:595:GLY:HA2	14	0.84
(1,1072)	1:A:594:LYS:HD2	1:A:595:GLY:HA3	14	0.84
(1,1072)	1:A:594:LYS:HD3	1:A:595:GLY:HA2	14	0.84
(1,1072)	1:A:594:LYS:HD3	1:A:595:GLY:HA3	14	0.84
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD11	2	0.83
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD12	2	0.83
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD13	2	0.83
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD21	2	0.83
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD22	2	0.83
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD23	2	0.83
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD11	2	0.82
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD12	2	0.82
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD13	2	0.82
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD21	2	0.82
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD22	2	0.82
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD23	2	0.82
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD11	10	0.82
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD12	10	0.82
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD13	10	0.82
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD21	10	0.82
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD22	10	0.82
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD23	10	0.82
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD1	5	0.82
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD2	5	0.82
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD1	5	0.82
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD2	5	0.82
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD1	5	0.82
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD2	5	0.82
(1,1039)	1:A:592:LEU:HD11	1:A:593:THR:H	2	0.82

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1039)	1:A:592:LEU:HD12	1:A:593:THR:H	2	0.82
(1,1039)	1:A:592:LEU:HD13	1:A:593:THR:H	2	0.82
(1,1039)	1:A:592:LEU:HD21	1:A:593:THR:H	2	0.82
(1,1039)	1:A:592:LEU:HD22	1:A:593:THR:H	2	0.82
(1,1039)	1:A:592:LEU:HD23	1:A:593:THR:H	2	0.82
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD11	9	0.81
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD12	9	0.81
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD13	9	0.81
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD21	9	0.81
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD22	9	0.81
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD23	9	0.81
(1,1043)	1:A:592:LEU:HD11	1:A:599:MET:H	11	0.81
(1,1043)	1:A:592:LEU:HD12	1:A:599:MET:H	11	0.81
(1,1043)	1:A:592:LEU:HD13	1:A:599:MET:H	11	0.81
(1,1043)	1:A:592:LEU:HD21	1:A:599:MET:H	11	0.81
(1,1043)	1:A:592:LEU:HD22	1:A:599:MET:H	11	0.81
(1,1043)	1:A:592:LEU:HD23	1:A:599:MET:H	11	0.81
(1,1039)	1:A:592:LEU:HD11	1:A:593:THR:H	1	0.8
(1,1039)	1:A:592:LEU:HD12	1:A:593:THR:H	1	0.8
(1,1039)	1:A:592:LEU:HD13	1:A:593:THR:H	1	0.8
(1,1039)	1:A:592:LEU:HD21	1:A:593:THR:H	1	0.8
(1,1039)	1:A:592:LEU:HD22	1:A:593:THR:H	1	0.8
(1,1039)	1:A:592:LEU:HD23	1:A:593:THR:H	1	0.8
(1,1039)	1:A:592:LEU:HD11	1:A:593:THR:H	9	0.8
(1,1039)	1:A:592:LEU:HD12	1:A:593:THR:H	9	0.8
(1,1039)	1:A:592:LEU:HD13	1:A:593:THR:H	9	0.8
(1,1039)	1:A:592:LEU:HD21	1:A:593:THR:H	9	0.8
(1,1039)	1:A:592:LEU:HD22	1:A:593:THR:H	9	0.8
(1,1039)	1:A:592:LEU:HD23	1:A:593:THR:H	9	0.8
(1,1039)	1:A:592:LEU:HD11	1:A:593:THR:H	13	0.8
(1,1039)	1:A:592:LEU:HD12	1:A:593:THR:H	13	0.8
(1,1039)	1:A:592:LEU:HD13	1:A:593:THR:H	13	0.8
(1,1039)	1:A:592:LEU:HD21	1:A:593:THR:H	13	0.8
(1,1039)	1:A:592:LEU:HD22	1:A:593:THR:H	13	0.8
(1,1039)	1:A:592:LEU:HD23	1:A:593:THR:H	13	0.8
(1,1039)	1:A:592:LEU:HD11	1:A:593:THR:H	5	0.79
(1,1039)	1:A:592:LEU:HD12	1:A:593:THR:H	5	0.79
(1,1039)	1:A:592:LEU:HD13	1:A:593:THR:H	5	0.79
(1,1039)	1:A:592:LEU:HD21	1:A:593:THR:H	5	0.79
(1,1039)	1:A:592:LEU:HD22	1:A:593:THR:H	5	0.79
(1,1039)	1:A:592:LEU:HD23	1:A:593:THR:H	5	0.79
(1,1039)	1:A:592:LEU:HD11	1:A:593:THR:H	14	0.79

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1039)	1:A:592:LEU:HD12	1:A:593:THR:H	14	0.79
(1,1039)	1:A:592:LEU:HD13	1:A:593:THR:H	14	0.79
(1,1039)	1:A:592:LEU:HD21	1:A:593:THR:H	14	0.79
(1,1039)	1:A:592:LEU:HD22	1:A:593:THR:H	14	0.79
(1,1039)	1:A:592:LEU:HD23	1:A:593:THR:H	14	0.79
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD11	10	0.78
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD12	10	0.78
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD13	10	0.78
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD11	10	0.78
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD12	10	0.78
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD13	10	0.78
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD11	14	0.78
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD12	14	0.78
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD13	14	0.78
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD21	14	0.78
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD22	14	0.78
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD23	14	0.78
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD2	11	0.78
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD3	11	0.78
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD2	11	0.78
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD3	11	0.78
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD2	11	0.78
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD3	11	0.78
(1,211)	1:A:542:MET:HE1	1:A:606:TYR:HD1	12	0.77
(1,211)	1:A:542:MET:HE1	1:A:606:TYR:HD2	12	0.77
(1,211)	1:A:542:MET:HE2	1:A:606:TYR:HD1	12	0.77
(1,211)	1:A:542:MET:HE2	1:A:606:TYR:HD2	12	0.77
(1,211)	1:A:542:MET:HE3	1:A:606:TYR:HD1	12	0.77
(1,211)	1:A:542:MET:HE3	1:A:606:TYR:HD2	12	0.77
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD11	13	0.77
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD12	13	0.77
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD13	13	0.77
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD21	13	0.77
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD22	13	0.77
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD23	13	0.77
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD11	8	0.76
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD12	8	0.76
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD13	8	0.76
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD21	8	0.76
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD22	8	0.76
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD23	8	0.76
(1,145)	1:A:538:LEU:HD11	1:A:605:SER:H	2	0.76

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,145)	1:A:538:LEU:HD12	1:A:605:SER:H	2	0.76
(1,145)	1:A:538:LEU:HD13	1:A:605:SER:H	2	0.76
(1,145)	1:A:538:LEU:HD21	1:A:605:SER:H	2	0.76
(1,145)	1:A:538:LEU:HD22	1:A:605:SER:H	2	0.76
(1,145)	1:A:538:LEU:HD23	1:A:605:SER:H	2	0.76
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB1	15	0.75
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB2	15	0.75
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB3	15	0.75
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB1	15	0.75
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB2	15	0.75
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB3	15	0.75
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD1	16	0.75
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD2	16	0.75
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD1	16	0.75
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD2	16	0.75
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD1	16	0.75
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD2	16	0.75
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD11	18	0.73
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD12	18	0.73
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD13	18	0.73
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD11	18	0.73
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD12	18	0.73
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD13	18	0.73
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD11	12	0.73
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD12	12	0.73
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD13	12	0.73
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD21	12	0.73
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD22	12	0.73
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD23	12	0.73
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD11	16	0.73
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD12	16	0.73
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD13	16	0.73
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD21	16	0.73
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD22	16	0.73
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD23	16	0.73
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB1	11	0.73
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB2	11	0.73
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB3	11	0.73
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB1	11	0.73
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB2	11	0.73
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB3	11	0.73
(1,1039)	1:A:592:LEU:HD11	1:A:593:THR:H	20	0.73

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1039)	1:A:592:LEU:HD12	1:A:593:THR:H	20	0.73
(1,1039)	1:A:592:LEU:HD13	1:A:593:THR:H	20	0.73
(1,1039)	1:A:592:LEU:HD21	1:A:593:THR:H	20	0.73
(1,1039)	1:A:592:LEU:HD22	1:A:593:THR:H	20	0.73
(1,1039)	1:A:592:LEU:HD23	1:A:593:THR:H	20	0.73
(1,141)	1:A:538:LEU:HD11	1:A:585:GLN:HB2	9	0.72
(1,141)	1:A:538:LEU:HD11	1:A:585:GLN:HB3	9	0.72
(1,141)	1:A:538:LEU:HD12	1:A:585:GLN:HB2	9	0.72
(1,141)	1:A:538:LEU:HD12	1:A:585:GLN:HB3	9	0.72
(1,141)	1:A:538:LEU:HD13	1:A:585:GLN:HB2	9	0.72
(1,141)	1:A:538:LEU:HD13	1:A:585:GLN:HB3	9	0.72
(1,141)	1:A:538:LEU:HD21	1:A:585:GLN:HB2	9	0.72
(1,141)	1:A:538:LEU:HD21	1:A:585:GLN:HB3	9	0.72
(1,141)	1:A:538:LEU:HD22	1:A:585:GLN:HB2	9	0.72
(1,141)	1:A:538:LEU:HD22	1:A:585:GLN:HB3	9	0.72
(1,141)	1:A:538:LEU:HD23	1:A:585:GLN:HB2	9	0.72
(1,141)	1:A:538:LEU:HD23	1:A:585:GLN:HB3	9	0.72
(1,1039)	1:A:592:LEU:HD11	1:A:593:THR:H	17	0.72
(1,1039)	1:A:592:LEU:HD12	1:A:593:THR:H	17	0.72
(1,1039)	1:A:592:LEU:HD13	1:A:593:THR:H	17	0.72
(1,1039)	1:A:592:LEU:HD21	1:A:593:THR:H	17	0.72
(1,1039)	1:A:592:LEU:HD22	1:A:593:THR:H	17	0.72
(1,1039)	1:A:592:LEU:HD23	1:A:593:THR:H	17	0.72
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD11	5	0.71
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD12	5	0.71
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD13	5	0.71
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD21	5	0.71
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD22	5	0.71
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD23	5	0.71
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB1	17	0.71
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB2	17	0.71
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB3	17	0.71
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB1	17	0.71
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB2	17	0.71
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB3	17	0.71
(1,1044)	1:A:592:LEU:HD11	1:A:623:ARG:H	12	0.71
(1,1044)	1:A:592:LEU:HD12	1:A:623:ARG:H	12	0.71
(1,1044)	1:A:592:LEU:HD13	1:A:623:ARG:H	12	0.71
(1,1044)	1:A:592:LEU:HD21	1:A:623:ARG:H	12	0.71
(1,1044)	1:A:592:LEU:HD22	1:A:623:ARG:H	12	0.71
(1,1044)	1:A:592:LEU:HD23	1:A:623:ARG:H	12	0.71
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD11	4	0.7

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD12	4	0.7
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD13	4	0.7
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD21	4	0.7
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD22	4	0.7
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD23	4	0.7
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD11	15	0.7
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD12	15	0.7
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD13	15	0.7
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD21	15	0.7
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD22	15	0.7
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD23	15	0.7
(1,235)	1:A:544:LEU:HD11	1:A:652:PHE:HD1	15	0.7
(1,235)	1:A:544:LEU:HD11	1:A:652:PHE:HD2	15	0.7
(1,235)	1:A:544:LEU:HD12	1:A:652:PHE:HD1	15	0.7
(1,235)	1:A:544:LEU:HD12	1:A:652:PHE:HD2	15	0.7
(1,235)	1:A:544:LEU:HD13	1:A:652:PHE:HD1	15	0.7
(1,235)	1:A:544:LEU:HD13	1:A:652:PHE:HD2	15	0.7
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD11	11	0.7
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD12	11	0.7
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD13	11	0.7
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD21	11	0.7
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD22	11	0.7
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD23	11	0.7
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD11	11	0.7
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD12	11	0.7
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD13	11	0.7
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD21	11	0.7
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD22	11	0.7
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD23	11	0.7
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD11	14	0.68
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD12	14	0.68
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD13	14	0.68
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD21	14	0.68
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD22	14	0.68
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD23	14	0.68
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG21	11	0.68
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG22	11	0.68
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG23	11	0.68
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG21	11	0.68
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG22	11	0.68
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG23	11	0.68
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB1	20	0.67

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB2	20	0.67
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB3	20	0.67
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB1	20	0.67
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB2	20	0.67
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB3	20	0.67
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD11	6	0.66
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD12	6	0.66
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD13	6	0.66
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD21	6	0.66
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD22	6	0.66
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD23	6	0.66
(1,1072)	1:A:594:LYS:HD2	1:A:595:GLY:HA2	16	0.66
(1,1072)	1:A:594:LYS:HD2	1:A:595:GLY:HA3	16	0.66
(1,1072)	1:A:594:LYS:HD3	1:A:595:GLY:HA2	16	0.66
(1,1072)	1:A:594:LYS:HD3	1:A:595:GLY:HA3	16	0.66
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD11	8	0.65
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD12	8	0.65
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD13	8	0.65
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD21	8	0.65
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD22	8	0.65
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD23	8	0.65
(1,842)	1:A:584:ILE:HD11	1:A:607:PHE:HD1	16	0.64
(1,842)	1:A:584:ILE:HD11	1:A:607:PHE:HD2	16	0.64
(1,842)	1:A:584:ILE:HD12	1:A:607:PHE:HD1	16	0.64
(1,842)	1:A:584:ILE:HD12	1:A:607:PHE:HD2	16	0.64
(1,842)	1:A:584:ILE:HD13	1:A:607:PHE:HD1	16	0.64
(1,842)	1:A:584:ILE:HD13	1:A:607:PHE:HD2	16	0.64
(1,235)	1:A:544:LEU:HD11	1:A:652:PHE:HD1	5	0.64
(1,235)	1:A:544:LEU:HD11	1:A:652:PHE:HD2	5	0.64
(1,235)	1:A:544:LEU:HD12	1:A:652:PHE:HD1	5	0.64
(1,235)	1:A:544:LEU:HD12	1:A:652:PHE:HD2	5	0.64
(1,235)	1:A:544:LEU:HD13	1:A:652:PHE:HD1	5	0.64
(1,235)	1:A:544:LEU:HD13	1:A:652:PHE:HD2	5	0.64
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD11	1	0.64
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD12	1	0.64
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD13	1	0.64
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD21	1	0.64
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD22	1	0.64
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD23	1	0.64
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD11	1	0.64
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD12	1	0.64
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD13	1	0.64

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD21	1	0.64
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD22	1	0.64
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD23	1	0.64
(1,1044)	1:A:592:LEU:HD11	1:A:623:ARG:H	6	0.64
(1,1044)	1:A:592:LEU:HD12	1:A:623:ARG:H	6	0.64
(1,1044)	1:A:592:LEU:HD13	1:A:623:ARG:H	6	0.64
(1,1044)	1:A:592:LEU:HD21	1:A:623:ARG:H	6	0.64
(1,1044)	1:A:592:LEU:HD22	1:A:623:ARG:H	6	0.64
(1,1044)	1:A:592:LEU:HD23	1:A:623:ARG:H	6	0.64
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD11	17	0.63
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD12	17	0.63
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD13	17	0.63
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD21	17	0.63
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD22	17	0.63
(1,990)	1:A:590:SER:HB2	1:A:592:LEU:HD23	17	0.63
(1,205)	1:A:542:MET:HE1	1:A:543:PRO:HG2	15	0.63
(1,205)	1:A:542:MET:HE1	1:A:543:PRO:HG3	15	0.63
(1,205)	1:A:542:MET:HE2	1:A:543:PRO:HG2	15	0.63
(1,205)	1:A:542:MET:HE2	1:A:543:PRO:HG3	15	0.63
(1,205)	1:A:542:MET:HE3	1:A:543:PRO:HG2	15	0.63
(1,205)	1:A:542:MET:HE3	1:A:543:PRO:HG3	15	0.63
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD2	13	0.62
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD3	13	0.62
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD2	13	0.62
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD3	13	0.62
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD2	13	0.62
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD3	13	0.62
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG21	13	0.62
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG22	13	0.62
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG23	13	0.62
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG21	13	0.62
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG22	13	0.62
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG23	13	0.62
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB1	18	0.62
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB2	18	0.62
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB3	18	0.62
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB1	18	0.62
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB2	18	0.62
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB3	18	0.62
(1,699)	1:A:574:GLU:HG2	1:A:575:GLY:HA2	1	0.61
(1,699)	1:A:574:GLU:HG2	1:A:575:GLY:HA3	1	0.61
(1,699)	1:A:574:GLU:HG3	1:A:575:GLY:HA2	1	0.61

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,699)	1:A:574:GLU:HG3	1:A:575:GLY:HA3	1	0.61
(1,699)	1:A:574:GLU:HG2	1:A:575:GLY:HA2	15	0.61
(1,699)	1:A:574:GLU:HG2	1:A:575:GLY:HA3	15	0.61
(1,699)	1:A:574:GLU:HG3	1:A:575:GLY:HA2	15	0.61
(1,699)	1:A:574:GLU:HG3	1:A:575:GLY:HA3	15	0.61
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD11	4	0.61
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD12	4	0.61
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD13	4	0.61
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD21	4	0.61
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD22	4	0.61
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD23	4	0.61
(1,145)	1:A:538:LEU:HD11	1:A:605:SER:H	6	0.61
(1,145)	1:A:538:LEU:HD12	1:A:605:SER:H	6	0.61
(1,145)	1:A:538:LEU:HD13	1:A:605:SER:H	6	0.61
(1,145)	1:A:538:LEU:HD21	1:A:605:SER:H	6	0.61
(1,145)	1:A:538:LEU:HD22	1:A:605:SER:H	6	0.61
(1,145)	1:A:538:LEU:HD23	1:A:605:SER:H	6	0.61
(1,209)	1:A:542:MET:HE1	1:A:545:PHE:HD1	7	0.6
(1,209)	1:A:542:MET:HE1	1:A:545:PHE:HD2	7	0.6
(1,209)	1:A:542:MET:HE2	1:A:545:PHE:HD1	7	0.6
(1,209)	1:A:542:MET:HE2	1:A:545:PHE:HD2	7	0.6
(1,209)	1:A:542:MET:HE3	1:A:545:PHE:HD1	7	0.6
(1,209)	1:A:542:MET:HE3	1:A:545:PHE:HD2	7	0.6
(1,1044)	1:A:592:LEU:HD11	1:A:623:ARG:H	3	0.6
(1,1044)	1:A:592:LEU:HD12	1:A:623:ARG:H	3	0.6
(1,1044)	1:A:592:LEU:HD13	1:A:623:ARG:H	3	0.6
(1,1044)	1:A:592:LEU:HD21	1:A:623:ARG:H	3	0.6
(1,1044)	1:A:592:LEU:HD22	1:A:623:ARG:H	3	0.6
(1,1044)	1:A:592:LEU:HD23	1:A:623:ARG:H	3	0.6
(1,842)	1:A:584:ILE:HD11	1:A:607:PHE:HD1	11	0.59
(1,842)	1:A:584:ILE:HD11	1:A:607:PHE:HD2	11	0.59
(1,842)	1:A:584:ILE:HD12	1:A:607:PHE:HD1	11	0.59
(1,842)	1:A:584:ILE:HD12	1:A:607:PHE:HD2	11	0.59
(1,842)	1:A:584:ILE:HD13	1:A:607:PHE:HD1	11	0.59
(1,842)	1:A:584:ILE:HD13	1:A:607:PHE:HD2	11	0.59
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD2	2	0.59
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD3	2	0.59
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD2	2	0.59
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD3	2	0.59
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD2	2	0.59
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD3	2	0.59
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD1	9	0.59

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD2	9	0.59
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD1	9	0.59
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD2	9	0.59
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD1	9	0.59
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD2	9	0.59
(1,1039)	1:A:592:LEU:HD11	1:A:593:THR:H	16	0.59
(1,1039)	1:A:592:LEU:HD12	1:A:593:THR:H	16	0.59
(1,1039)	1:A:592:LEU:HD13	1:A:593:THR:H	16	0.59
(1,1039)	1:A:592:LEU:HD21	1:A:593:THR:H	16	0.59
(1,1039)	1:A:592:LEU:HD22	1:A:593:THR:H	16	0.59
(1,1039)	1:A:592:LEU:HD23	1:A:593:THR:H	16	0.59
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB1	4	0.58
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB2	4	0.58
(1,1513)	1:A:650:ARG:HD2	1:A:651:ALA:HB3	4	0.58
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB1	4	0.58
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB2	4	0.58
(1,1513)	1:A:650:ARG:HD3	1:A:651:ALA:HB3	4	0.58
(1,136)	1:A:538:LEU:HD11	1:A:541:SER:H	12	0.58
(1,136)	1:A:538:LEU:HD12	1:A:541:SER:H	12	0.58
(1,136)	1:A:538:LEU:HD13	1:A:541:SER:H	12	0.58
(1,136)	1:A:538:LEU:HD21	1:A:541:SER:H	12	0.58
(1,136)	1:A:538:LEU:HD22	1:A:541:SER:H	12	0.58
(1,136)	1:A:538:LEU:HD23	1:A:541:SER:H	12	0.58
(1,1041)	1:A:592:LEU:HD11	1:A:598:GLU:HG2	10	0.58
(1,1041)	1:A:592:LEU:HD12	1:A:598:GLU:HG2	10	0.58
(1,1041)	1:A:592:LEU:HD13	1:A:598:GLU:HG2	10	0.58
(1,1041)	1:A:592:LEU:HD21	1:A:598:GLU:HG2	10	0.58
(1,1041)	1:A:592:LEU:HD22	1:A:598:GLU:HG2	10	0.58
(1,1041)	1:A:592:LEU:HD23	1:A:598:GLU:HG2	10	0.58
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD2	14	0.57
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD3	14	0.57
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD2	14	0.57
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD3	14	0.57
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD2	14	0.57
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD3	14	0.57
(1,1039)	1:A:592:LEU:HD11	1:A:593:THR:H	12	0.57
(1,1039)	1:A:592:LEU:HD12	1:A:593:THR:H	12	0.57
(1,1039)	1:A:592:LEU:HD13	1:A:593:THR:H	12	0.57
(1,1039)	1:A:592:LEU:HD21	1:A:593:THR:H	12	0.57
(1,1039)	1:A:592:LEU:HD22	1:A:593:THR:H	12	0.57
(1,1039)	1:A:592:LEU:HD23	1:A:593:THR:H	12	0.57
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD11	12	0.56

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD12	12	0.56
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD13	12	0.56
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD21	12	0.56
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD22	12	0.56
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD23	12	0.56
(1,139)	1:A:538:LEU:HD11	1:A:585:GLN:HA	9	0.56
(1,139)	1:A:538:LEU:HD12	1:A:585:GLN:HA	9	0.56
(1,139)	1:A:538:LEU:HD13	1:A:585:GLN:HA	9	0.56
(1,139)	1:A:538:LEU:HD21	1:A:585:GLN:HA	9	0.56
(1,139)	1:A:538:LEU:HD22	1:A:585:GLN:HA	9	0.56
(1,139)	1:A:538:LEU:HD23	1:A:585:GLN:HA	9	0.56
(1,137)	1:A:538:LEU:HD11	1:A:584:ILE:H	12	0.56
(1,137)	1:A:538:LEU:HD12	1:A:584:ILE:H	12	0.56
(1,137)	1:A:538:LEU:HD13	1:A:584:ILE:H	12	0.56
(1,137)	1:A:538:LEU:HD21	1:A:584:ILE:H	12	0.56
(1,137)	1:A:538:LEU:HD22	1:A:584:ILE:H	12	0.56
(1,137)	1:A:538:LEU:HD23	1:A:584:ILE:H	12	0.56
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD11	7	0.56
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD12	7	0.56
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD13	7	0.56
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD21	7	0.56
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD22	7	0.56
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD23	7	0.56
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD11	7	0.56
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD12	7	0.56
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD13	7	0.56
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD21	7	0.56
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD22	7	0.56
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD23	7	0.56
(1,1045)	1:A:592:LEU:HD11	1:A:623:ARG:HD2	13	0.56
(1,1045)	1:A:592:LEU:HD12	1:A:623:ARG:HD2	13	0.56
(1,1045)	1:A:592:LEU:HD13	1:A:623:ARG:HD2	13	0.56
(1,1045)	1:A:592:LEU:HD21	1:A:623:ARG:HD2	13	0.56
(1,1045)	1:A:592:LEU:HD22	1:A:623:ARG:HD2	13	0.56
(1,1045)	1:A:592:LEU:HD23	1:A:623:ARG:HD2	13	0.56
(1,1045)	1:A:592:LEU:HD11	1:A:623:ARG:HD3	13	0.56
(1,1045)	1:A:592:LEU:HD12	1:A:623:ARG:HD3	13	0.56
(1,1045)	1:A:592:LEU:HD13	1:A:623:ARG:HD3	13	0.56
(1,1045)	1:A:592:LEU:HD21	1:A:623:ARG:HD3	13	0.56
(1,1045)	1:A:592:LEU:HD22	1:A:623:ARG:HD3	13	0.56
(1,1045)	1:A:592:LEU:HD23	1:A:623:ARG:HD3	13	0.56
(1,1039)	1:A:592:LEU:HD11	1:A:593:THR:H	3	0.56

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1039)	1:A:592:LEU:HD12	1:A:593:THR:H	3	0.56
(1,1039)	1:A:592:LEU:HD13	1:A:593:THR:H	3	0.56
(1,1039)	1:A:592:LEU:HD21	1:A:593:THR:H	3	0.56
(1,1039)	1:A:592:LEU:HD22	1:A:593:THR:H	3	0.56
(1,1039)	1:A:592:LEU:HD23	1:A:593:THR:H	3	0.56
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD11	18	0.55
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD12	18	0.55
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD13	18	0.55
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD21	18	0.55
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD22	18	0.55
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD23	18	0.55
(1,235)	1:A:544:LEU:HD11	1:A:652:PHE:HD1	4	0.55
(1,235)	1:A:544:LEU:HD11	1:A:652:PHE:HD2	4	0.55
(1,235)	1:A:544:LEU:HD12	1:A:652:PHE:HD1	4	0.55
(1,235)	1:A:544:LEU:HD12	1:A:652:PHE:HD2	4	0.55
(1,235)	1:A:544:LEU:HD13	1:A:652:PHE:HD1	4	0.55
(1,235)	1:A:544:LEU:HD13	1:A:652:PHE:HD2	4	0.55
(1,142)	1:A:538:LEU:HD11	1:A:586:HIS:H	9	0.55
(1,142)	1:A:538:LEU:HD12	1:A:586:HIS:H	9	0.55
(1,142)	1:A:538:LEU:HD13	1:A:586:HIS:H	9	0.55
(1,142)	1:A:538:LEU:HD21	1:A:586:HIS:H	9	0.55
(1,142)	1:A:538:LEU:HD22	1:A:586:HIS:H	9	0.55
(1,142)	1:A:538:LEU:HD23	1:A:586:HIS:H	9	0.55
(1,1044)	1:A:592:LEU:HD11	1:A:623:ARG:H	7	0.55
(1,1044)	1:A:592:LEU:HD12	1:A:623:ARG:H	7	0.55
(1,1044)	1:A:592:LEU:HD13	1:A:623:ARG:H	7	0.55
(1,1044)	1:A:592:LEU:HD21	1:A:623:ARG:H	7	0.55
(1,1044)	1:A:592:LEU:HD22	1:A:623:ARG:H	7	0.55
(1,1044)	1:A:592:LEU:HD23	1:A:623:ARG:H	7	0.55
(1,1041)	1:A:592:LEU:HD11	1:A:598:GLU:HG2	8	0.55
(1,1041)	1:A:592:LEU:HD12	1:A:598:GLU:HG2	8	0.55
(1,1041)	1:A:592:LEU:HD13	1:A:598:GLU:HG2	8	0.55
(1,1041)	1:A:592:LEU:HD21	1:A:598:GLU:HG2	8	0.55
(1,1041)	1:A:592:LEU:HD22	1:A:598:GLU:HG2	8	0.55
(1,1041)	1:A:592:LEU:HD23	1:A:598:GLU:HG2	8	0.55
(1,1039)	1:A:592:LEU:HD11	1:A:593:THR:H	10	0.55
(1,1039)	1:A:592:LEU:HD12	1:A:593:THR:H	10	0.55
(1,1039)	1:A:592:LEU:HD13	1:A:593:THR:H	10	0.55
(1,1039)	1:A:592:LEU:HD21	1:A:593:THR:H	10	0.55
(1,1039)	1:A:592:LEU:HD22	1:A:593:THR:H	10	0.55
(1,1039)	1:A:592:LEU:HD23	1:A:593:THR:H	10	0.55
(1,577)	1:A:566:GLN:HG2	1:A:627:TYR:HD1	5	0.54

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,577)	1:A:566:GLN:HG2	1:A:627:TYR:HD2	5	0.54
(1,577)	1:A:566:GLN:HG3	1:A:627:TYR:HD1	5	0.54
(1,577)	1:A:566:GLN:HG3	1:A:627:TYR:HD2	5	0.54
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD11	15	0.54
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD12	15	0.54
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD13	15	0.54
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD21	15	0.54
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD22	15	0.54
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD23	15	0.54
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD1	6	0.54
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD2	6	0.54
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD1	6	0.54
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD2	6	0.54
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD1	6	0.54
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD2	6	0.54
(1,1072)	1:A:594:LYS:HD2	1:A:595:GLY:HA2	4	0.54
(1,1072)	1:A:594:LYS:HD2	1:A:595:GLY:HA3	4	0.54
(1,1072)	1:A:594:LYS:HD3	1:A:595:GLY:HA2	4	0.54
(1,1072)	1:A:594:LYS:HD3	1:A:595:GLY:HA3	4	0.54
(1,1044)	1:A:592:LEU:HD11	1:A:623:ARG:H	13	0.54
(1,1044)	1:A:592:LEU:HD12	1:A:623:ARG:H	13	0.54
(1,1044)	1:A:592:LEU:HD13	1:A:623:ARG:H	13	0.54
(1,1044)	1:A:592:LEU:HD21	1:A:623:ARG:H	13	0.54
(1,1044)	1:A:592:LEU:HD22	1:A:623:ARG:H	13	0.54
(1,1044)	1:A:592:LEU:HD23	1:A:623:ARG:H	13	0.54
(1,1039)	1:A:592:LEU:HD11	1:A:593:THR:H	8	0.54
(1,1039)	1:A:592:LEU:HD12	1:A:593:THR:H	8	0.54
(1,1039)	1:A:592:LEU:HD13	1:A:593:THR:H	8	0.54
(1,1039)	1:A:592:LEU:HD21	1:A:593:THR:H	8	0.54
(1,1039)	1:A:592:LEU:HD22	1:A:593:THR:H	8	0.54
(1,1039)	1:A:592:LEU:HD23	1:A:593:THR:H	8	0.54
(1,500)	1:A:562:PHE:HE1	1:A:629:ARG:HG2	2	0.53
(1,500)	1:A:562:PHE:HE1	1:A:629:ARG:HG3	2	0.53
(1,500)	1:A:562:PHE:HE2	1:A:629:ARG:HG2	2	0.53
(1,500)	1:A:562:PHE:HE2	1:A:629:ARG:HG3	2	0.53
(1,145)	1:A:538:LEU:HD11	1:A:605:SER:H	9	0.53
(1,145)	1:A:538:LEU:HD12	1:A:605:SER:H	9	0.53
(1,145)	1:A:538:LEU:HD13	1:A:605:SER:H	9	0.53
(1,145)	1:A:538:LEU:HD21	1:A:605:SER:H	9	0.53
(1,145)	1:A:538:LEU:HD22	1:A:605:SER:H	9	0.53
(1,145)	1:A:538:LEU:HD23	1:A:605:SER:H	9	0.53
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD11	19	0.53

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD12	19	0.53
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD13	19	0.53
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD21	19	0.53
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD22	19	0.53
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD23	19	0.53
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD11	19	0.53
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD12	19	0.53
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD13	19	0.53
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD21	19	0.53
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD22	19	0.53
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD23	19	0.53
(1,235)	1:A:544:LEU:HD11	1:A:652:PHE:HD1	8	0.52
(1,235)	1:A:544:LEU:HD11	1:A:652:PHE:HD2	8	0.52
(1,235)	1:A:544:LEU:HD12	1:A:652:PHE:HD1	8	0.52
(1,235)	1:A:544:LEU:HD12	1:A:652:PHE:HD2	8	0.52
(1,235)	1:A:544:LEU:HD13	1:A:652:PHE:HD1	8	0.52
(1,235)	1:A:544:LEU:HD13	1:A:652:PHE:HD2	8	0.52
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD11	3	0.51
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD12	3	0.51
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD13	3	0.51
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD21	3	0.51
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD22	3	0.51
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD23	3	0.51
(1,1100)	1:A:597:LYS:HG2	1:A:597:LYS:HE2	12	0.51
(1,1100)	1:A:597:LYS:HG2	1:A:597:LYS:HE3	12	0.51
(1,1100)	1:A:597:LYS:HG3	1:A:597:LYS:HE2	12	0.51
(1,1100)	1:A:597:LYS:HG3	1:A:597:LYS:HE3	12	0.51
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD11	7	0.5
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD12	7	0.5
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD13	7	0.5
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD21	7	0.5
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD22	7	0.5
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD23	7	0.5
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD11	6	0.5
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD12	6	0.5
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD13	6	0.5
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD21	6	0.5
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD22	6	0.5
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD23	6	0.5
(1,842)	1:A:584:ILE:HD11	1:A:607:PHE:HD1	9	0.49
(1,842)	1:A:584:ILE:HD11	1:A:607:PHE:HD2	9	0.49
(1,842)	1:A:584:ILE:HD12	1:A:607:PHE:HD1	9	0.49

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,842)	1:A:584:ILE:HD12	1:A:607:PHE:HD2	9	0.49
(1,842)	1:A:584:ILE:HD13	1:A:607:PHE:HD1	9	0.49
(1,842)	1:A:584:ILE:HD13	1:A:607:PHE:HD2	9	0.49
(1,699)	1:A:574:GLU:HG2	1:A:575:GLY:HA2	7	0.49
(1,699)	1:A:574:GLU:HG2	1:A:575:GLY:HA3	7	0.49
(1,699)	1:A:574:GLU:HG3	1:A:575:GLY:HA2	7	0.49
(1,699)	1:A:574:GLU:HG3	1:A:575:GLY:HA3	7	0.49
(1,699)	1:A:574:GLU:HG2	1:A:575:GLY:HA2	8	0.49
(1,699)	1:A:574:GLU:HG2	1:A:575:GLY:HA3	8	0.49
(1,699)	1:A:574:GLU:HG3	1:A:575:GLY:HA2	8	0.49
(1,699)	1:A:574:GLU:HG3	1:A:575:GLY:HA3	8	0.49
(1,500)	1:A:562:PHE:HE1	1:A:629:ARG:HG2	8	0.49
(1,500)	1:A:562:PHE:HE1	1:A:629:ARG:HG3	8	0.49
(1,500)	1:A:562:PHE:HE2	1:A:629:ARG:HG2	8	0.49
(1,500)	1:A:562:PHE:HE2	1:A:629:ARG:HG3	8	0.49
(1,138)	1:A:538:LEU:HD11	1:A:585:GLN:H	9	0.49
(1,138)	1:A:538:LEU:HD12	1:A:585:GLN:H	9	0.49
(1,138)	1:A:538:LEU:HD13	1:A:585:GLN:H	9	0.49
(1,138)	1:A:538:LEU:HD21	1:A:585:GLN:H	9	0.49
(1,138)	1:A:538:LEU:HD22	1:A:585:GLN:H	9	0.49
(1,138)	1:A:538:LEU:HD23	1:A:585:GLN:H	9	0.49
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD11	8	0.49
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD12	8	0.49
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD13	8	0.49
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD21	8	0.49
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD22	8	0.49
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD23	8	0.49
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD11	8	0.49
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD12	8	0.49
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD13	8	0.49
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD21	8	0.49
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD22	8	0.49
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD23	8	0.49
(1,1100)	1:A:597:LYS:HG2	1:A:597:LYS:HE2	1	0.48
(1,1100)	1:A:597:LYS:HG2	1:A:597:LYS:HE3	1	0.48
(1,1100)	1:A:597:LYS:HG3	1:A:597:LYS:HE2	1	0.48
(1,1100)	1:A:597:LYS:HG3	1:A:597:LYS:HE3	1	0.48
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD11	4	0.47
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD12	4	0.47
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD13	4	0.47
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD21	4	0.47
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD22	4	0.47

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD23	4	0.47
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD11	17	0.47
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD12	17	0.47
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD13	17	0.47
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD21	17	0.47
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD22	17	0.47
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD23	17	0.47
(1,1100)	1:A:597:LYS:HG2	1:A:597:LYS:HE2	4	0.47
(1,1100)	1:A:597:LYS:HG2	1:A:597:LYS:HE3	4	0.47
(1,1100)	1:A:597:LYS:HG3	1:A:597:LYS:HE2	4	0.47
(1,1100)	1:A:597:LYS:HG3	1:A:597:LYS:HE3	4	0.47
(1,1100)	1:A:597:LYS:HG2	1:A:597:LYS:HE2	18	0.47
(1,1100)	1:A:597:LYS:HG2	1:A:597:LYS:HE3	18	0.47
(1,1100)	1:A:597:LYS:HG3	1:A:597:LYS:HE2	18	0.47
(1,1100)	1:A:597:LYS:HG3	1:A:597:LYS:HE3	18	0.47
(1,1072)	1:A:594:LYS:HD2	1:A:595:GLY:HA2	13	0.47
(1,1072)	1:A:594:LYS:HD2	1:A:595:GLY:HA3	13	0.47
(1,1072)	1:A:594:LYS:HD3	1:A:595:GLY:HA2	13	0.47
(1,1072)	1:A:594:LYS:HD3	1:A:595:GLY:HA3	13	0.47
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD1	1	0.46
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD2	1	0.46
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD1	1	0.46
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD2	1	0.46
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD1	1	0.46
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD2	1	0.46
(1,145)	1:A:538:LEU:HD11	1:A:605:SER:H	18	0.46
(1,145)	1:A:538:LEU:HD12	1:A:605:SER:H	18	0.46
(1,145)	1:A:538:LEU:HD13	1:A:605:SER:H	18	0.46
(1,145)	1:A:538:LEU:HD21	1:A:605:SER:H	18	0.46
(1,145)	1:A:538:LEU:HD22	1:A:605:SER:H	18	0.46
(1,145)	1:A:538:LEU:HD23	1:A:605:SER:H	18	0.46
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD11	6	0.46
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD12	6	0.46
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD13	6	0.46
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD21	6	0.46
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD22	6	0.46
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD23	6	0.46
(1,1100)	1:A:597:LYS:HG2	1:A:597:LYS:HE2	3	0.46
(1,1100)	1:A:597:LYS:HG2	1:A:597:LYS:HE3	3	0.46
(1,1100)	1:A:597:LYS:HG3	1:A:597:LYS:HE2	3	0.46
(1,1100)	1:A:597:LYS:HG3	1:A:597:LYS:HE3	3	0.46
(1,1100)	1:A:597:LYS:HG2	1:A:597:LYS:HE2	20	0.46

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1100)	1:A:597:LYS:HG2	1:A:597:LYS:HE3	20	0.46
(1,1100)	1:A:597:LYS:HG3	1:A:597:LYS:HE2	20	0.46
(1,1100)	1:A:597:LYS:HG3	1:A:597:LYS:HE3	20	0.46
(1,1042)	1:A:592:LEU:HD11	1:A:598:GLU:HB2	11	0.46
(1,1042)	1:A:592:LEU:HD11	1:A:598:GLU:HB3	11	0.46
(1,1042)	1:A:592:LEU:HD12	1:A:598:GLU:HB2	11	0.46
(1,1042)	1:A:592:LEU:HD12	1:A:598:GLU:HB3	11	0.46
(1,1042)	1:A:592:LEU:HD13	1:A:598:GLU:HB2	11	0.46
(1,1042)	1:A:592:LEU:HD13	1:A:598:GLU:HB3	11	0.46
(1,1042)	1:A:592:LEU:HD21	1:A:598:GLU:HB2	11	0.46
(1,1042)	1:A:592:LEU:HD21	1:A:598:GLU:HB3	11	0.46
(1,1042)	1:A:592:LEU:HD22	1:A:598:GLU:HB2	11	0.46
(1,1042)	1:A:592:LEU:HD22	1:A:598:GLU:HB3	11	0.46
(1,1042)	1:A:592:LEU:HD23	1:A:598:GLU:HB2	11	0.46
(1,1042)	1:A:592:LEU:HD23	1:A:598:GLU:HB3	11	0.46
(1,699)	1:A:574:GLU:HG2	1:A:575:GLY:HA2	10	0.45
(1,699)	1:A:574:GLU:HG2	1:A:575:GLY:HA3	10	0.45
(1,699)	1:A:574:GLU:HG3	1:A:575:GLY:HA2	10	0.45
(1,699)	1:A:574:GLU:HG3	1:A:575:GLY:HA3	10	0.45
(1,500)	1:A:562:PHE:HE1	1:A:629:ARG:HG2	18	0.45
(1,500)	1:A:562:PHE:HE1	1:A:629:ARG:HG3	18	0.45
(1,500)	1:A:562:PHE:HE2	1:A:629:ARG:HG2	18	0.45
(1,500)	1:A:562:PHE:HE2	1:A:629:ARG:HG3	18	0.45
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD11	2	0.45
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD12	2	0.45
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD13	2	0.45
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD21	2	0.45
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD22	2	0.45
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD23	2	0.45
(1,405)	1:A:556:MET:HE1	1:A:638:PHE:HD1	5	0.45
(1,405)	1:A:556:MET:HE1	1:A:638:PHE:HD2	5	0.45
(1,405)	1:A:556:MET:HE2	1:A:638:PHE:HD1	5	0.45
(1,405)	1:A:556:MET:HE2	1:A:638:PHE:HD2	5	0.45
(1,405)	1:A:556:MET:HE3	1:A:638:PHE:HD1	5	0.45
(1,405)	1:A:556:MET:HE3	1:A:638:PHE:HD2	5	0.45
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD11	15	0.45
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD12	15	0.45
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD13	15	0.45
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD21	15	0.45
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD22	15	0.45
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD23	15	0.45
(1,1044)	1:A:592:LEU:HD11	1:A:623:ARG:H	11	0.45

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1044)	1:A:592:LEU:HD12	1:A:623:ARG:H	11	0.45
(1,1044)	1:A:592:LEU:HD13	1:A:623:ARG:H	11	0.45
(1,1044)	1:A:592:LEU:HD21	1:A:623:ARG:H	11	0.45
(1,1044)	1:A:592:LEU:HD22	1:A:623:ARG:H	11	0.45
(1,1044)	1:A:592:LEU:HD23	1:A:623:ARG:H	11	0.45
(1,1039)	1:A:592:LEU:HD11	1:A:593:THR:H	19	0.45
(1,1039)	1:A:592:LEU:HD12	1:A:593:THR:H	19	0.45
(1,1039)	1:A:592:LEU:HD13	1:A:593:THR:H	19	0.45
(1,1039)	1:A:592:LEU:HD21	1:A:593:THR:H	19	0.45
(1,1039)	1:A:592:LEU:HD22	1:A:593:THR:H	19	0.45
(1,1039)	1:A:592:LEU:HD23	1:A:593:THR:H	19	0.45
(1,842)	1:A:584:ILE:HD11	1:A:607:PHE:HD1	15	0.44
(1,842)	1:A:584:ILE:HD11	1:A:607:PHE:HD2	15	0.44
(1,842)	1:A:584:ILE:HD12	1:A:607:PHE:HD1	15	0.44
(1,842)	1:A:584:ILE:HD12	1:A:607:PHE:HD2	15	0.44
(1,842)	1:A:584:ILE:HD13	1:A:607:PHE:HD1	15	0.44
(1,842)	1:A:584:ILE:HD13	1:A:607:PHE:HD2	15	0.44
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD11	6	0.44
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD12	6	0.44
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD13	6	0.44
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD21	6	0.44
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD22	6	0.44
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD23	6	0.44
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD1	17	0.44
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD2	17	0.44
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD1	17	0.44
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD2	17	0.44
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD1	17	0.44
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD2	17	0.44
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD2	19	0.43
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD3	19	0.43
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD2	19	0.43
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD3	19	0.43
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD2	19	0.43
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD3	19	0.43
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD11	5	0.43
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD12	5	0.43
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD13	5	0.43
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD21	5	0.43
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD22	5	0.43
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD23	5	0.43
(1,1039)	1:A:592:LEU:HD11	1:A:593:THR:H	6	0.43

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1039)	1:A:592:LEU:HD12	1:A:593:THR:H	6	0.43
(1,1039)	1:A:592:LEU:HD13	1:A:593:THR:H	6	0.43
(1,1039)	1:A:592:LEU:HD21	1:A:593:THR:H	6	0.43
(1,1039)	1:A:592:LEU:HD22	1:A:593:THR:H	6	0.43
(1,1039)	1:A:592:LEU:HD23	1:A:593:THR:H	6	0.43
(1,455)	1:A:560:LEU:HD11	1:A:631:TYR:HD1	5	0.42
(1,455)	1:A:560:LEU:HD11	1:A:631:TYR:HD2	5	0.42
(1,455)	1:A:560:LEU:HD12	1:A:631:TYR:HD1	5	0.42
(1,455)	1:A:560:LEU:HD12	1:A:631:TYR:HD2	5	0.42
(1,455)	1:A:560:LEU:HD13	1:A:631:TYR:HD1	5	0.42
(1,455)	1:A:560:LEU:HD13	1:A:631:TYR:HD2	5	0.42
(1,405)	1:A:556:MET:HE1	1:A:638:PHE:HD1	16	0.42
(1,405)	1:A:556:MET:HE1	1:A:638:PHE:HD2	16	0.42
(1,405)	1:A:556:MET:HE2	1:A:638:PHE:HD1	16	0.42
(1,405)	1:A:556:MET:HE2	1:A:638:PHE:HD2	16	0.42
(1,405)	1:A:556:MET:HE3	1:A:638:PHE:HD1	16	0.42
(1,405)	1:A:556:MET:HE3	1:A:638:PHE:HD2	16	0.42
(1,1608)	1:A:662:ARG:HB2	1:A:662:ARG:HD2	7	0.42
(1,1608)	1:A:662:ARG:HB2	1:A:662:ARG:HD3	7	0.42
(1,1608)	1:A:662:ARG:HB3	1:A:662:ARG:HD2	7	0.42
(1,1608)	1:A:662:ARG:HB3	1:A:662:ARG:HD3	7	0.42
(1,1100)	1:A:597:LYS:HG2	1:A:597:LYS:HE2	5	0.42
(1,1100)	1:A:597:LYS:HG2	1:A:597:LYS:HE3	5	0.42
(1,1100)	1:A:597:LYS:HG3	1:A:597:LYS:HE2	5	0.42
(1,1100)	1:A:597:LYS:HG3	1:A:597:LYS:HE3	5	0.42
(1,1044)	1:A:592:LEU:HD11	1:A:623:ARG:H	16	0.42
(1,1044)	1:A:592:LEU:HD12	1:A:623:ARG:H	16	0.42
(1,1044)	1:A:592:LEU:HD13	1:A:623:ARG:H	16	0.42
(1,1044)	1:A:592:LEU:HD21	1:A:623:ARG:H	16	0.42
(1,1044)	1:A:592:LEU:HD22	1:A:623:ARG:H	16	0.42
(1,1044)	1:A:592:LEU:HD23	1:A:623:ARG:H	16	0.42
(1,842)	1:A:584:ILE:HD11	1:A:607:PHE:HD1	14	0.41
(1,842)	1:A:584:ILE:HD11	1:A:607:PHE:HD2	14	0.41
(1,842)	1:A:584:ILE:HD12	1:A:607:PHE:HD1	14	0.41
(1,842)	1:A:584:ILE:HD12	1:A:607:PHE:HD2	14	0.41
(1,842)	1:A:584:ILE:HD13	1:A:607:PHE:HD1	14	0.41
(1,842)	1:A:584:ILE:HD13	1:A:607:PHE:HD2	14	0.41
(1,699)	1:A:574:GLU:HG2	1:A:575:GLY:HA2	5	0.41
(1,699)	1:A:574:GLU:HG2	1:A:575:GLY:HA3	5	0.41
(1,699)	1:A:574:GLU:HG3	1:A:575:GLY:HA2	5	0.41
(1,699)	1:A:574:GLU:HG3	1:A:575:GLY:HA3	5	0.41
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG21	6	0.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG22	6	0.41
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG23	6	0.41
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG21	6	0.41
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG22	6	0.41
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG23	6	0.41
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD11	17	0.41
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD12	17	0.41
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD13	17	0.41
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD21	17	0.41
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD22	17	0.41
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD23	17	0.41
(1,842)	1:A:584:ILE:HD11	1:A:607:PHE:HD1	8	0.4
(1,842)	1:A:584:ILE:HD11	1:A:607:PHE:HD2	8	0.4
(1,842)	1:A:584:ILE:HD12	1:A:607:PHE:HD1	8	0.4
(1,842)	1:A:584:ILE:HD12	1:A:607:PHE:HD2	8	0.4
(1,842)	1:A:584:ILE:HD13	1:A:607:PHE:HD1	8	0.4
(1,842)	1:A:584:ILE:HD13	1:A:607:PHE:HD2	8	0.4
(1,842)	1:A:584:ILE:HD11	1:A:607:PHE:HD1	19	0.4
(1,842)	1:A:584:ILE:HD11	1:A:607:PHE:HD2	19	0.4
(1,842)	1:A:584:ILE:HD12	1:A:607:PHE:HD1	19	0.4
(1,842)	1:A:584:ILE:HD12	1:A:607:PHE:HD2	19	0.4
(1,842)	1:A:584:ILE:HD13	1:A:607:PHE:HD1	19	0.4
(1,842)	1:A:584:ILE:HD13	1:A:607:PHE:HD2	19	0.4
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD11	3	0.4
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD12	3	0.4
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD13	3	0.4
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD21	3	0.4
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD22	3	0.4
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD23	3	0.4
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD1	7	0.4
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD2	7	0.4
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD1	7	0.4
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD2	7	0.4
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD1	7	0.4
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD2	7	0.4
(1,137)	1:A:538:LEU:HD11	1:A:584:ILE:H	18	0.4
(1,137)	1:A:538:LEU:HD12	1:A:584:ILE:H	18	0.4
(1,137)	1:A:538:LEU:HD13	1:A:584:ILE:H	18	0.4
(1,137)	1:A:538:LEU:HD21	1:A:584:ILE:H	18	0.4
(1,137)	1:A:538:LEU:HD22	1:A:584:ILE:H	18	0.4
(1,137)	1:A:538:LEU:HD23	1:A:584:ILE:H	18	0.4
(1,1045)	1:A:592:LEU:HD11	1:A:623:ARG:HD2	11	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1045)	1:A:592:LEU:HD12	1:A:623:ARG:HD2	11	0.4
(1,1045)	1:A:592:LEU:HD13	1:A:623:ARG:HD2	11	0.4
(1,1045)	1:A:592:LEU:HD21	1:A:623:ARG:HD2	11	0.4
(1,1045)	1:A:592:LEU:HD22	1:A:623:ARG:HD2	11	0.4
(1,1045)	1:A:592:LEU:HD23	1:A:623:ARG:HD2	11	0.4
(1,1045)	1:A:592:LEU:HD11	1:A:623:ARG:HD3	11	0.4
(1,1045)	1:A:592:LEU:HD12	1:A:623:ARG:HD3	11	0.4
(1,1045)	1:A:592:LEU:HD13	1:A:623:ARG:HD3	11	0.4
(1,1045)	1:A:592:LEU:HD21	1:A:623:ARG:HD3	11	0.4
(1,1045)	1:A:592:LEU:HD22	1:A:623:ARG:HD3	11	0.4
(1,1045)	1:A:592:LEU:HD23	1:A:623:ARG:HD3	11	0.4
(1,141)	1:A:538:LEU:HD11	1:A:585:GLN:HB2	11	0.39
(1,141)	1:A:538:LEU:HD11	1:A:585:GLN:HB3	11	0.39
(1,141)	1:A:538:LEU:HD12	1:A:585:GLN:HB2	11	0.39
(1,141)	1:A:538:LEU:HD12	1:A:585:GLN:HB3	11	0.39
(1,141)	1:A:538:LEU:HD13	1:A:585:GLN:HB2	11	0.39
(1,141)	1:A:538:LEU:HD13	1:A:585:GLN:HB3	11	0.39
(1,141)	1:A:538:LEU:HD21	1:A:585:GLN:HB2	11	0.39
(1,141)	1:A:538:LEU:HD21	1:A:585:GLN:HB3	11	0.39
(1,141)	1:A:538:LEU:HD22	1:A:585:GLN:HB2	11	0.39
(1,141)	1:A:538:LEU:HD22	1:A:585:GLN:HB3	11	0.39
(1,141)	1:A:538:LEU:HD23	1:A:585:GLN:HB2	11	0.39
(1,141)	1:A:538:LEU:HD23	1:A:585:GLN:HB3	11	0.39
(1,932)	1:A:588:VAL:HG11	1:A:602:SER:HB3	18	0.38
(1,932)	1:A:588:VAL:HG12	1:A:602:SER:HB3	18	0.38
(1,932)	1:A:588:VAL:HG13	1:A:602:SER:HB3	18	0.38
(1,932)	1:A:588:VAL:HG21	1:A:602:SER:HB3	18	0.38
(1,932)	1:A:588:VAL:HG22	1:A:602:SER:HB3	18	0.38
(1,932)	1:A:588:VAL:HG23	1:A:602:SER:HB3	18	0.38
(1,500)	1:A:562:PHE:HE1	1:A:629:ARG:HG2	17	0.38
(1,500)	1:A:562:PHE:HE1	1:A:629:ARG:HG3	17	0.38
(1,500)	1:A:562:PHE:HE2	1:A:629:ARG:HG2	17	0.38
(1,500)	1:A:562:PHE:HE2	1:A:629:ARG:HG3	17	0.38
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD2	5	0.38
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD3	5	0.38
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD2	5	0.38
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD3	5	0.38
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD2	5	0.38
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD3	5	0.38
(1,138)	1:A:538:LEU:HD11	1:A:585:GLN:H	11	0.38
(1,138)	1:A:538:LEU:HD12	1:A:585:GLN:H	11	0.38
(1,138)	1:A:538:LEU:HD13	1:A:585:GLN:H	11	0.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,138)	1:A:538:LEU:HD21	1:A:585:GLN:H	11	0.38
(1,138)	1:A:538:LEU:HD22	1:A:585:GLN:H	11	0.38
(1,138)	1:A:538:LEU:HD23	1:A:585:GLN:H	11	0.38
(1,1041)	1:A:592:LEU:HD11	1:A:598:GLU:HG2	2	0.38
(1,1041)	1:A:592:LEU:HD12	1:A:598:GLU:HG2	2	0.38
(1,1041)	1:A:592:LEU:HD13	1:A:598:GLU:HG2	2	0.38
(1,1041)	1:A:592:LEU:HD21	1:A:598:GLU:HG2	2	0.38
(1,1041)	1:A:592:LEU:HD22	1:A:598:GLU:HG2	2	0.38
(1,1041)	1:A:592:LEU:HD23	1:A:598:GLU:HG2	2	0.38
(1,1039)	1:A:592:LEU:HD11	1:A:593:THR:H	7	0.38
(1,1039)	1:A:592:LEU:HD12	1:A:593:THR:H	7	0.38
(1,1039)	1:A:592:LEU:HD13	1:A:593:THR:H	7	0.38
(1,1039)	1:A:592:LEU:HD21	1:A:593:THR:H	7	0.38
(1,1039)	1:A:592:LEU:HD22	1:A:593:THR:H	7	0.38
(1,1039)	1:A:592:LEU:HD23	1:A:593:THR:H	7	0.38
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD11	13	0.37
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD12	13	0.37
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD13	13	0.37
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD21	13	0.37
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD22	13	0.37
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD23	13	0.37
(1,235)	1:A:544:LEU:HD11	1:A:652:PHE:HD1	17	0.37
(1,235)	1:A:544:LEU:HD11	1:A:652:PHE:HD2	17	0.37
(1,235)	1:A:544:LEU:HD12	1:A:652:PHE:HD1	17	0.37
(1,235)	1:A:544:LEU:HD12	1:A:652:PHE:HD2	17	0.37
(1,235)	1:A:544:LEU:HD13	1:A:652:PHE:HD1	17	0.37
(1,235)	1:A:544:LEU:HD13	1:A:652:PHE:HD2	17	0.37
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD2	7	0.37
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD3	7	0.37
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD2	7	0.37
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD3	7	0.37
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD2	7	0.37
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD3	7	0.37
(1,137)	1:A:538:LEU:HD11	1:A:584:ILE:H	17	0.37
(1,137)	1:A:538:LEU:HD12	1:A:584:ILE:H	17	0.37
(1,137)	1:A:538:LEU:HD13	1:A:584:ILE:H	17	0.37
(1,137)	1:A:538:LEU:HD21	1:A:584:ILE:H	17	0.37
(1,137)	1:A:538:LEU:HD22	1:A:584:ILE:H	17	0.37
(1,137)	1:A:538:LEU:HD23	1:A:584:ILE:H	17	0.37
(1,1031)	1:A:592:LEU:HA	1:A:592:LEU:HD11	11	0.37
(1,1031)	1:A:592:LEU:HA	1:A:592:LEU:HD12	11	0.37
(1,1031)	1:A:592:LEU:HA	1:A:592:LEU:HD13	11	0.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1031)	1:A:592:LEU:HA	1:A:592:LEU:HD21	11	0.37
(1,1031)	1:A:592:LEU:HA	1:A:592:LEU:HD22	11	0.37
(1,1031)	1:A:592:LEU:HA	1:A:592:LEU:HD23	11	0.37
(1,577)	1:A:566:GLN:HG2	1:A:627:TYR:HD1	15	0.36
(1,577)	1:A:566:GLN:HG2	1:A:627:TYR:HD2	15	0.36
(1,577)	1:A:566:GLN:HG3	1:A:627:TYR:HD1	15	0.36
(1,577)	1:A:566:GLN:HG3	1:A:627:TYR:HD2	15	0.36
(1,405)	1:A:556:MET:HE1	1:A:638:PHE:HD1	15	0.36
(1,405)	1:A:556:MET:HE1	1:A:638:PHE:HD2	15	0.36
(1,405)	1:A:556:MET:HE2	1:A:638:PHE:HD1	15	0.36
(1,405)	1:A:556:MET:HE2	1:A:638:PHE:HD2	15	0.36
(1,405)	1:A:556:MET:HE3	1:A:638:PHE:HD1	15	0.36
(1,405)	1:A:556:MET:HE3	1:A:638:PHE:HD2	15	0.36
(1,211)	1:A:542:MET:HE1	1:A:606:TYR:HD1	9	0.36
(1,211)	1:A:542:MET:HE1	1:A:606:TYR:HD2	9	0.36
(1,211)	1:A:542:MET:HE2	1:A:606:TYR:HD1	9	0.36
(1,211)	1:A:542:MET:HE2	1:A:606:TYR:HD2	9	0.36
(1,211)	1:A:542:MET:HE3	1:A:606:TYR:HD1	9	0.36
(1,211)	1:A:542:MET:HE3	1:A:606:TYR:HD2	9	0.36
(1,1100)	1:A:597:LYS:HG2	1:A:597:LYS:HE2	8	0.36
(1,1100)	1:A:597:LYS:HG2	1:A:597:LYS:HE3	8	0.36
(1,1100)	1:A:597:LYS:HG3	1:A:597:LYS:HE2	8	0.36
(1,1100)	1:A:597:LYS:HG3	1:A:597:LYS:HE3	8	0.36
(1,1100)	1:A:597:LYS:HG2	1:A:597:LYS:HE2	14	0.36
(1,1100)	1:A:597:LYS:HG2	1:A:597:LYS:HE3	14	0.36
(1,1100)	1:A:597:LYS:HG3	1:A:597:LYS:HE2	14	0.36
(1,1100)	1:A:597:LYS:HG3	1:A:597:LYS:HE3	14	0.36
(1,1100)	1:A:597:LYS:HG2	1:A:597:LYS:HE2	16	0.36
(1,1100)	1:A:597:LYS:HG2	1:A:597:LYS:HE3	16	0.36
(1,1100)	1:A:597:LYS:HG3	1:A:597:LYS:HE2	16	0.36
(1,1100)	1:A:597:LYS:HG3	1:A:597:LYS:HE3	16	0.36
(1,1100)	1:A:597:LYS:HG2	1:A:597:LYS:HE2	19	0.36
(1,1100)	1:A:597:LYS:HG2	1:A:597:LYS:HE3	19	0.36
(1,1100)	1:A:597:LYS:HG3	1:A:597:LYS:HE2	19	0.36
(1,1100)	1:A:597:LYS:HG3	1:A:597:LYS:HE3	19	0.36
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG21	9	0.35
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG22	9	0.35
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG23	9	0.35
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG21	9	0.35
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG22	9	0.35
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG23	9	0.35
(1,968)	1:A:589:VAL:HG21	1:A:607:PHE:HD1	12	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,968)	1:A:589:VAL:HG21	1:A:607:PHE:HD2	12	0.34
(1,968)	1:A:589:VAL:HG22	1:A:607:PHE:HD1	12	0.34
(1,968)	1:A:589:VAL:HG22	1:A:607:PHE:HD2	12	0.34
(1,968)	1:A:589:VAL:HG23	1:A:607:PHE:HD1	12	0.34
(1,968)	1:A:589:VAL:HG23	1:A:607:PHE:HD2	12	0.34
(1,145)	1:A:538:LEU:HD11	1:A:605:SER:H	1	0.34
(1,145)	1:A:538:LEU:HD12	1:A:605:SER:H	1	0.34
(1,145)	1:A:538:LEU:HD13	1:A:605:SER:H	1	0.34
(1,145)	1:A:538:LEU:HD21	1:A:605:SER:H	1	0.34
(1,145)	1:A:538:LEU:HD22	1:A:605:SER:H	1	0.34
(1,145)	1:A:538:LEU:HD23	1:A:605:SER:H	1	0.34
(1,145)	1:A:538:LEU:HD11	1:A:605:SER:H	10	0.34
(1,145)	1:A:538:LEU:HD12	1:A:605:SER:H	10	0.34
(1,145)	1:A:538:LEU:HD13	1:A:605:SER:H	10	0.34
(1,145)	1:A:538:LEU:HD21	1:A:605:SER:H	10	0.34
(1,145)	1:A:538:LEU:HD22	1:A:605:SER:H	10	0.34
(1,145)	1:A:538:LEU:HD23	1:A:605:SER:H	10	0.34
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD11	1	0.34
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD12	1	0.34
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD13	1	0.34
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD21	1	0.34
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD22	1	0.34
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD23	1	0.34
(1,1045)	1:A:592:LEU:HD11	1:A:623:ARG:HD2	4	0.34
(1,1045)	1:A:592:LEU:HD12	1:A:623:ARG:HD2	4	0.34
(1,1045)	1:A:592:LEU:HD13	1:A:623:ARG:HD2	4	0.34
(1,1045)	1:A:592:LEU:HD21	1:A:623:ARG:HD2	4	0.34
(1,1045)	1:A:592:LEU:HD22	1:A:623:ARG:HD2	4	0.34
(1,1045)	1:A:592:LEU:HD23	1:A:623:ARG:HD2	4	0.34
(1,1045)	1:A:592:LEU:HD11	1:A:623:ARG:HD3	4	0.34
(1,1045)	1:A:592:LEU:HD12	1:A:623:ARG:HD3	4	0.34
(1,1045)	1:A:592:LEU:HD13	1:A:623:ARG:HD3	4	0.34
(1,1045)	1:A:592:LEU:HD21	1:A:623:ARG:HD3	4	0.34
(1,1045)	1:A:592:LEU:HD22	1:A:623:ARG:HD3	4	0.34
(1,1045)	1:A:592:LEU:HD23	1:A:623:ARG:HD3	4	0.34
(1,1041)	1:A:592:LEU:HD11	1:A:598:GLU:HG2	14	0.34
(1,1041)	1:A:592:LEU:HD12	1:A:598:GLU:HG2	14	0.34
(1,1041)	1:A:592:LEU:HD13	1:A:598:GLU:HG2	14	0.34
(1,1041)	1:A:592:LEU:HD21	1:A:598:GLU:HG2	14	0.34
(1,1041)	1:A:592:LEU:HD22	1:A:598:GLU:HG2	14	0.34
(1,1041)	1:A:592:LEU:HD23	1:A:598:GLU:HG2	14	0.34
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD11	18	0.33

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD12	18	0.33
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD13	18	0.33
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD21	18	0.33
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD22	18	0.33
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD23	18	0.33
(1,932)	1:A:588:VAL:HG11	1:A:602:SER:HB3	6	0.33
(1,932)	1:A:588:VAL:HG12	1:A:602:SER:HB3	6	0.33
(1,932)	1:A:588:VAL:HG13	1:A:602:SER:HB3	6	0.33
(1,932)	1:A:588:VAL:HG21	1:A:602:SER:HB3	6	0.33
(1,932)	1:A:588:VAL:HG22	1:A:602:SER:HB3	6	0.33
(1,932)	1:A:588:VAL:HG23	1:A:602:SER:HB3	6	0.33
(1,500)	1:A:562:PHE:HE1	1:A:629:ARG:HG2	19	0.33
(1,500)	1:A:562:PHE:HE1	1:A:629:ARG:HG3	19	0.33
(1,500)	1:A:562:PHE:HE2	1:A:629:ARG:HG2	19	0.33
(1,500)	1:A:562:PHE:HE2	1:A:629:ARG:HG3	19	0.33
(1,137)	1:A:538:LEU:HD11	1:A:584:ILE:H	4	0.33
(1,137)	1:A:538:LEU:HD12	1:A:584:ILE:H	4	0.33
(1,137)	1:A:538:LEU:HD13	1:A:584:ILE:H	4	0.33
(1,137)	1:A:538:LEU:HD21	1:A:584:ILE:H	4	0.33
(1,137)	1:A:538:LEU:HD22	1:A:584:ILE:H	4	0.33
(1,137)	1:A:538:LEU:HD23	1:A:584:ILE:H	4	0.33
(1,968)	1:A:589:VAL:HG21	1:A:607:PHE:HD1	14	0.32
(1,968)	1:A:589:VAL:HG21	1:A:607:PHE:HD2	14	0.32
(1,968)	1:A:589:VAL:HG22	1:A:607:PHE:HD1	14	0.32
(1,968)	1:A:589:VAL:HG22	1:A:607:PHE:HD2	14	0.32
(1,968)	1:A:589:VAL:HG23	1:A:607:PHE:HD1	14	0.32
(1,968)	1:A:589:VAL:HG23	1:A:607:PHE:HD2	14	0.32
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD11	4	0.32
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD12	4	0.32
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD13	4	0.32
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD21	4	0.32
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD22	4	0.32
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD23	4	0.32
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD1	12	0.32
(1,1484)	1:A:648:MET:HE1	1:A:652:PHE:HD2	12	0.32
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD1	12	0.32
(1,1484)	1:A:648:MET:HE2	1:A:652:PHE:HD2	12	0.32
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD1	12	0.32
(1,1484)	1:A:648:MET:HE3	1:A:652:PHE:HD2	12	0.32
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD11	3	0.32
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD12	3	0.32
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD13	3	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD21	3	0.32
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD22	3	0.32
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD23	3	0.32
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD11	8	0.32
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD12	8	0.32
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD13	8	0.32
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD21	8	0.32
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD22	8	0.32
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD23	8	0.32
(1,235)	1:A:544:LEU:HD11	1:A:652:PHE:HD1	9	0.31
(1,235)	1:A:544:LEU:HD11	1:A:652:PHE:HD2	9	0.31
(1,235)	1:A:544:LEU:HD12	1:A:652:PHE:HD1	9	0.31
(1,235)	1:A:544:LEU:HD12	1:A:652:PHE:HD2	9	0.31
(1,235)	1:A:544:LEU:HD13	1:A:652:PHE:HD1	9	0.31
(1,235)	1:A:544:LEU:HD13	1:A:652:PHE:HD2	9	0.31
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD11	7	0.31
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD12	7	0.31
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD13	7	0.31
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD21	7	0.31
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD22	7	0.31
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD23	7	0.31
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD11	7	0.31
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD12	7	0.31
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD13	7	0.31
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD21	7	0.31
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD22	7	0.31
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD23	7	0.31
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD11	9	0.3
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD12	9	0.3
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD13	9	0.3
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD11	9	0.3
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD12	9	0.3
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD13	9	0.3
(1,577)	1:A:566:GLN:HG2	1:A:627:TYR:HD1	2	0.3
(1,577)	1:A:566:GLN:HG2	1:A:627:TYR:HD2	2	0.3
(1,577)	1:A:566:GLN:HG3	1:A:627:TYR:HD1	2	0.3
(1,577)	1:A:566:GLN:HG3	1:A:627:TYR:HD2	2	0.3
(1,500)	1:A:562:PHE:HE1	1:A:629:ARG:HG2	15	0.3
(1,500)	1:A:562:PHE:HE1	1:A:629:ARG:HG3	15	0.3
(1,500)	1:A:562:PHE:HE2	1:A:629:ARG:HG2	15	0.3
(1,500)	1:A:562:PHE:HE2	1:A:629:ARG:HG3	15	0.3
(1,1072)	1:A:594:LYS:HD2	1:A:595:GLY:HA2	17	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1072)	1:A:594:LYS:HD2	1:A:595:GLY:HA3	17	0.3
(1,1072)	1:A:594:LYS:HD3	1:A:595:GLY:HA2	17	0.3
(1,1072)	1:A:594:LYS:HD3	1:A:595:GLY:HA3	17	0.3
(1,1041)	1:A:592:LEU:HD11	1:A:598:GLU:HG2	17	0.3
(1,1041)	1:A:592:LEU:HD12	1:A:598:GLU:HG2	17	0.3
(1,1041)	1:A:592:LEU:HD13	1:A:598:GLU:HG2	17	0.3
(1,1041)	1:A:592:LEU:HD21	1:A:598:GLU:HG2	17	0.3
(1,1041)	1:A:592:LEU:HD22	1:A:598:GLU:HG2	17	0.3
(1,1041)	1:A:592:LEU:HD23	1:A:598:GLU:HG2	17	0.3
(1,932)	1:A:588:VAL:HG11	1:A:602:SER:HB3	7	0.29
(1,932)	1:A:588:VAL:HG12	1:A:602:SER:HB3	7	0.29
(1,932)	1:A:588:VAL:HG13	1:A:602:SER:HB3	7	0.29
(1,932)	1:A:588:VAL:HG21	1:A:602:SER:HB3	7	0.29
(1,932)	1:A:588:VAL:HG22	1:A:602:SER:HB3	7	0.29
(1,932)	1:A:588:VAL:HG23	1:A:602:SER:HB3	7	0.29
(1,932)	1:A:588:VAL:HG11	1:A:602:SER:HB3	13	0.29
(1,932)	1:A:588:VAL:HG12	1:A:602:SER:HB3	13	0.29
(1,932)	1:A:588:VAL:HG13	1:A:602:SER:HB3	13	0.29
(1,932)	1:A:588:VAL:HG21	1:A:602:SER:HB3	13	0.29
(1,932)	1:A:588:VAL:HG22	1:A:602:SER:HB3	13	0.29
(1,932)	1:A:588:VAL:HG23	1:A:602:SER:HB3	13	0.29
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD11	13	0.29
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD12	13	0.29
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD13	13	0.29
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD21	13	0.29
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD22	13	0.29
(1,449)	1:A:560:LEU:HA	1:A:633:LEU:HD23	13	0.29
(1,142)	1:A:538:LEU:HD11	1:A:586:HIS:H	11	0.29
(1,142)	1:A:538:LEU:HD12	1:A:586:HIS:H	11	0.29
(1,142)	1:A:538:LEU:HD13	1:A:586:HIS:H	11	0.29
(1,142)	1:A:538:LEU:HD21	1:A:586:HIS:H	11	0.29
(1,142)	1:A:538:LEU:HD22	1:A:586:HIS:H	11	0.29
(1,142)	1:A:538:LEU:HD23	1:A:586:HIS:H	11	0.29
(1,1044)	1:A:592:LEU:HD11	1:A:623:ARG:H	14	0.29
(1,1044)	1:A:592:LEU:HD12	1:A:623:ARG:H	14	0.29
(1,1044)	1:A:592:LEU:HD13	1:A:623:ARG:H	14	0.29
(1,1044)	1:A:592:LEU:HD21	1:A:623:ARG:H	14	0.29
(1,1044)	1:A:592:LEU:HD22	1:A:623:ARG:H	14	0.29
(1,1044)	1:A:592:LEU:HD23	1:A:623:ARG:H	14	0.29
(1,1045)	1:A:592:LEU:HD11	1:A:623:ARG:HD2	9	0.28
(1,1045)	1:A:592:LEU:HD12	1:A:623:ARG:HD2	9	0.28
(1,1045)	1:A:592:LEU:HD13	1:A:623:ARG:HD2	9	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1045)	1:A:592:LEU:HD21	1:A:623:ARG:HD2	9	0.28
(1,1045)	1:A:592:LEU:HD22	1:A:623:ARG:HD2	9	0.28
(1,1045)	1:A:592:LEU:HD23	1:A:623:ARG:HD2	9	0.28
(1,1045)	1:A:592:LEU:HD11	1:A:623:ARG:HD3	9	0.28
(1,1045)	1:A:592:LEU:HD12	1:A:623:ARG:HD3	9	0.28
(1,1045)	1:A:592:LEU:HD13	1:A:623:ARG:HD3	9	0.28
(1,1045)	1:A:592:LEU:HD21	1:A:623:ARG:HD3	9	0.28
(1,1045)	1:A:592:LEU:HD22	1:A:623:ARG:HD3	9	0.28
(1,1045)	1:A:592:LEU:HD23	1:A:623:ARG:HD3	9	0.28
(1,235)	1:A:544:LEU:HD11	1:A:652:PHE:HD1	13	0.27
(1,235)	1:A:544:LEU:HD11	1:A:652:PHE:HD2	13	0.27
(1,235)	1:A:544:LEU:HD12	1:A:652:PHE:HD1	13	0.27
(1,235)	1:A:544:LEU:HD12	1:A:652:PHE:HD2	13	0.27
(1,235)	1:A:544:LEU:HD13	1:A:652:PHE:HD1	13	0.27
(1,235)	1:A:544:LEU:HD13	1:A:652:PHE:HD2	13	0.27
(1,1612)	1:A:663:ILE:HA	1:A:663:ILE:HG12	8	0.27
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD2	12	0.27
(1,1581)	1:A:656:ALA:HB1	1:A:659:ARG:HD3	12	0.27
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD2	12	0.27
(1,1581)	1:A:656:ALA:HB2	1:A:659:ARG:HD3	12	0.27
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD2	12	0.27
(1,1581)	1:A:656:ALA:HB3	1:A:659:ARG:HD3	12	0.27
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD11	16	0.27
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD12	16	0.27
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD13	16	0.27
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD21	16	0.27
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD22	16	0.27
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD23	16	0.27
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD11	19	0.26
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD12	19	0.26
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD13	19	0.26
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD21	19	0.26
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD22	19	0.26
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD23	19	0.26
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD11	8	0.26
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD12	8	0.26
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD13	8	0.26
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD11	8	0.26
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD12	8	0.26
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD13	8	0.26
(1,405)	1:A:556:MET:HE1	1:A:638:PHE:HD1	8	0.26
(1,405)	1:A:556:MET:HE1	1:A:638:PHE:HD2	8	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,405)	1:A:556:MET:HE2	1:A:638:PHE:HD1	8	0.26
(1,405)	1:A:556:MET:HE2	1:A:638:PHE:HD2	8	0.26
(1,405)	1:A:556:MET:HE3	1:A:638:PHE:HD1	8	0.26
(1,405)	1:A:556:MET:HE3	1:A:638:PHE:HD2	8	0.26
(1,209)	1:A:542:MET:HE1	1:A:545:PHE:HD1	16	0.26
(1,209)	1:A:542:MET:HE1	1:A:545:PHE:HD2	16	0.26
(1,209)	1:A:542:MET:HE2	1:A:545:PHE:HD1	16	0.26
(1,209)	1:A:542:MET:HE2	1:A:545:PHE:HD2	16	0.26
(1,209)	1:A:542:MET:HE3	1:A:545:PHE:HD1	16	0.26
(1,209)	1:A:542:MET:HE3	1:A:545:PHE:HD2	16	0.26
(1,1612)	1:A:663:ILE:HA	1:A:663:ILE:HG12	20	0.26
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD11	13	0.26
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD12	13	0.26
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD13	13	0.26
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD21	13	0.26
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD22	13	0.26
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD23	13	0.26
(1,405)	1:A:556:MET:HE1	1:A:638:PHE:HD1	6	0.25
(1,405)	1:A:556:MET:HE1	1:A:638:PHE:HD2	6	0.25
(1,405)	1:A:556:MET:HE2	1:A:638:PHE:HD1	6	0.25
(1,405)	1:A:556:MET:HE2	1:A:638:PHE:HD2	6	0.25
(1,405)	1:A:556:MET:HE3	1:A:638:PHE:HD1	6	0.25
(1,405)	1:A:556:MET:HE3	1:A:638:PHE:HD2	6	0.25
(1,405)	1:A:556:MET:HE1	1:A:638:PHE:HD1	17	0.25
(1,405)	1:A:556:MET:HE1	1:A:638:PHE:HD2	17	0.25
(1,405)	1:A:556:MET:HE2	1:A:638:PHE:HD1	17	0.25
(1,405)	1:A:556:MET:HE2	1:A:638:PHE:HD2	17	0.25
(1,405)	1:A:556:MET:HE3	1:A:638:PHE:HD1	17	0.25
(1,405)	1:A:556:MET:HE3	1:A:638:PHE:HD2	17	0.25
(1,209)	1:A:542:MET:HE1	1:A:545:PHE:HD1	10	0.25
(1,209)	1:A:542:MET:HE1	1:A:545:PHE:HD2	10	0.25
(1,209)	1:A:542:MET:HE2	1:A:545:PHE:HD1	10	0.25
(1,209)	1:A:542:MET:HE2	1:A:545:PHE:HD2	10	0.25
(1,209)	1:A:542:MET:HE3	1:A:545:PHE:HD1	10	0.25
(1,209)	1:A:542:MET:HE3	1:A:545:PHE:HD2	10	0.25
(1,205)	1:A:542:MET:HE1	1:A:543:PRO:HG2	3	0.25
(1,205)	1:A:542:MET:HE1	1:A:543:PRO:HG3	3	0.25
(1,205)	1:A:542:MET:HE2	1:A:543:PRO:HG2	3	0.25
(1,205)	1:A:542:MET:HE2	1:A:543:PRO:HG3	3	0.25
(1,205)	1:A:542:MET:HE3	1:A:543:PRO:HG2	3	0.25
(1,205)	1:A:542:MET:HE3	1:A:543:PRO:HG3	3	0.25
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG21	14	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG22	14	0.25
(1,1514)	1:A:650:ARG:HD2	1:A:654:THR:HG23	14	0.25
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG21	14	0.25
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG22	14	0.25
(1,1514)	1:A:650:ARG:HD3	1:A:654:THR:HG23	14	0.25
(1,1506)	1:A:650:ARG:HB2	1:A:650:ARG:HD2	6	0.25
(1,1506)	1:A:650:ARG:HB2	1:A:650:ARG:HD3	6	0.25
(1,1506)	1:A:650:ARG:HB3	1:A:650:ARG:HD2	6	0.25
(1,1506)	1:A:650:ARG:HB3	1:A:650:ARG:HD3	6	0.25
(1,1506)	1:A:650:ARG:HB2	1:A:650:ARG:HD2	13	0.25
(1,1506)	1:A:650:ARG:HB2	1:A:650:ARG:HD3	13	0.25
(1,1506)	1:A:650:ARG:HB3	1:A:650:ARG:HD2	13	0.25
(1,1506)	1:A:650:ARG:HB3	1:A:650:ARG:HD3	13	0.25
(1,141)	1:A:538:LEU:HD11	1:A:585:GLN:HB2	16	0.25
(1,141)	1:A:538:LEU:HD11	1:A:585:GLN:HB3	16	0.25
(1,141)	1:A:538:LEU:HD12	1:A:585:GLN:HB2	16	0.25
(1,141)	1:A:538:LEU:HD12	1:A:585:GLN:HB3	16	0.25
(1,141)	1:A:538:LEU:HD13	1:A:585:GLN:HB2	16	0.25
(1,141)	1:A:538:LEU:HD13	1:A:585:GLN:HB3	16	0.25
(1,141)	1:A:538:LEU:HD21	1:A:585:GLN:HB2	16	0.25
(1,141)	1:A:538:LEU:HD21	1:A:585:GLN:HB3	16	0.25
(1,141)	1:A:538:LEU:HD22	1:A:585:GLN:HB2	16	0.25
(1,141)	1:A:538:LEU:HD22	1:A:585:GLN:HB3	16	0.25
(1,141)	1:A:538:LEU:HD23	1:A:585:GLN:HB2	16	0.25
(1,141)	1:A:538:LEU:HD23	1:A:585:GLN:HB3	16	0.25
(1,1072)	1:A:594:LYS:HD2	1:A:595:GLY:HA2	9	0.25
(1,1072)	1:A:594:LYS:HD2	1:A:595:GLY:HA3	9	0.25
(1,1072)	1:A:594:LYS:HD3	1:A:595:GLY:HA2	9	0.25
(1,1072)	1:A:594:LYS:HD3	1:A:595:GLY:HA3	9	0.25
(1,1041)	1:A:592:LEU:HD11	1:A:598:GLU:HG2	9	0.25
(1,1041)	1:A:592:LEU:HD12	1:A:598:GLU:HG2	9	0.25
(1,1041)	1:A:592:LEU:HD13	1:A:598:GLU:HG2	9	0.25
(1,1041)	1:A:592:LEU:HD21	1:A:598:GLU:HG2	9	0.25
(1,1041)	1:A:592:LEU:HD22	1:A:598:GLU:HG2	9	0.25
(1,1041)	1:A:592:LEU:HD23	1:A:598:GLU:HG2	9	0.25
(1,842)	1:A:584:ILE:HD11	1:A:607:PHE:HD1	12	0.24
(1,842)	1:A:584:ILE:HD11	1:A:607:PHE:HD2	12	0.24
(1,842)	1:A:584:ILE:HD12	1:A:607:PHE:HD1	12	0.24
(1,842)	1:A:584:ILE:HD12	1:A:607:PHE:HD2	12	0.24
(1,842)	1:A:584:ILE:HD13	1:A:607:PHE:HD1	12	0.24
(1,842)	1:A:584:ILE:HD13	1:A:607:PHE:HD2	12	0.24
(1,577)	1:A:566:GLN:HG2	1:A:627:TYR:HD1	8	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,577)	1:A:566:GLN:HG2	1:A:627:TYR:HD2	8	0.24
(1,577)	1:A:566:GLN:HG3	1:A:627:TYR:HD1	8	0.24
(1,577)	1:A:566:GLN:HG3	1:A:627:TYR:HD2	8	0.24
(1,235)	1:A:544:LEU:HD11	1:A:652:PHE:HD1	11	0.24
(1,235)	1:A:544:LEU:HD11	1:A:652:PHE:HD2	11	0.24
(1,235)	1:A:544:LEU:HD12	1:A:652:PHE:HD1	11	0.24
(1,235)	1:A:544:LEU:HD12	1:A:652:PHE:HD2	11	0.24
(1,235)	1:A:544:LEU:HD13	1:A:652:PHE:HD1	11	0.24
(1,235)	1:A:544:LEU:HD13	1:A:652:PHE:HD2	11	0.24
(1,145)	1:A:538:LEU:HD11	1:A:605:SER:H	15	0.24
(1,145)	1:A:538:LEU:HD12	1:A:605:SER:H	15	0.24
(1,145)	1:A:538:LEU:HD13	1:A:605:SER:H	15	0.24
(1,145)	1:A:538:LEU:HD21	1:A:605:SER:H	15	0.24
(1,145)	1:A:538:LEU:HD22	1:A:605:SER:H	15	0.24
(1,145)	1:A:538:LEU:HD23	1:A:605:SER:H	15	0.24
(1,1043)	1:A:592:LEU:HD11	1:A:599:MET:H	10	0.24
(1,1043)	1:A:592:LEU:HD12	1:A:599:MET:H	10	0.24
(1,1043)	1:A:592:LEU:HD13	1:A:599:MET:H	10	0.24
(1,1043)	1:A:592:LEU:HD21	1:A:599:MET:H	10	0.24
(1,1043)	1:A:592:LEU:HD22	1:A:599:MET:H	10	0.24
(1,1043)	1:A:592:LEU:HD23	1:A:599:MET:H	10	0.24
(1,1039)	1:A:592:LEU:HD11	1:A:593:THR:H	15	0.24
(1,1039)	1:A:592:LEU:HD12	1:A:593:THR:H	15	0.24
(1,1039)	1:A:592:LEU:HD13	1:A:593:THR:H	15	0.24
(1,1039)	1:A:592:LEU:HD21	1:A:593:THR:H	15	0.24
(1,1039)	1:A:592:LEU:HD22	1:A:593:THR:H	15	0.24
(1,1039)	1:A:592:LEU:HD23	1:A:593:THR:H	15	0.24
(1,500)	1:A:562:PHE:HE1	1:A:629:ARG:HG2	6	0.23
(1,500)	1:A:562:PHE:HE1	1:A:629:ARG:HG3	6	0.23
(1,500)	1:A:562:PHE:HE2	1:A:629:ARG:HG2	6	0.23
(1,500)	1:A:562:PHE:HE2	1:A:629:ARG:HG3	6	0.23
(1,405)	1:A:556:MET:HE1	1:A:638:PHE:HD1	1	0.23
(1,405)	1:A:556:MET:HE1	1:A:638:PHE:HD2	1	0.23
(1,405)	1:A:556:MET:HE2	1:A:638:PHE:HD1	1	0.23
(1,405)	1:A:556:MET:HE2	1:A:638:PHE:HD2	1	0.23
(1,405)	1:A:556:MET:HE3	1:A:638:PHE:HD1	1	0.23
(1,405)	1:A:556:MET:HE3	1:A:638:PHE:HD2	1	0.23
(1,405)	1:A:556:MET:HE1	1:A:638:PHE:HD1	14	0.23
(1,405)	1:A:556:MET:HE1	1:A:638:PHE:HD2	14	0.23
(1,405)	1:A:556:MET:HE2	1:A:638:PHE:HD1	14	0.23
(1,405)	1:A:556:MET:HE2	1:A:638:PHE:HD2	14	0.23
(1,405)	1:A:556:MET:HE3	1:A:638:PHE:HD1	14	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,405)	1:A:556:MET:HE3	1:A:638:PHE:HD2	14	0.23
(1,145)	1:A:538:LEU:HD11	1:A:605:SER:H	8	0.23
(1,145)	1:A:538:LEU:HD12	1:A:605:SER:H	8	0.23
(1,145)	1:A:538:LEU:HD13	1:A:605:SER:H	8	0.23
(1,145)	1:A:538:LEU:HD21	1:A:605:SER:H	8	0.23
(1,145)	1:A:538:LEU:HD22	1:A:605:SER:H	8	0.23
(1,145)	1:A:538:LEU:HD23	1:A:605:SER:H	8	0.23
(1,1071)	1:A:594:LYS:HB2	1:A:594:LYS:HD2	19	0.23
(1,1071)	1:A:594:LYS:HB2	1:A:594:LYS:HD3	19	0.23
(1,1071)	1:A:594:LYS:HB3	1:A:594:LYS:HD2	19	0.23
(1,1071)	1:A:594:LYS:HB3	1:A:594:LYS:HD3	19	0.23
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD11	20	0.22
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD12	20	0.22
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD13	20	0.22
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD21	20	0.22
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD22	20	0.22
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD23	20	0.22
(1,500)	1:A:562:PHE:HE1	1:A:629:ARG:HG2	12	0.22
(1,500)	1:A:562:PHE:HE1	1:A:629:ARG:HG3	12	0.22
(1,500)	1:A:562:PHE:HE2	1:A:629:ARG:HG2	12	0.22
(1,500)	1:A:562:PHE:HE2	1:A:629:ARG:HG3	12	0.22
(1,137)	1:A:538:LEU:HD11	1:A:584:ILE:H	9	0.22
(1,137)	1:A:538:LEU:HD12	1:A:584:ILE:H	9	0.22
(1,137)	1:A:538:LEU:HD13	1:A:584:ILE:H	9	0.22
(1,137)	1:A:538:LEU:HD21	1:A:584:ILE:H	9	0.22
(1,137)	1:A:538:LEU:HD22	1:A:584:ILE:H	9	0.22
(1,137)	1:A:538:LEU:HD23	1:A:584:ILE:H	9	0.22
(1,577)	1:A:566:GLN:HG2	1:A:627:TYR:HD1	12	0.21
(1,577)	1:A:566:GLN:HG2	1:A:627:TYR:HD2	12	0.21
(1,577)	1:A:566:GLN:HG3	1:A:627:TYR:HD1	12	0.21
(1,577)	1:A:566:GLN:HG3	1:A:627:TYR:HD2	12	0.21
(1,405)	1:A:556:MET:HE1	1:A:638:PHE:HD1	20	0.21
(1,405)	1:A:556:MET:HE1	1:A:638:PHE:HD2	20	0.21
(1,405)	1:A:556:MET:HE2	1:A:638:PHE:HD1	20	0.21
(1,405)	1:A:556:MET:HE2	1:A:638:PHE:HD2	20	0.21
(1,405)	1:A:556:MET:HE3	1:A:638:PHE:HD1	20	0.21
(1,405)	1:A:556:MET:HE3	1:A:638:PHE:HD2	20	0.21
(1,145)	1:A:538:LEU:HD11	1:A:605:SER:H	14	0.21
(1,145)	1:A:538:LEU:HD12	1:A:605:SER:H	14	0.21
(1,145)	1:A:538:LEU:HD13	1:A:605:SER:H	14	0.21
(1,145)	1:A:538:LEU:HD21	1:A:605:SER:H	14	0.21
(1,145)	1:A:538:LEU:HD22	1:A:605:SER:H	14	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,145)	1:A:538:LEU:HD23	1:A:605:SER:H	14	0.21
(1,1041)	1:A:592:LEU:HD11	1:A:598:GLU:HG2	18	0.21
(1,1041)	1:A:592:LEU:HD12	1:A:598:GLU:HG2	18	0.21
(1,1041)	1:A:592:LEU:HD13	1:A:598:GLU:HG2	18	0.21
(1,1041)	1:A:592:LEU:HD21	1:A:598:GLU:HG2	18	0.21
(1,1041)	1:A:592:LEU:HD22	1:A:598:GLU:HG2	18	0.21
(1,1041)	1:A:592:LEU:HD23	1:A:598:GLU:HG2	18	0.21
(1,986)	1:A:590:SER:HA	1:A:600:LYS:H	16	0.2
(1,577)	1:A:566:GLN:HG2	1:A:627:TYR:HD1	3	0.2
(1,577)	1:A:566:GLN:HG2	1:A:627:TYR:HD2	3	0.2
(1,577)	1:A:566:GLN:HG3	1:A:627:TYR:HD1	3	0.2
(1,577)	1:A:566:GLN:HG3	1:A:627:TYR:HD2	3	0.2
(1,240)	1:A:544:LEU:HD21	1:A:652:PHE:HD1	3	0.2
(1,240)	1:A:544:LEU:HD21	1:A:652:PHE:HD2	3	0.2
(1,240)	1:A:544:LEU:HD22	1:A:652:PHE:HD1	3	0.2
(1,240)	1:A:544:LEU:HD22	1:A:652:PHE:HD2	3	0.2
(1,240)	1:A:544:LEU:HD23	1:A:652:PHE:HD1	3	0.2
(1,240)	1:A:544:LEU:HD23	1:A:652:PHE:HD2	3	0.2
(1,143)	1:A:538:LEU:HD11	1:A:604:GLY:H	11	0.2
(1,143)	1:A:538:LEU:HD12	1:A:604:GLY:H	11	0.2
(1,143)	1:A:538:LEU:HD13	1:A:604:GLY:H	11	0.2
(1,143)	1:A:538:LEU:HD21	1:A:604:GLY:H	11	0.2
(1,143)	1:A:538:LEU:HD22	1:A:604:GLY:H	11	0.2
(1,143)	1:A:538:LEU:HD23	1:A:604:GLY:H	11	0.2
(1,1429)	1:A:643:GLU:HB2	1:A:643:GLU:HG2	1	0.2
(1,1097)	1:A:597:LYS:HB3	1:A:598:GLU:HA	19	0.2
(1,1042)	1:A:592:LEU:HD11	1:A:598:GLU:HB2	20	0.2
(1,1042)	1:A:592:LEU:HD11	1:A:598:GLU:HB3	20	0.2
(1,1042)	1:A:592:LEU:HD12	1:A:598:GLU:HB2	20	0.2
(1,1042)	1:A:592:LEU:HD12	1:A:598:GLU:HB3	20	0.2
(1,1042)	1:A:592:LEU:HD13	1:A:598:GLU:HB2	20	0.2
(1,1042)	1:A:592:LEU:HD13	1:A:598:GLU:HB3	20	0.2
(1,1042)	1:A:592:LEU:HD21	1:A:598:GLU:HB2	20	0.2
(1,1042)	1:A:592:LEU:HD21	1:A:598:GLU:HB3	20	0.2
(1,1042)	1:A:592:LEU:HD22	1:A:598:GLU:HB2	20	0.2
(1,1042)	1:A:592:LEU:HD22	1:A:598:GLU:HB3	20	0.2
(1,1042)	1:A:592:LEU:HD23	1:A:598:GLU:HB2	20	0.2
(1,1042)	1:A:592:LEU:HD23	1:A:598:GLU:HB3	20	0.2
(1,577)	1:A:566:GLN:HG2	1:A:627:TYR:HD1	1	0.19
(1,577)	1:A:566:GLN:HG2	1:A:627:TYR:HD2	1	0.19
(1,577)	1:A:566:GLN:HG3	1:A:627:TYR:HD1	1	0.19
(1,577)	1:A:566:GLN:HG3	1:A:627:TYR:HD2	1	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1041)	1:A:592:LEU:HD11	1:A:598:GLU:HG2	1	0.19
(1,1041)	1:A:592:LEU:HD12	1:A:598:GLU:HG2	1	0.19
(1,1041)	1:A:592:LEU:HD13	1:A:598:GLU:HG2	1	0.19
(1,1041)	1:A:592:LEU:HD21	1:A:598:GLU:HG2	1	0.19
(1,1041)	1:A:592:LEU:HD22	1:A:598:GLU:HG2	1	0.19
(1,1041)	1:A:592:LEU:HD23	1:A:598:GLU:HG2	1	0.19
(1,986)	1:A:590:SER:HA	1:A:600:LYS:H	5	0.18
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD11	5	0.18
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD12	5	0.18
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD13	5	0.18
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD21	5	0.18
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD22	5	0.18
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD23	5	0.18
(1,205)	1:A:542:MET:HE1	1:A:543:PRO:HG2	8	0.18
(1,205)	1:A:542:MET:HE1	1:A:543:PRO:HG3	8	0.18
(1,205)	1:A:542:MET:HE2	1:A:543:PRO:HG2	8	0.18
(1,205)	1:A:542:MET:HE2	1:A:543:PRO:HG3	8	0.18
(1,205)	1:A:542:MET:HE3	1:A:543:PRO:HG2	8	0.18
(1,205)	1:A:542:MET:HE3	1:A:543:PRO:HG3	8	0.18
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD11	14	0.18
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD12	14	0.18
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD13	14	0.18
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD21	14	0.18
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD22	14	0.18
(1,127)	1:A:538:LEU:H	1:A:538:LEU:HD23	14	0.18
(1,1044)	1:A:592:LEU:HD11	1:A:623:ARG:H	9	0.18
(1,1044)	1:A:592:LEU:HD12	1:A:623:ARG:H	9	0.18
(1,1044)	1:A:592:LEU:HD13	1:A:623:ARG:H	9	0.18
(1,1044)	1:A:592:LEU:HD21	1:A:623:ARG:H	9	0.18
(1,1044)	1:A:592:LEU:HD22	1:A:623:ARG:H	9	0.18
(1,1044)	1:A:592:LEU:HD23	1:A:623:ARG:H	9	0.18
(1,1022)	1:A:591:VAL:HG21	1:A:600:LYS:HA	5	0.18
(1,1022)	1:A:591:VAL:HG22	1:A:600:LYS:HA	5	0.18
(1,1022)	1:A:591:VAL:HG23	1:A:600:LYS:HA	5	0.18
(1,1022)	1:A:591:VAL:HG21	1:A:600:LYS:HA	11	0.18
(1,1022)	1:A:591:VAL:HG22	1:A:600:LYS:HA	11	0.18
(1,1022)	1:A:591:VAL:HG23	1:A:600:LYS:HA	11	0.18
(1,1022)	1:A:591:VAL:HG21	1:A:600:LYS:HA	14	0.18
(1,1022)	1:A:591:VAL:HG22	1:A:600:LYS:HA	14	0.18
(1,1022)	1:A:591:VAL:HG23	1:A:600:LYS:HA	14	0.18
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD11	6	0.17
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD12	6	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD13	6	0.17
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD11	6	0.17
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD12	6	0.17
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD13	6	0.17
(1,729)	1:A:577:ILE:HB	1:A:577:ILE:HD11	16	0.17
(1,729)	1:A:577:ILE:HB	1:A:577:ILE:HD12	16	0.17
(1,729)	1:A:577:ILE:HB	1:A:577:ILE:HD13	16	0.17
(1,139)	1:A:538:LEU:HD11	1:A:585:GLN:HA	11	0.17
(1,139)	1:A:538:LEU:HD12	1:A:585:GLN:HA	11	0.17
(1,139)	1:A:538:LEU:HD13	1:A:585:GLN:HA	11	0.17
(1,139)	1:A:538:LEU:HD21	1:A:585:GLN:HA	11	0.17
(1,139)	1:A:538:LEU:HD22	1:A:585:GLN:HA	11	0.17
(1,139)	1:A:538:LEU:HD23	1:A:585:GLN:HA	11	0.17
(1,1327)	1:A:635:VAL:HG21	1:A:636:ASP:HA	5	0.17
(1,1327)	1:A:635:VAL:HG22	1:A:636:ASP:HA	5	0.17
(1,1327)	1:A:635:VAL:HG23	1:A:636:ASP:HA	5	0.17
(1,1185)	1:A:611:CYS:HA	1:A:614:THR:H	20	0.17
(1,1022)	1:A:591:VAL:HG21	1:A:600:LYS:HA	1	0.17
(1,1022)	1:A:591:VAL:HG22	1:A:600:LYS:HA	1	0.17
(1,1022)	1:A:591:VAL:HG23	1:A:600:LYS:HA	1	0.17
(1,1022)	1:A:591:VAL:HG21	1:A:600:LYS:HA	7	0.17
(1,1022)	1:A:591:VAL:HG22	1:A:600:LYS:HA	7	0.17
(1,1022)	1:A:591:VAL:HG23	1:A:600:LYS:HA	7	0.17
(1,1022)	1:A:591:VAL:HG21	1:A:600:LYS:HA	12	0.17
(1,1022)	1:A:591:VAL:HG22	1:A:600:LYS:HA	12	0.17
(1,1022)	1:A:591:VAL:HG23	1:A:600:LYS:HA	12	0.17
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD11	1	0.16
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD12	1	0.16
(1,788)	1:A:582:TYR:HD1	1:A:630:LEU:HD13	1	0.16
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD11	1	0.16
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD12	1	0.16
(1,788)	1:A:582:TYR:HD2	1:A:630:LEU:HD13	1	0.16
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD11	11	0.16
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD12	11	0.16
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD13	11	0.16
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD21	11	0.16
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD22	11	0.16
(1,1592)	1:A:660:LEU:HA	1:A:660:LEU:HD23	11	0.16
(1,1585)	1:A:657:ILE:HB	1:A:657:ILE:HD11	7	0.16
(1,1585)	1:A:657:ILE:HB	1:A:657:ILE:HD12	7	0.16
(1,1585)	1:A:657:ILE:HB	1:A:657:ILE:HD13	7	0.16
(1,1506)	1:A:650:ARG:HB2	1:A:650:ARG:HD2	9	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1506)	1:A:650:ARG:HB2	1:A:650:ARG:HD3	9	0.16
(1,1506)	1:A:650:ARG:HB3	1:A:650:ARG:HD2	9	0.16
(1,1506)	1:A:650:ARG:HB3	1:A:650:ARG:HD3	9	0.16
(1,1383)	1:A:640:GLU:H	1:A:640:GLU:HG2	16	0.16
(1,1327)	1:A:635:VAL:HG21	1:A:636:ASP:HA	6	0.16
(1,1327)	1:A:635:VAL:HG22	1:A:636:ASP:HA	6	0.16
(1,1327)	1:A:635:VAL:HG23	1:A:636:ASP:HA	6	0.16
(1,1327)	1:A:635:VAL:HG21	1:A:636:ASP:HA	17	0.16
(1,1327)	1:A:635:VAL:HG22	1:A:636:ASP:HA	17	0.16
(1,1327)	1:A:635:VAL:HG23	1:A:636:ASP:HA	17	0.16
(1,1264)	1:A:626:THR:H	1:A:628:CYS:HB2	16	0.16
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD11	4	0.16
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD12	4	0.16
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD13	4	0.16
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD21	4	0.16
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD22	4	0.16
(1,124)	1:A:537:LYS:HD2	1:A:538:LEU:HD23	4	0.16
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD11	4	0.16
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD12	4	0.16
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD13	4	0.16
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD21	4	0.16
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD22	4	0.16
(1,124)	1:A:537:LYS:HD3	1:A:538:LEU:HD23	4	0.16
(1,1022)	1:A:591:VAL:HG21	1:A:600:LYS:HA	4	0.16
(1,1022)	1:A:591:VAL:HG22	1:A:600:LYS:HA	4	0.16
(1,1022)	1:A:591:VAL:HG23	1:A:600:LYS:HA	4	0.16
(1,1022)	1:A:591:VAL:HG21	1:A:600:LYS:HA	6	0.16
(1,1022)	1:A:591:VAL:HG22	1:A:600:LYS:HA	6	0.16
(1,1022)	1:A:591:VAL:HG23	1:A:600:LYS:HA	6	0.16
(1,1022)	1:A:591:VAL:HG21	1:A:600:LYS:HA	9	0.16
(1,1022)	1:A:591:VAL:HG22	1:A:600:LYS:HA	9	0.16
(1,1022)	1:A:591:VAL:HG23	1:A:600:LYS:HA	9	0.16
(1,1022)	1:A:591:VAL:HG21	1:A:600:LYS:HA	13	0.16
(1,1022)	1:A:591:VAL:HG22	1:A:600:LYS:HA	13	0.16
(1,1022)	1:A:591:VAL:HG23	1:A:600:LYS:HA	13	0.16
(1,1019)	1:A:591:VAL:HG21	1:A:599:MET:HA	17	0.16
(1,1019)	1:A:591:VAL:HG22	1:A:599:MET:HA	17	0.16
(1,1019)	1:A:591:VAL:HG23	1:A:599:MET:HA	17	0.16
(1,986)	1:A:590:SER:HA	1:A:600:LYS:H	1	0.15
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD11	3	0.15
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD12	3	0.15
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD13	3	0.15

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD21	3	0.15
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD22	3	0.15
(1,439)	1:A:559:LYS:HE2	1:A:633:LEU:HD23	3	0.15
(1,1264)	1:A:626:THR:H	1:A:628:CYS:HB2	1	0.15
(1,1264)	1:A:626:THR:H	1:A:628:CYS:HB2	10	0.15
(1,1041)	1:A:592:LEU:HD11	1:A:598:GLU:HG2	16	0.15
(1,1041)	1:A:592:LEU:HD12	1:A:598:GLU:HG2	16	0.15
(1,1041)	1:A:592:LEU:HD13	1:A:598:GLU:HG2	16	0.15
(1,1041)	1:A:592:LEU:HD21	1:A:598:GLU:HG2	16	0.15
(1,1041)	1:A:592:LEU:HD22	1:A:598:GLU:HG2	16	0.15
(1,1041)	1:A:592:LEU:HD23	1:A:598:GLU:HG2	16	0.15
(1,1022)	1:A:591:VAL:HG21	1:A:600:LYS:HA	2	0.15
(1,1022)	1:A:591:VAL:HG22	1:A:600:LYS:HA	2	0.15
(1,1022)	1:A:591:VAL:HG23	1:A:600:LYS:HA	2	0.15
(1,1022)	1:A:591:VAL:HG21	1:A:600:LYS:HA	16	0.15
(1,1022)	1:A:591:VAL:HG22	1:A:600:LYS:HA	16	0.15
(1,1022)	1:A:591:VAL:HG23	1:A:600:LYS:HA	16	0.15
(1,1022)	1:A:591:VAL:HG21	1:A:600:LYS:HA	17	0.15
(1,1022)	1:A:591:VAL:HG22	1:A:600:LYS:HA	17	0.15
(1,1022)	1:A:591:VAL:HG23	1:A:600:LYS:HA	17	0.15
(1,1019)	1:A:591:VAL:HG21	1:A:599:MET:HA	2	0.15
(1,1019)	1:A:591:VAL:HG22	1:A:599:MET:HA	2	0.15
(1,1019)	1:A:591:VAL:HG23	1:A:599:MET:HA	2	0.15
(1,1019)	1:A:591:VAL:HG21	1:A:599:MET:HA	6	0.15
(1,1019)	1:A:591:VAL:HG22	1:A:599:MET:HA	6	0.15
(1,1019)	1:A:591:VAL:HG23	1:A:599:MET:HA	6	0.15
(1,1019)	1:A:591:VAL:HG21	1:A:599:MET:HA	7	0.15
(1,1019)	1:A:591:VAL:HG22	1:A:599:MET:HA	7	0.15
(1,1019)	1:A:591:VAL:HG23	1:A:599:MET:HA	7	0.15
(1,1015)	1:A:591:VAL:HG11	1:A:593:THR:H	17	0.15
(1,1015)	1:A:591:VAL:HG12	1:A:593:THR:H	17	0.15
(1,1015)	1:A:591:VAL:HG13	1:A:593:THR:H	17	0.15
(1,986)	1:A:590:SER:HA	1:A:600:LYS:H	3	0.14
(1,986)	1:A:590:SER:HA	1:A:600:LYS:H	4	0.14
(1,986)	1:A:590:SER:HA	1:A:600:LYS:H	7	0.14
(1,986)	1:A:590:SER:HA	1:A:600:LYS:H	9	0.14
(1,986)	1:A:590:SER:HA	1:A:600:LYS:H	12	0.14
(1,986)	1:A:590:SER:HA	1:A:600:LYS:H	14	0.14
(1,1427)	1:A:643:GLU:H	1:A:643:GLU:HB2	9	0.14
(1,1427)	1:A:643:GLU:H	1:A:643:GLU:HB2	13	0.14
(1,1327)	1:A:635:VAL:HG21	1:A:636:ASP:HA	1	0.14
(1,1327)	1:A:635:VAL:HG22	1:A:636:ASP:HA	1	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1327)	1:A:635:VAL:HG23	1:A:636:ASP:HA	1	0.14
(1,1327)	1:A:635:VAL:HG21	1:A:636:ASP:HA	8	0.14
(1,1327)	1:A:635:VAL:HG22	1:A:636:ASP:HA	8	0.14
(1,1327)	1:A:635:VAL:HG23	1:A:636:ASP:HA	8	0.14
(1,1327)	1:A:635:VAL:HG21	1:A:636:ASP:HA	15	0.14
(1,1327)	1:A:635:VAL:HG22	1:A:636:ASP:HA	15	0.14
(1,1327)	1:A:635:VAL:HG23	1:A:636:ASP:HA	15	0.14
(1,1264)	1:A:626:THR:H	1:A:628:CYS:HB2	5	0.14
(1,1044)	1:A:592:LEU:HD11	1:A:623:ARG:H	4	0.14
(1,1044)	1:A:592:LEU:HD12	1:A:623:ARG:H	4	0.14
(1,1044)	1:A:592:LEU:HD13	1:A:623:ARG:H	4	0.14
(1,1044)	1:A:592:LEU:HD21	1:A:623:ARG:H	4	0.14
(1,1044)	1:A:592:LEU:HD22	1:A:623:ARG:H	4	0.14
(1,1044)	1:A:592:LEU:HD23	1:A:623:ARG:H	4	0.14
(1,1022)	1:A:591:VAL:HG21	1:A:600:LYS:HA	3	0.14
(1,1022)	1:A:591:VAL:HG22	1:A:600:LYS:HA	3	0.14
(1,1022)	1:A:591:VAL:HG23	1:A:600:LYS:HA	3	0.14
(1,986)	1:A:590:SER:HA	1:A:600:LYS:H	2	0.13
(1,986)	1:A:590:SER:HA	1:A:600:LYS:H	11	0.13
(1,728)	1:A:577:ILE:HA	1:A:618:ARG:H	16	0.13
(1,696)	1:A:574:GLU:HA	1:A:579:LYS:HD2	9	0.13
(1,696)	1:A:574:GLU:HA	1:A:579:LYS:HD3	9	0.13
(1,1506)	1:A:650:ARG:HB2	1:A:650:ARG:HD2	14	0.13
(1,1506)	1:A:650:ARG:HB2	1:A:650:ARG:HD3	14	0.13
(1,1506)	1:A:650:ARG:HB3	1:A:650:ARG:HD2	14	0.13
(1,1506)	1:A:650:ARG:HB3	1:A:650:ARG:HD3	14	0.13
(1,1264)	1:A:626:THR:H	1:A:628:CYS:HB2	4	0.13
(1,1264)	1:A:626:THR:H	1:A:628:CYS:HB2	11	0.13
(1,1127)	1:A:600:LYS:HD3	1:A:601:LEU:H	13	0.13
(1,1043)	1:A:592:LEU:HD11	1:A:599:MET:H	19	0.13
(1,1043)	1:A:592:LEU:HD12	1:A:599:MET:H	19	0.13
(1,1043)	1:A:592:LEU:HD13	1:A:599:MET:H	19	0.13
(1,1043)	1:A:592:LEU:HD21	1:A:599:MET:H	19	0.13
(1,1043)	1:A:592:LEU:HD22	1:A:599:MET:H	19	0.13
(1,1043)	1:A:592:LEU:HD23	1:A:599:MET:H	19	0.13
(1,1019)	1:A:591:VAL:HG21	1:A:599:MET:HA	5	0.13
(1,1019)	1:A:591:VAL:HG22	1:A:599:MET:HA	5	0.13
(1,1019)	1:A:591:VAL:HG23	1:A:599:MET:HA	5	0.13
(1,1015)	1:A:591:VAL:HG11	1:A:593:THR:H	2	0.13
(1,1015)	1:A:591:VAL:HG12	1:A:593:THR:H	2	0.13
(1,1015)	1:A:591:VAL:HG13	1:A:593:THR:H	2	0.13
(1,986)	1:A:590:SER:HA	1:A:600:LYS:H	6	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,986)	1:A:590:SER:HA	1:A:600:LYS:H	17	0.12
(1,743)	1:A:578:GLY:H	1:A:579:LYS:HA	16	0.12
(1,653)	1:A:572:ILE:H	1:A:572:ILE:HG12	14	0.12
(1,205)	1:A:542:MET:HE1	1:A:543:PRO:HG2	9	0.12
(1,205)	1:A:542:MET:HE1	1:A:543:PRO:HG3	9	0.12
(1,205)	1:A:542:MET:HE2	1:A:543:PRO:HG2	9	0.12
(1,205)	1:A:542:MET:HE2	1:A:543:PRO:HG3	9	0.12
(1,205)	1:A:542:MET:HE3	1:A:543:PRO:HG2	9	0.12
(1,205)	1:A:542:MET:HE3	1:A:543:PRO:HG3	9	0.12
(1,1619)	1:A:663:ILE:HG21	1:A:663:ILE:HG13	1	0.12
(1,1619)	1:A:663:ILE:HG22	1:A:663:ILE:HG13	1	0.12
(1,1619)	1:A:663:ILE:HG23	1:A:663:ILE:HG13	1	0.12
(1,1429)	1:A:643:GLU:HB2	1:A:643:GLU:HG2	4	0.12
(1,1264)	1:A:626:THR:H	1:A:628:CYS:HB2	19	0.12
(1,118)	1:A:537:LYS:HA	1:A:537:LYS:HD2	19	0.12
(1,118)	1:A:537:LYS:HA	1:A:537:LYS:HD3	19	0.12
(1,1015)	1:A:591:VAL:HG11	1:A:593:THR:H	1	0.12
(1,1015)	1:A:591:VAL:HG12	1:A:593:THR:H	1	0.12
(1,1015)	1:A:591:VAL:HG13	1:A:593:THR:H	1	0.12
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD11	10	0.11
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD12	10	0.11
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD13	10	0.11
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD21	10	0.11
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD22	10	0.11
(1,994)	1:A:590:SER:HB3	1:A:592:LEU:HD23	10	0.11
(1,696)	1:A:574:GLU:HA	1:A:579:LYS:HD2	12	0.11
(1,696)	1:A:574:GLU:HA	1:A:579:LYS:HD3	12	0.11
(1,567)	1:A:566:GLN:HA	1:A:627:TYR:HB3	18	0.11
(1,257)	1:A:546:ALA:H	1:A:547:ASN:HB3	3	0.11
(1,1588)	1:A:659:ARG:H	1:A:659:ARG:HB2	1	0.11
(1,1588)	1:A:659:ARG:H	1:A:659:ARG:HB2	14	0.11
(1,1427)	1:A:643:GLU:H	1:A:643:GLU:HB2	14	0.11
(1,140)	1:A:538:LEU:HD11	1:A:585:GLN:HG2	12	0.11
(1,140)	1:A:538:LEU:HD12	1:A:585:GLN:HG2	12	0.11
(1,140)	1:A:538:LEU:HD13	1:A:585:GLN:HG2	12	0.11
(1,140)	1:A:538:LEU:HD21	1:A:585:GLN:HG2	12	0.11
(1,140)	1:A:538:LEU:HD22	1:A:585:GLN:HG2	12	0.11
(1,140)	1:A:538:LEU:HD23	1:A:585:GLN:HG2	12	0.11
(1,140)	1:A:538:LEU:HD11	1:A:585:GLN:HG3	12	0.11
(1,140)	1:A:538:LEU:HD12	1:A:585:GLN:HG3	12	0.11
(1,140)	1:A:538:LEU:HD13	1:A:585:GLN:HG3	12	0.11
(1,140)	1:A:538:LEU:HD21	1:A:585:GLN:HG3	12	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,140)	1:A:538:LEU:HD22	1:A:585:GLN:HG3	12	0.11
(1,140)	1:A:538:LEU:HD23	1:A:585:GLN:HG3	12	0.11
(1,1392)	1:A:640:GLU:HB3	1:A:641:VAL:HG11	4	0.11
(1,1392)	1:A:640:GLU:HB3	1:A:641:VAL:HG12	4	0.11
(1,1392)	1:A:640:GLU:HB3	1:A:641:VAL:HG13	4	0.11
(1,1317)	1:A:635:VAL:H	1:A:636:ASP:HB2	4	0.11
(1,1127)	1:A:600:LYS:HD3	1:A:601:LEU:H	11	0.11
(1,1127)	1:A:600:LYS:HD3	1:A:601:LEU:H	17	0.11
(1,1106)	1:A:598:GLU:HG3	1:A:599:MET:H	3	0.11
(1,1100)	1:A:597:LYS:HG2	1:A:597:LYS:HE2	2	0.11
(1,1100)	1:A:597:LYS:HG2	1:A:597:LYS:HE3	2	0.11
(1,1100)	1:A:597:LYS:HG3	1:A:597:LYS:HE2	2	0.11
(1,1100)	1:A:597:LYS:HG3	1:A:597:LYS:HE3	2	0.11
(1,1074)	1:A:595:GLY:HA2	1:A:596:ASN:HB3	10	0.11
(1,1074)	1:A:595:GLY:HA3	1:A:596:ASN:HB3	10	0.11
(1,1074)	1:A:595:GLY:HA2	1:A:596:ASN:HB3	17	0.11
(1,1074)	1:A:595:GLY:HA3	1:A:596:ASN:HB3	17	0.11
(1,1045)	1:A:592:LEU:HD11	1:A:623:ARG:HD2	16	0.11
(1,1045)	1:A:592:LEU:HD12	1:A:623:ARG:HD2	16	0.11
(1,1045)	1:A:592:LEU:HD13	1:A:623:ARG:HD2	16	0.11
(1,1045)	1:A:592:LEU:HD21	1:A:623:ARG:HD2	16	0.11
(1,1045)	1:A:592:LEU:HD22	1:A:623:ARG:HD2	16	0.11
(1,1045)	1:A:592:LEU:HD23	1:A:623:ARG:HD2	16	0.11
(1,1045)	1:A:592:LEU:HD11	1:A:623:ARG:HD3	16	0.11
(1,1045)	1:A:592:LEU:HD12	1:A:623:ARG:HD3	16	0.11
(1,1045)	1:A:592:LEU:HD13	1:A:623:ARG:HD3	16	0.11
(1,1045)	1:A:592:LEU:HD21	1:A:623:ARG:HD3	16	0.11
(1,1045)	1:A:592:LEU:HD22	1:A:623:ARG:HD3	16	0.11
(1,1045)	1:A:592:LEU:HD23	1:A:623:ARG:HD3	16	0.11
(1,1019)	1:A:591:VAL:HG21	1:A:599:MET:HA	1	0.11
(1,1019)	1:A:591:VAL:HG22	1:A:599:MET:HA	1	0.11
(1,1019)	1:A:591:VAL:HG23	1:A:599:MET:HA	1	0.11
(1,1019)	1:A:591:VAL:HG21	1:A:599:MET:HA	12	0.11
(1,1019)	1:A:591:VAL:HG22	1:A:599:MET:HA	12	0.11
(1,1019)	1:A:591:VAL:HG23	1:A:599:MET:HA	12	0.11
(1,1019)	1:A:591:VAL:HG21	1:A:599:MET:HA	14	0.11
(1,1019)	1:A:591:VAL:HG22	1:A:599:MET:HA	14	0.11
(1,1019)	1:A:591:VAL:HG23	1:A:599:MET:HA	14	0.11
(1,1019)	1:A:591:VAL:HG21	1:A:599:MET:HA	16	0.11
(1,1019)	1:A:591:VAL:HG22	1:A:599:MET:HA	16	0.11
(1,1019)	1:A:591:VAL:HG23	1:A:599:MET:HA	16	0.11
(1,1015)	1:A:591:VAL:HG11	1:A:593:THR:H	7	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1015)	1:A:591:VAL:HG12	1:A:593:THR:H	7	0.11
(1,1015)	1:A:591:VAL:HG13	1:A:593:THR:H	7	0.11
(1,1015)	1:A:591:VAL:HG11	1:A:593:THR:H	9	0.11
(1,1015)	1:A:591:VAL:HG12	1:A:593:THR:H	9	0.11
(1,1015)	1:A:591:VAL:HG13	1:A:593:THR:H	9	0.11
(1,1014)	1:A:591:VAL:HG11	1:A:592:LEU:HA	14	0.11
(1,1014)	1:A:591:VAL:HG12	1:A:592:LEU:HA	14	0.11
(1,1014)	1:A:591:VAL:HG13	1:A:592:LEU:HA	14	0.11

10 Dihedral-angle violation analysis ⓘ

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value