



Full wwPDB NMR Structure Validation Report ⓘ

Mar 23, 2026 – 06:47 AM UTC

PDB ID : 2BZE / pdb_00002bze
BMRB ID : 7351
Title : NMR Structure of human RTF1 PLUS3 domain.
Authors : Truffault, V.; Diercks, T.; Ab, E.; De Jong, R.N.; Daniels, M.A.; Kaptein, R.;
Folkers, G.E.; Structural Proteomics in Europe (SPINE)
Deposited on : 2005-08-16

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 ⓘ symbol.

The types of validation reports are described at

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

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

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

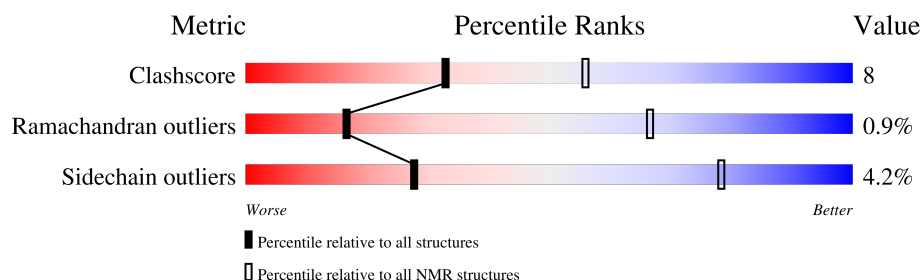
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 91%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	153	

2 Ensemble composition and analysis

This entry contains 25 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:-1-A:-1, A:345-A:365, A:370-A:382, A:392-A:476 (120)	0.52	10

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

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

NmrClust was unable to cluster the ensemble.

Error message: 1 Unexpected character

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2451 atoms, of which 1220 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called KIAA0252 PROTEIN.

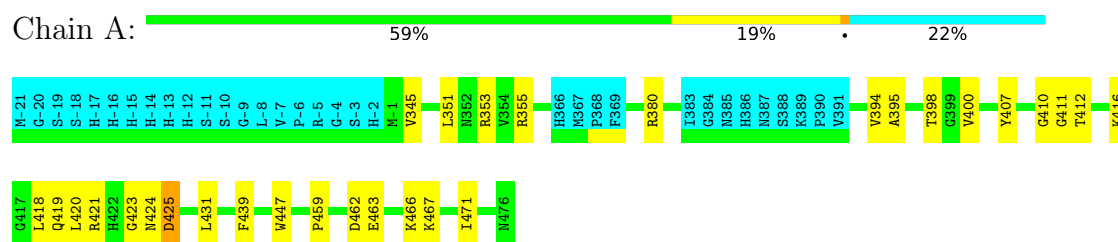
Mol	Chain	Residues	Atoms						Trace
1	A	153	Total	C	H	N	O	S	0
			2451	773	1220	233	217	8	

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: KIAA0252 PROTEIN

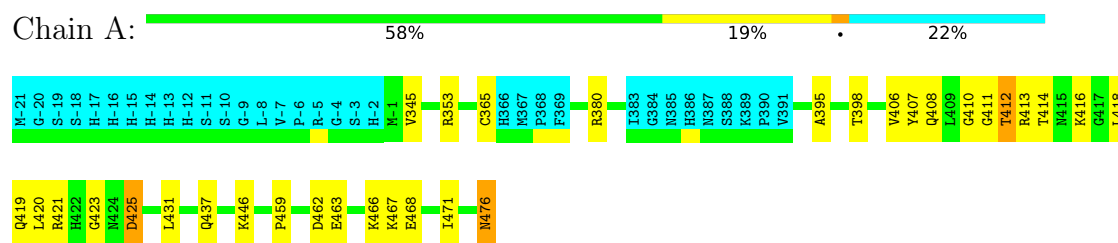


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

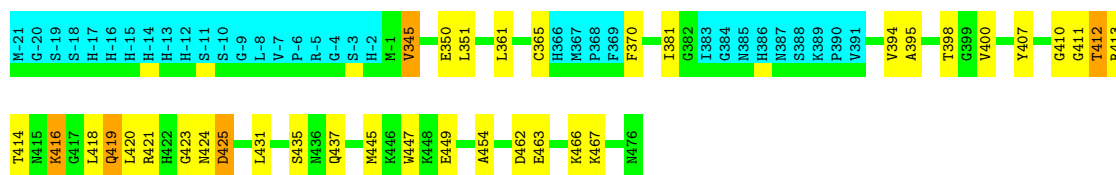
• Molecule 1: KIAA0252 PROTEIN



4.2.2 Score per residue for model 2

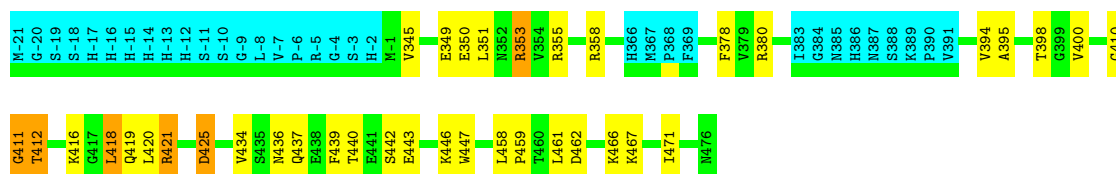
• Molecule 1: KIAA0252 PROTEIN





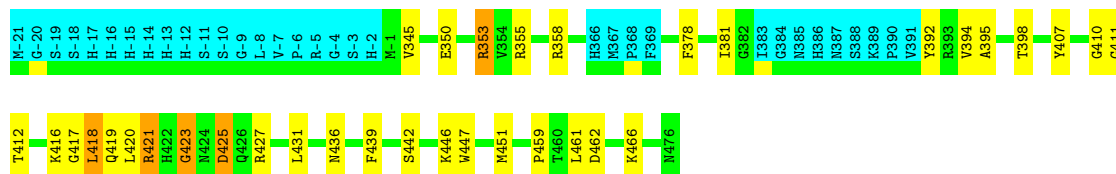
4.2.3 Score per residue for model 3

- Molecule 1: KIAA0252 PROTEIN



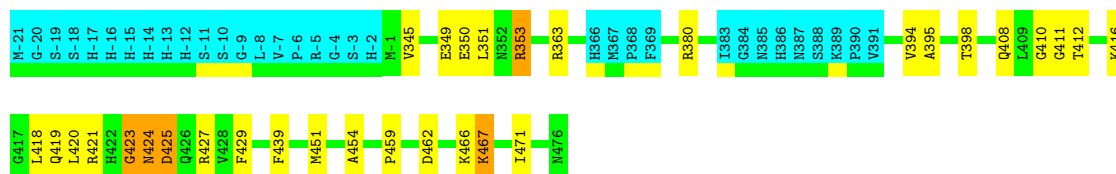
4.2.4 Score per residue for model 4

- Molecule 1: KIAA0252 PROTEIN



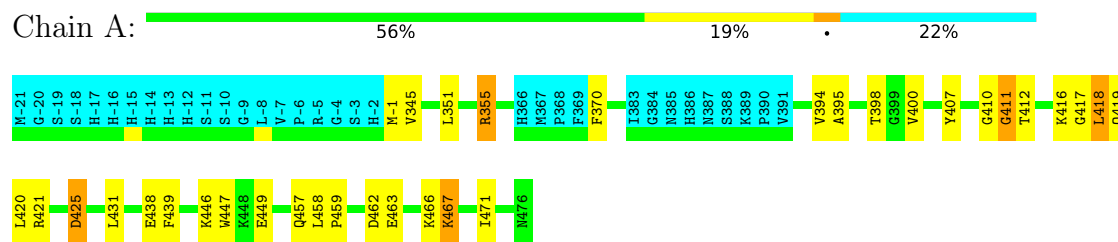
4.2.5 Score per residue for model 5

- Molecule 1: KIAA0252 PROTEIN



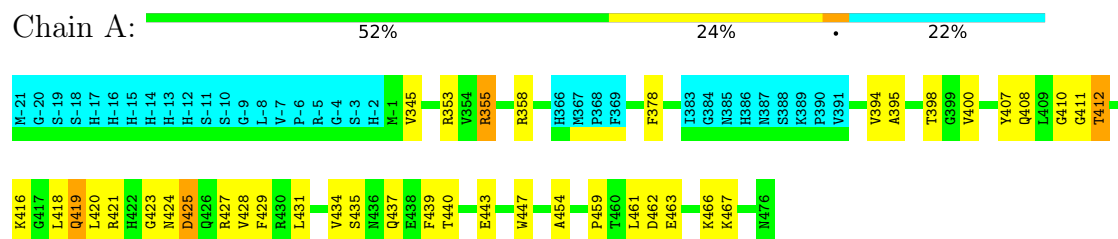
4.2.6 Score per residue for model 6

- Molecule 1: KIAA0252 PROTEIN



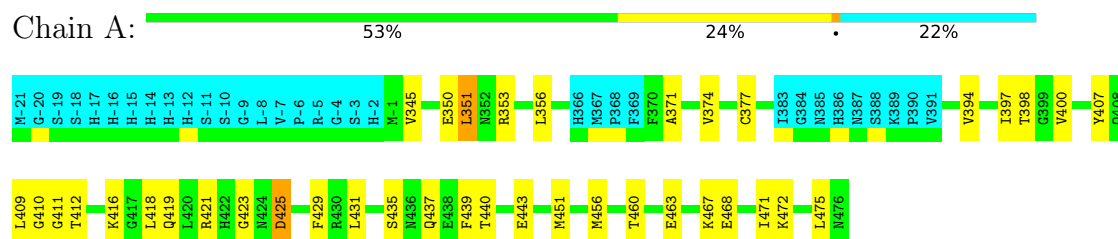
4.2.7 Score per residue for model 7

- Molecule 1: KIAA0252 PROTEIN



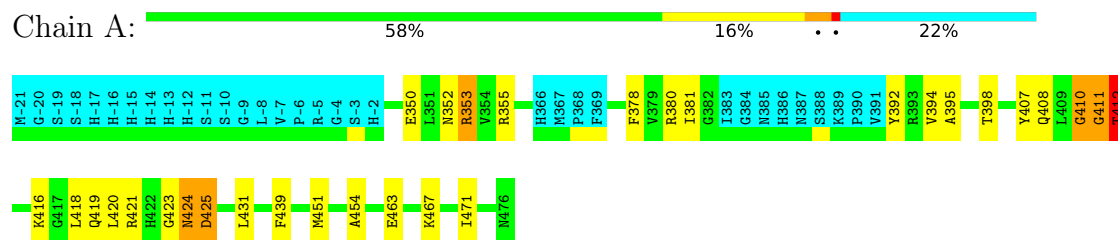
4.2.8 Score per residue for model 8

- Molecule 1: KIAA0252 PROTEIN



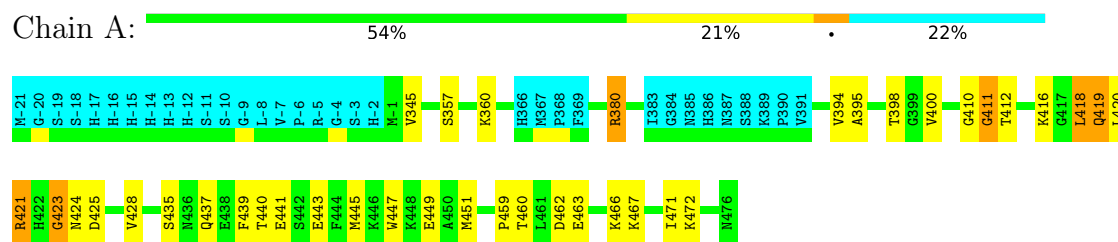
4.2.9 Score per residue for model 9

- Molecule 1: KIAA0252 PROTEIN



4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: KIAA0252 PROTEIN



4.2.11 Score per residue for model 11

- Molecule 1: KIAA0252 PROTEIN



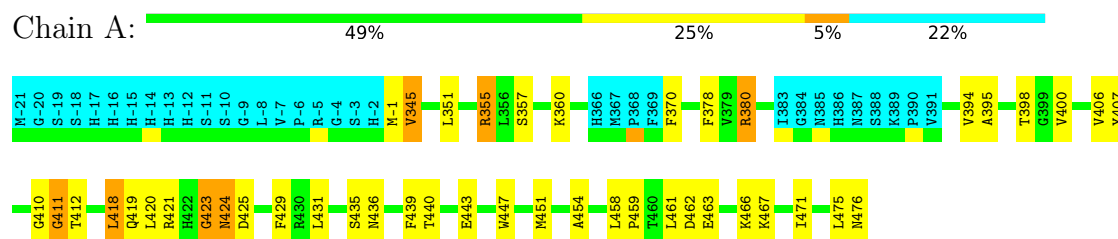
4.2.12 Score per residue for model 12

- Molecule 1: KIAA0252 PROTEIN



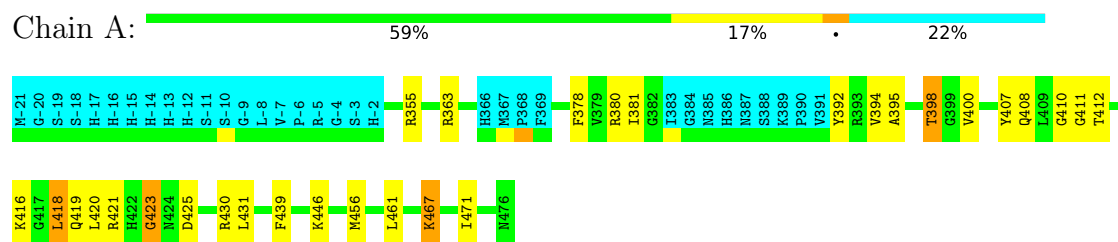
4.2.13 Score per residue for model 13

- Molecule 1: KIAA0252 PROTEIN



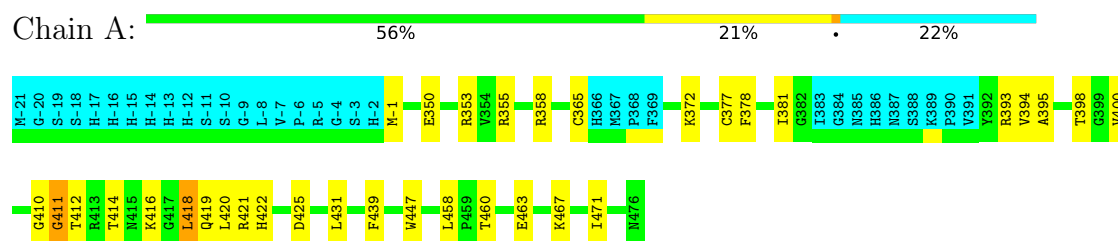
4.2.14 Score per residue for model 14

- Molecule 1: KIAA0252 PROTEIN



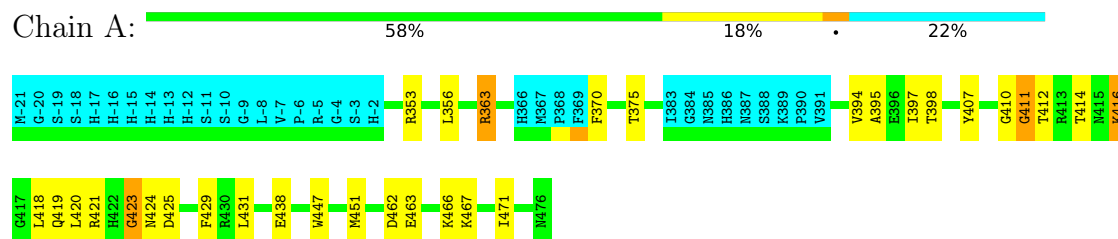
4.2.15 Score per residue for model 15

- Molecule 1: KIAA0252 PROTEIN



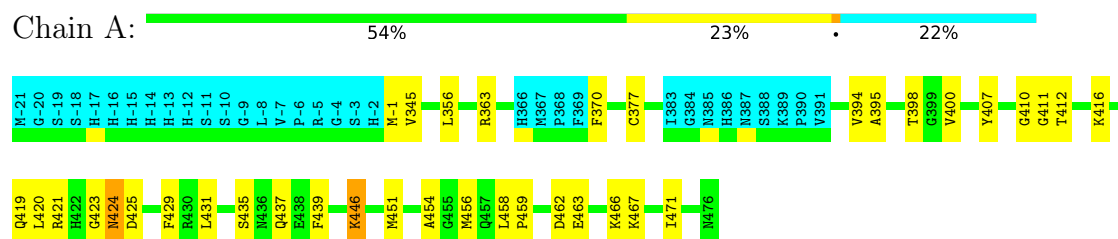
4.2.16 Score per residue for model 16

- Molecule 1: KIAA0252 PROTEIN



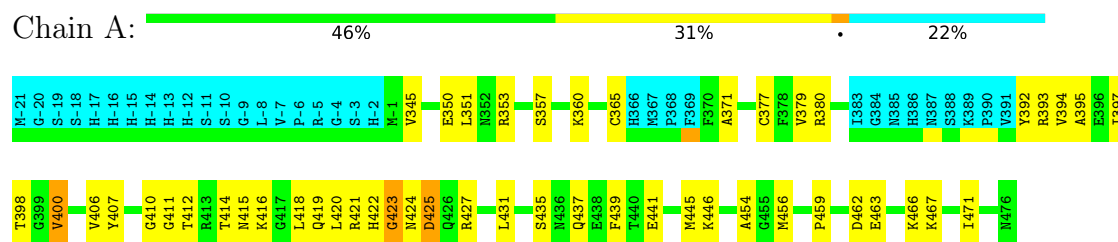
4.2.17 Score per residue for model 17

- Molecule 1: KIAA0252 PROTEIN



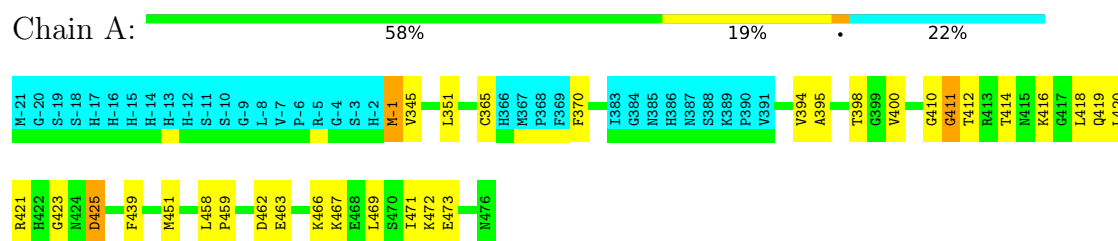
4.2.18 Score per residue for model 18

- Molecule 1: KIAA0252 PROTEIN



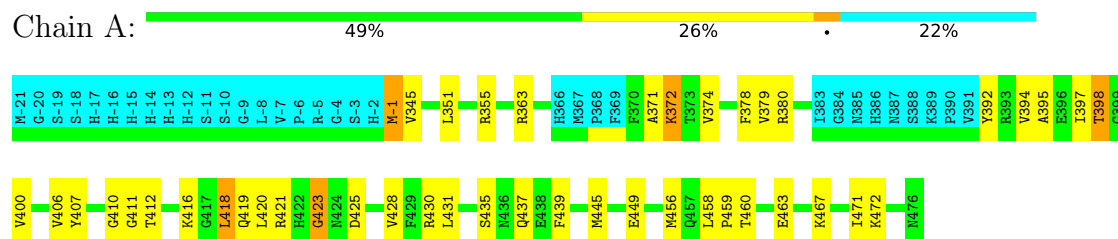
4.2.19 Score per residue for model 19

- Molecule 1: KIAA0252 PROTEIN



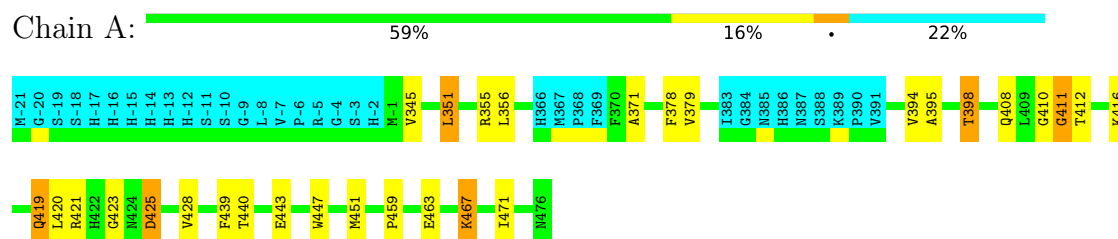
4.2.20 Score per residue for model 20

- Molecule 1: KIAA0252 PROTEIN



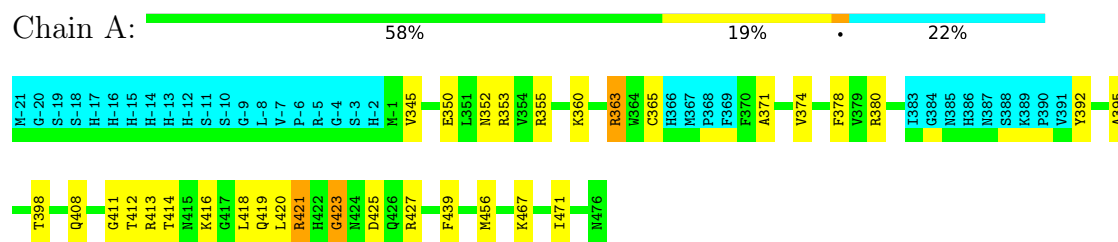
4.2.21 Score per residue for model 21

- Molecule 1: KIAA0252 PROTEIN



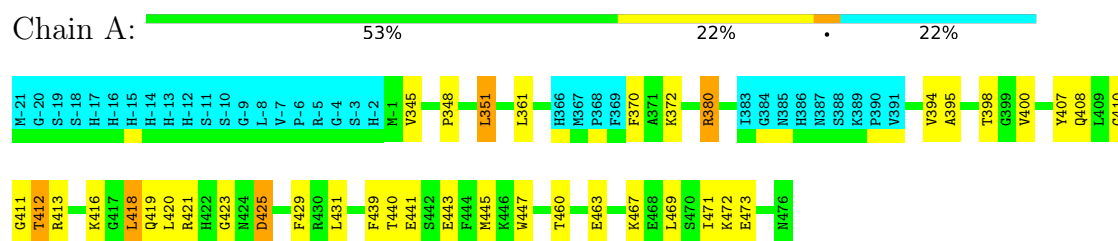
4.2.22 Score per residue for model 22

- Molecule 1: KIAA0252 PROTEIN



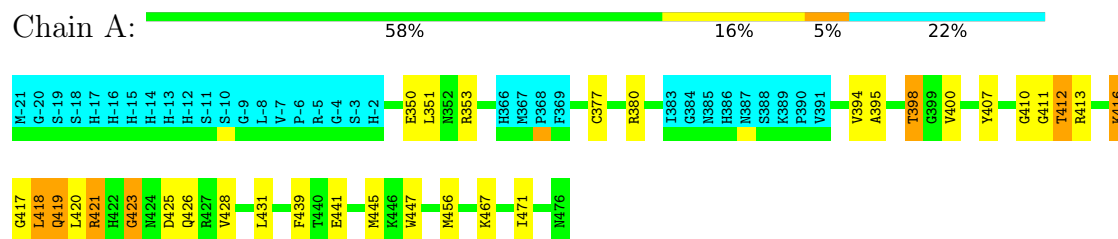
4.2.23 Score per residue for model 23

- Molecule 1: KIAA0252 PROTEIN



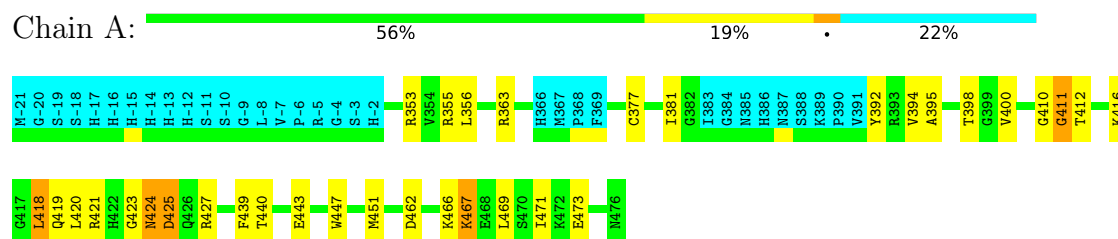
4.2.24 Score per residue for model 24

- Molecule 1: KIAA0252 PROTEIN



4.2.25 Score per residue for model 25

- Molecule 1: KIAA0252 PROTEIN



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 25 were deposited, based on the following criterion: *LOW ENERGY*.

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

Software name	Classification	Version
CNS	refinement	
Sparky	structure solution	
CYANA	structure solution	

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	1828
Number of shifts mapped to atoms	1828
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

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	1.28±0.03	4±1/991 (0.4± 0.1%)	1.06±0.02	1±1/1329 (0.1± 0.1%)
All	All	1.28	107/24775 (0.4%)	1.06	19/33225 (0.1%)

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	1.8±0.9
All	All	0	44

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	412	THR	N-CA	-10.14	1.33	1.46	15	25
1	A	456	MET	N-CA	-7.18	1.36	1.45	8	3
1	A	381	ILE	C-N	-7.02	1.30	1.33	15	2
1	A	411	GLY	C-N	-6.68	1.25	1.33	15	10
1	A	423	GLY	C-N	-6.51	1.25	1.33	13	14
1	A	446	LYS	N-CA	-6.50	1.38	1.46	1	3
1	A	370	PHE	N-CA	-6.37	1.37	1.46	23	4
1	A	425	ASP	CA-C	-6.29	1.45	1.53	1	5
1	A	418	LEU	CA-C	-5.97	1.45	1.52	20	10
1	A	400	VAL	N-CA	-5.69	1.39	1.46	17	2
1	A	425	ASP	C-N	-5.63	1.24	1.33	4	13
1	A	413	ARG	CA-C	-5.63	1.46	1.53	22	1
1	A	416	LYS	C-N	-5.53	1.28	1.33	24	1
1	A	417	GLY	C-N	-5.43	1.25	1.33	24	2
1	A	-1	MET	CA-C	-5.43	1.46	1.52	20	1
1	A	398	THR	N-CA	-5.23	1.39	1.46	21	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	397	ILE	C-N	-5.18	1.27	1.33	8	1
1	A	348	PRO	C-O	-5.18	1.17	1.24	23	1
1	A	356	LEU	N-CA	-5.17	1.39	1.46	11	1
1	A	409	LEU	C-N	5.14	1.41	1.33	8	1
1	A	427	ARG	C-N	-5.11	1.27	1.33	22	1
1	A	380	ARG	NE-CZ	5.07	1.38	1.33	11	1
1	A	417	GLY	CA-C	-5.03	1.47	1.52	6	1

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(°)	Ideal(°)	Models	
								Worst	Total
1	A	424	ASN	CA-CB-CG	6.26	118.86	112.60	13	5
1	A	411	GLY	CA-C-N	6.17	131.53	122.39	15	3
1	A	411	GLY	C-N-CA	6.17	131.53	122.39	15	3
1	A	412	THR	N-CA-CB	-5.67	101.53	110.77	15	2
1	A	456	MET	N-CA-CB	-5.34	101.92	110.46	17	2
1	A	370	PHE	CA-CB-CG	5.24	119.04	113.80	17	2
1	A	409	LEU	CA-C-O	-5.21	115.53	121.68	8	1
1	A	412	THR	N-CA-C	-5.07	101.37	109.23	20	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	410	GLY	Peptide	24
1	A	353	ARG	Sidechain	8
1	A	421	ARG	Sidechain	5
1	A	427	ARG	Sidechain	3
1	A	380	ARG	Sidechain	3
1	A	363	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	975	990	990	17±3
All	All	24375	24750	24750	415

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:407:TYR:OH	1:A:431:LEU:HG	0.65	1.89	1	16
1:A:421:ARG:HA	1:A:425:ASP:O	0.65	1.92	2	25
1:A:371:ALA:HB2	1:A:400:VAL:HG12	0.65	1.66	18	1
1:A:398:THR:O	1:A:419:GLN:HB3	0.61	1.96	2	25
1:A:380:ARG:HD3	1:A:439:PHE:CZ	0.60	2.32	9	2
1:A:423:GLY:HA2	1:A:451:MET:SD	0.59	2.37	17	12
1:A:395:ALA:HB1	1:A:420:LEU:HB3	0.59	1.74	21	24
1:A:462:ASP:O	1:A:466:LYS:HD3	0.58	1.98	16	3
1:A:-1:MET:SD	1:A:458:LEU:HB2	0.58	2.39	15	6
1:A:394:VAL:HG22	1:A:439:PHE:CE1	0.58	2.34	13	12
1:A:440:THR:OG1	1:A:443:GLU:HG2	0.58	1.99	25	8
1:A:365:CYS:SG	1:A:414:THR:HB	0.58	2.38	18	4
1:A:355:ARG:HA	1:A:378:PHE:O	0.57	1.99	15	10
1:A:394:VAL:HG22	1:A:439:PHE:CE2	0.57	2.35	15	8
1:A:467:LYS:O	1:A:471:ILE:HG12	0.56	2.00	17	15
1:A:350:GLU:O	1:A:353:ARG:HG2	0.56	2.01	3	9
1:A:407:TYR:CE2	1:A:430:ARG:HD2	0.56	2.35	20	1
1:A:419:GLN:NE2	1:A:428:VAL:HB	0.55	2.17	12	1
1:A:400:VAL:HG22	1:A:418:LEU:CD2	0.55	2.31	6	7
1:A:345:VAL:HG23	1:A:459:PRO:O	0.55	2.02	3	6
1:A:468:GLU:O	1:A:472:LYS:HG3	0.55	2.02	8	1
1:A:469:LEU:O	1:A:473:GLU:HG2	0.54	2.02	19	4
1:A:407:TYR:CD2	1:A:430:ARG:HD2	0.54	2.37	14	1
1:A:392:TYR:CE1	1:A:435:SER:HB2	0.54	2.37	18	2
1:A:445:MET:O	1:A:449:GLU:HG3	0.54	2.03	10	3
1:A:427:ARG:HD2	1:A:429:PHE:CZ	0.54	2.37	7	2
1:A:377:CYS:SG	1:A:471:ILE:HD11	0.54	2.43	18	5
1:A:345:VAL:HG12	1:A:459:PRO:O	0.53	2.03	13	6
1:A:462:ASP:O	1:A:466:LYS:HG2	0.53	2.03	3	12
1:A:463:GLU:O	1:A:467:LYS:HG2	0.53	2.03	9	13
1:A:410:GLY:O	1:A:412:THR:HB	0.53	2.03	9	1
1:A:435:SER:HB3	1:A:437:GLN:OE1	0.53	2.04	2	1
1:A:424:ASN:HB2	1:A:454:ALA:CB	0.52	2.34	18	3
1:A:351:LEU:HD21	1:A:394:VAL:HG11	0.52	1.80	24	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:345:VAL:HG11	1:A:351:LEU:HD23	0.52	1.81	21	3
1:A:380:ARG:NH1	1:A:437:GLN:HB2	0.52	2.20	1	4
1:A:356:LEU:HD21	1:A:471:ILE:HD12	0.51	1.83	25	4
1:A:400:VAL:HG22	1:A:418:LEU:CD1	0.51	2.36	13	8
1:A:357:SER:OG	1:A:360:LYS:HG3	0.51	2.05	10	3
1:A:419:GLN:NE2	1:A:428:VAL:HG22	0.50	2.22	10	5
1:A:393:ARG:HB3	1:A:422:HIS:CD2	0.50	2.41	18	1
1:A:467:LYS:HA	1:A:467:LYS:HE3	0.49	1.84	6	2
1:A:424:ASN:HB2	1:A:454:ALA:HB2	0.49	1.82	18	1
1:A:365:CYS:SG	1:A:414:THR:HG21	0.49	2.48	15	2
1:A:407:TYR:CE2	1:A:430:ARG:HB3	0.48	2.43	12	1
1:A:380:ARG:HG3	1:A:439:PHE:CZ	0.48	2.43	24	1
1:A:435:SER:HB3	1:A:437:GLN:NE2	0.48	2.24	17	2
1:A:394:VAL:HB	1:A:447:TRP:CB	0.47	2.38	3	2
1:A:377:CYS:SG	1:A:467:LYS:HB3	0.47	2.49	17	2
1:A:421:ARG:NH1	1:A:426:GLN:HG3	0.47	2.24	24	1
1:A:394:VAL:HB	1:A:447:TRP:HB2	0.47	1.86	7	10
1:A:424:ASN:HB3	1:A:454:ALA:HB1	0.47	1.86	5	2
1:A:467:LYS:O	1:A:471:ILE:HG13	0.47	2.09	22	5
1:A:424:ASN:HB3	1:A:454:ALA:CB	0.47	2.39	5	1
1:A:394:VAL:HB	1:A:447:TRP:CG	0.47	2.44	3	4
1:A:371:ALA:HB2	1:A:400:VAL:CG1	0.47	2.39	18	1
1:A:358:ARG:HD3	1:A:434:VAL:O	0.47	2.10	7	2
1:A:461:LEU:H	1:A:461:LEU:HD22	0.47	1.70	4	4
1:A:380:ARG:HD3	1:A:439:PHE:CE2	0.46	2.44	9	1
1:A:442:SER:O	1:A:446:LYS:HG3	0.46	2.10	4	3
1:A:351:LEU:HD13	1:A:394:VAL:HG11	0.46	1.87	3	1
1:A:372:LYS:HD3	1:A:372:LYS:C	0.46	2.36	15	1
1:A:351:LEU:HD11	1:A:447:TRP:CZ3	0.46	2.45	3	2
1:A:371:ALA:HA	1:A:374:VAL:HG22	0.46	1.87	22	4
1:A:424:ASN:HB2	1:A:454:ALA:HB1	0.46	1.88	13	1
1:A:380:ARG:HD2	1:A:392:TYR:HB3	0.46	1.86	22	1
1:A:345:VAL:CG1	1:A:459:PRO:HD2	0.46	2.41	20	3
1:A:400:VAL:HG22	1:A:418:LEU:HD13	0.45	1.88	10	7
1:A:475:LEU:HD12	1:A:476:ASN:N	0.45	2.26	13	2
1:A:406:VAL:HG22	1:A:415:ASN:HB3	0.45	1.88	18	1
1:A:412:THR:C	1:A:413:ARG:HD2	0.45	2.37	23	5
1:A:400:VAL:HG13	1:A:416:LYS:HZ3	0.45	1.72	2	1
1:A:442:SER:O	1:A:446:LYS:HG2	0.45	2.12	3	1
1:A:380:ARG:HH11	1:A:437:GLN:HB2	0.45	1.72	10	1
1:A:423:GLY:O	1:A:456:MET:HE2	0.44	2.12	20	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:457:GLN:HG2	1:A:458:LEU:O	0.44	2.12	6	1
1:A:441:GLU:O	1:A:445:MET:HG3	0.44	2.12	23	3
1:A:352:ASN:HA	1:A:355:ARG:HB2	0.44	1.88	22	2
1:A:361:LEU:HD13	1:A:431:LEU:HD22	0.44	1.90	2	2
1:A:380:ARG:HB3	1:A:435:SER:OG	0.44	2.12	13	1
1:A:358:ARG:HB2	1:A:431:LEU:O	0.44	2.12	15	1
1:A:414:THR:OG1	1:A:416:LYS:HG3	0.44	2.13	16	1
1:A:460:THR:O	1:A:463:GLU:HG2	0.44	2.12	8	3
1:A:381:ILE:O	1:A:392:TYR:HA	0.43	2.13	25	4
1:A:355:ARG:NH2	1:A:438:GLU:HA	0.43	2.27	6	1
1:A:356:LEU:HB2	1:A:379:VAL:HG12	0.43	1.90	21	1
1:A:392:TYR:HB2	1:A:443:GLU:OE2	0.42	2.14	11	1
1:A:435:SER:HB3	1:A:437:GLN:CD	0.42	2.39	8	1
1:A:360:LYS:O	1:A:363:ARG:HG3	0.42	2.14	22	1
1:A:471:ILE:O	1:A:475:LEU:HG	0.42	2.15	8	1
1:A:460:THR:OG1	1:A:463:GLU:HG2	0.42	2.14	20	1
1:A:447:TRP:CZ3	1:A:458:LEU:HD23	0.42	2.50	3	1
1:A:400:VAL:HG22	1:A:418:LEU:HD23	0.42	1.92	24	3
1:A:420:LEU:HD12	1:A:429:PHE:CD1	0.42	2.50	17	3
1:A:438:GLU:H	1:A:438:GLU:CD	0.42	2.22	16	1
1:A:351:LEU:O	1:A:355:ARG:HB3	0.41	2.15	13	1
1:A:380:ARG:NH1	1:A:392:TYR:HB3	0.41	2.30	14	1
1:A:421:ARG:HG3	1:A:423:GLY:O	0.41	2.15	16	1
1:A:414:THR:OG1	1:A:416:LYS:HE3	0.41	2.15	22	1
1:A:406:VAL:CG2	1:A:415:ASN:HB3	0.41	2.45	18	1
1:A:424:ASN:CG	1:A:454:ALA:HB1	0.41	2.41	9	1
1:A:393:ARG:HD3	1:A:422:HIS:NE2	0.41	2.30	15	1
1:A:441:GLU:O	1:A:445:MET:HG2	0.41	2.15	18	1
1:A:372:LYS:HD2	1:A:372:LYS:C	0.41	2.40	20	1
1:A:394:VAL:HG22	1:A:439:PHE:CD1	0.41	2.50	8	1
1:A:375:THR:HA	1:A:397:ILE:O	0.41	2.16	16	1
1:A:358:ARG:HG2	1:A:436:ASN:OD1	0.41	2.16	4	1
1:A:379:VAL:CG1	1:A:397:ILE:HD11	0.41	2.46	18	2
1:A:355:ARG:HG3	1:A:439:PHE:CE1	0.40	2.51	21	1
1:A:353:ARG:HD3	1:A:468:GLU:CD	0.40	2.41	1	1
1:A:476:ASN:HD22	1:A:476:ASN:C	0.40	2.23	1	1
1:A:345:VAL:HG23	1:A:350:GLU:HB2	0.40	1.94	2	1
1:A:357:SER:HB3	1:A:436:ASN:HA	0.40	1.94	12	1
1:A:446:LYS:O	1:A:449:GLU:HG2	0.40	2.17	6	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	119/153 (78%)	114±1 (96±1%)	4±1 (3±1%)	1±0 (1±0%)	16	66
All	All	2975/3825 (78%)	2856 (96%)	92 (3%)	27 (1%)	16	66

All 2 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	411	GLY	25
1	A	-1	MET	2

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	106/135 (79%)	102±2 (96±2%)	4±2 (4±2%)	28	78
All	All	2650/3375 (79%)	2538 (96%)	112 (4%)	28	78

All 23 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	416	LYS	23
1	A	408	GLN	10
1	A	418	LEU	9
1	A	351	LEU	8
1	A	363	ARG	7
1	A	419	GLN	6
1	A	467	LYS	6
1	A	355	ARG	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	472	LYS	5
1	A	406	VAL	4
1	A	370	PHE	4
1	A	424	ASN	4
1	A	345	VAL	3
1	A	412	THR	3
1	A	349	GLU	2
1	A	436	ASN	2
1	A	380	ARG	2
1	A	461	LEU	2
1	A	446	LYS	2
1	A	372	LYS	2
1	A	476	ASN	1
1	A	463	GLU	1
1	A	435	SER	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 91% 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	1828
Number of shifts mapped to atoms	1828
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	14

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	144	2.67 ± 0.11	Should be applied
$^{13}\text{C}_\beta$	132	2.84 ± 0.21	Should be applied
$^{13}\text{C}'$	140	2.61 ± 0.14	Should be applied
^{15}N	136	-0.15 ± 0.38	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 91%, i.e. 1568 atoms were assigned a chemical shift out of a possible 1719. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	602/604 (100%)	246/246 (100%)	238/240 (99%)	118/118 (100%)
Sidechain	870/989 (88%)	590/638 (92%)	263/301 (87%)	17/50 (34%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	96/126 (76%)	54/63 (86%)	40/59 (68%)	2/4 (50%)
Overall	1568/1719 (91%)	890/947 (94%)	541/600 (90%)	137/172 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 1828 atoms were assigned a chemical shift out of a possible 2141. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	716/767 (93%)	296/313 (95%)	284/306 (93%)	136/148 (92%)
Sidechain	1010/1175 (86%)	686/761 (90%)	305/358 (85%)	19/56 (34%)
Aromatic	102/199 (51%)	58/104 (56%)	42/82 (51%)	2/13 (15%)
Overall	1828/2141 (85%)	1040/1178 (88%)	631/746 (85%)	157/217 (72%)

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.

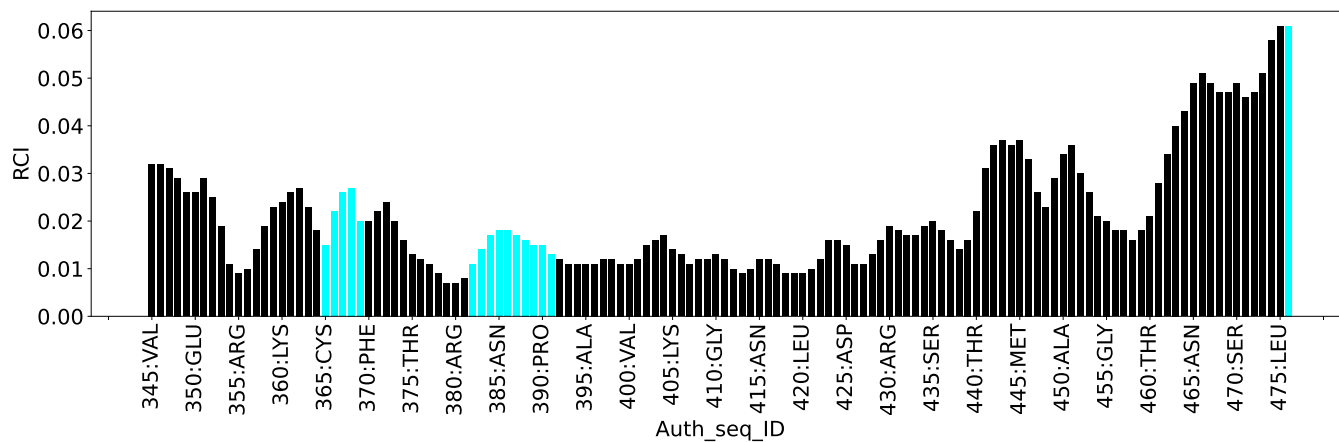
List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	380	ARG	NE	114.68	76.53 – 92.65	18.7
1	A	427	ARG	NE	113.19	76.53 – 92.65	17.7
1	A	353	ARG	NE	112.29	76.53 – 92.65	17.2
1	A	358	ARG	NE	111.51	76.53 – 92.65	16.7
1	A	421	ARG	NE	109.64	76.53 – 92.65	15.5
1	A	355	ARG	NE	109.59	76.53 – 92.65	15.5
1	A	432	GLU	HG3	0.82	1.20 – 3.30	-6.8
1	A	355	ARG	HD3	1.66	1.81 – 4.39	-5.6
1	A	394	VAL	HG11	-0.62	-0.48 – 2.12	-5.5
1	A	394	VAL	HG12	-0.62	-0.48 – 2.12	-5.5
1	A	394	VAL	HG13	-0.62	-0.48 – 2.12	-5.5
1	A	451	MET	HG3	0.41	0.54 – 4.26	-5.3
1	A	414	THR	CG2	15.83	16.06 – 27.03	-5.2
1	A	432	GLU	HG2	1.20	1.24 – 3.30	-5.2

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

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	3424
Intra-residue ($ i-j =0$)	864
Sequential ($ i-j =1$)	913
Medium range ($ i-j >1$ and $ i-j <5$)	606
Long range ($ i-j \geq 5$)	1041
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	22.4
Number of long range restraints per residue ¹	6.8

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	25.8	0.2
0.2-0.5 (Medium)	2.9	0.44
>0.5 (Large)	0.1	1.15

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

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

9 Distance violation analysis ⓘ

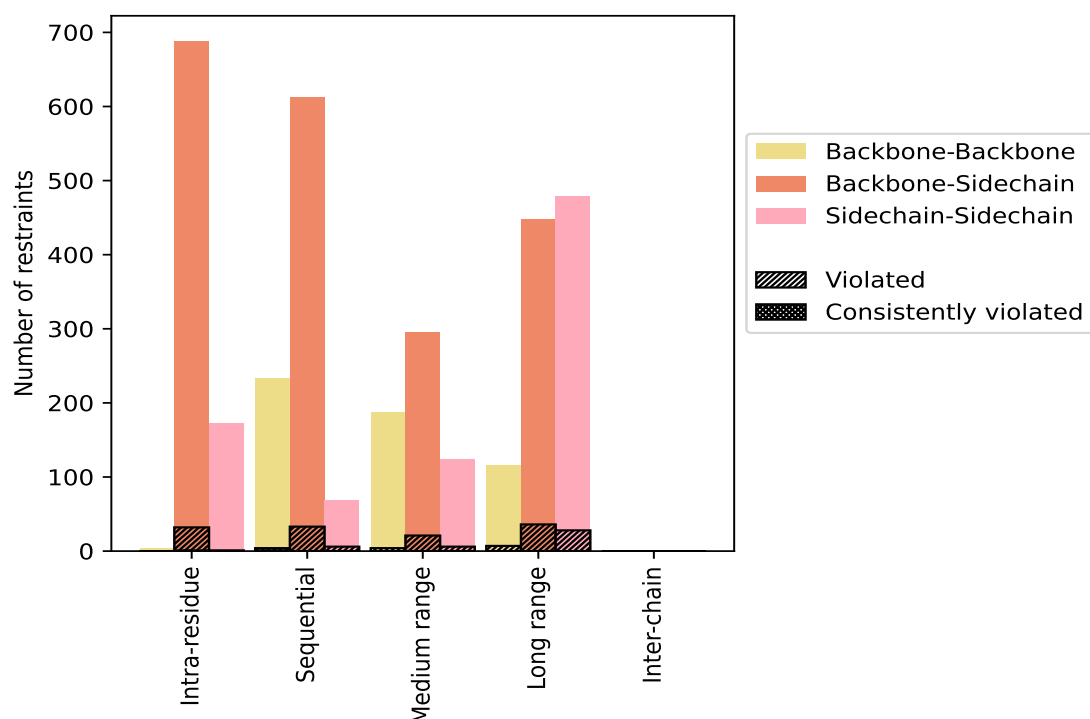
9.1 Summary of distance violations ⓘ

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

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	864	25.2	33	3.8	1.0	1	0.1	0.0
Backbone-Backbone	4	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	688	20.1	32	4.7	0.9	1	0.1	0.0
Sidechain-Sidechain	172	5.0	1	0.6	0.0	0	0.0	0.0
Sequential ($i-j =1$)	913	26.7	43	4.7	1.3	1	0.1	0.0
Backbone-Backbone	233	6.8	4	1.7	0.1	1	0.4	0.0
Backbone-Sidechain	612	17.9	33	5.4	1.0	0	0.0	0.0
Sidechain-Sidechain	68	2.0	6	8.8	0.2	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	606	17.7	31	5.1	0.9	0	0.0	0.0
Backbone-Backbone	187	5.5	4	2.1	0.1	0	0.0	0.0
Backbone-Sidechain	295	8.6	21	7.1	0.6	0	0.0	0.0
Sidechain-Sidechain	124	3.6	6	4.8	0.2	0	0.0	0.0
Long range ($i-j \geq 5$)	1041	30.4	71	6.8	2.1	0	0.0	0.0
Backbone-Backbone	115	3.4	7	6.1	0.2	0	0.0	0.0
Backbone-Sidechain	448	13.1	36	8.0	1.1	0	0.0	0.0
Sidechain-Sidechain	478	14.0	28	5.9	0.8	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	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3424	100.0	178	5.2	5.2	2	0.1	0.1
Backbone-Backbone	539	15.7	15	2.8	0.4	1	0.2	0.0
Backbone-Sidechain	2043	59.7	122	6.0	3.6	1	0.0	0.0
Sidechain-Sidechain	842	24.6	41	4.9	1.2	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 [i](#)



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	8	6	4	12	0	30	0.15	0.26	0.04	0.14
2	6	10	3	14	0	33	0.14	0.26	0.04	0.13
3	5	10	5	10	0	30	0.14	0.2	0.03	0.14
4	5	8	3	11	0	27	0.14	0.24	0.04	0.14
5	3	9	5	10	0	27	0.17	1.15	0.19	0.12
6	7	10	2	11	0	30	0.18	0.89	0.14	0.16
7	2	9	5	13	0	29	0.15	0.41	0.07	0.12
8	8	11	6	17	0	42	0.14	0.28	0.04	0.12
9	5	7	5	10	0	27	0.16	0.34	0.05	0.14
10	4	9	2	16	0	31	0.15	0.23	0.03	0.14

Continued on next page...

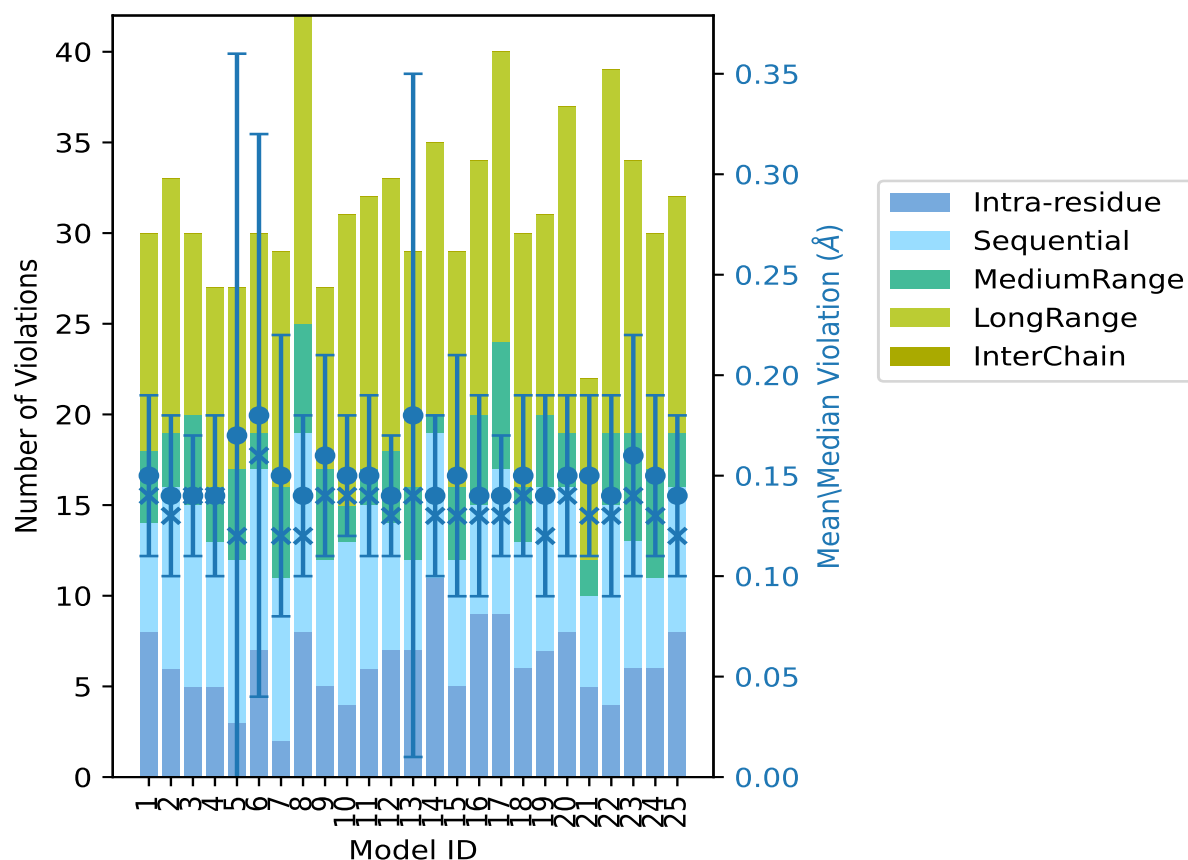
Continued from previous page...

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	6	9	2	15	0	32	0.15	0.24	0.04	0.14
12	7	7	4	15	0	33	0.14	0.22	0.03	0.13
13	7	5	4	13	0	29	0.18	1.06	0.17	0.14
14	11	8	1	15	0	35	0.14	0.23	0.04	0.13
15	5	7	4	13	0	29	0.15	0.4	0.06	0.13
16	9	6	5	14	0	34	0.14	0.39	0.05	0.13
17	9	8	7	16	0	40	0.14	0.22	0.03	0.13
18	6	7	3	14	0	30	0.15	0.24	0.04	0.14
19	7	9	4	11	0	31	0.14	0.28	0.05	0.12
20	8	8	3	18	0	37	0.15	0.25	0.04	0.14
21	5	5	2	10	0	22	0.15	0.26	0.04	0.13
22	4	11	4	20	0	39	0.14	0.3	0.05	0.13
23	6	7	6	15	0	34	0.16	0.44	0.06	0.14
24	6	5	6	13	0	30	0.15	0.28	0.04	0.13
25	8	8	3	13	0	32	0.14	0.26	0.04	0.12

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

⁵Inter-chain restraints, ⁶Standard deviation

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



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

9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3246(IR:831, SQ:870, MR:575, LR:970, 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	%
11	14	17	28	0	70	1	4.0
5	10	4	13	0	32	2	8.0
5	4	2	4	0	15	3	12.0
0	4	0	6	0	10	4	16.0
3	4	2	3	0	12	5	20.0
1	1	2	2	0	6	6	24.0

Continued on next page...

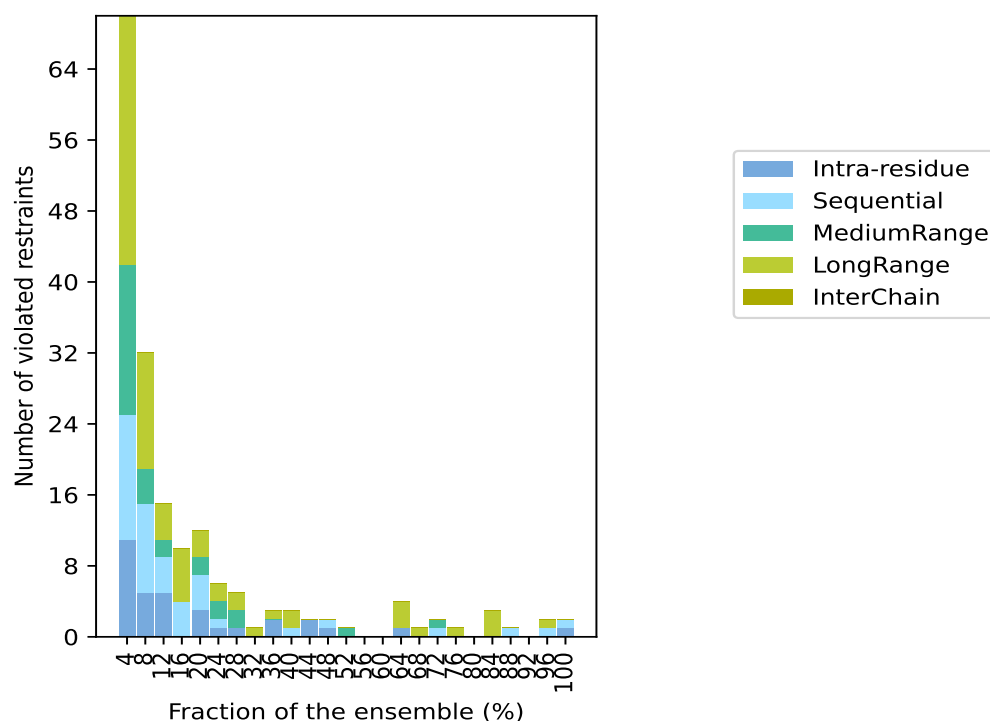
Continued from previous page...

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
1	0	2	2	0	5	7	28.0
0	0	0	1	0	1	8	32.0
2	0	0	1	0	3	9	36.0
0	1	0	2	0	3	10	40.0
2	0	0	0	0	2	11	44.0
1	1	0	0	0	2	12	48.0
0	0	1	0	0	1	13	52.0
0	0	0	0	0	0	14	56.0
0	0	0	0	0	0	15	60.0
1	0	0	3	0	4	16	64.0
0	0	0	1	0	1	17	68.0
0	1	1	0	0	2	18	72.0
0	0	0	1	0	1	19	76.0
0	0	0	0	0	0	20	80.0
0	0	0	3	0	3	21	84.0
0	1	0	0	0	1	22	88.0
0	0	0	0	0	0	23	92.0
0	1	0	1	0	2	24	96.0
1	1	0	0	0	2	25	100.0

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

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

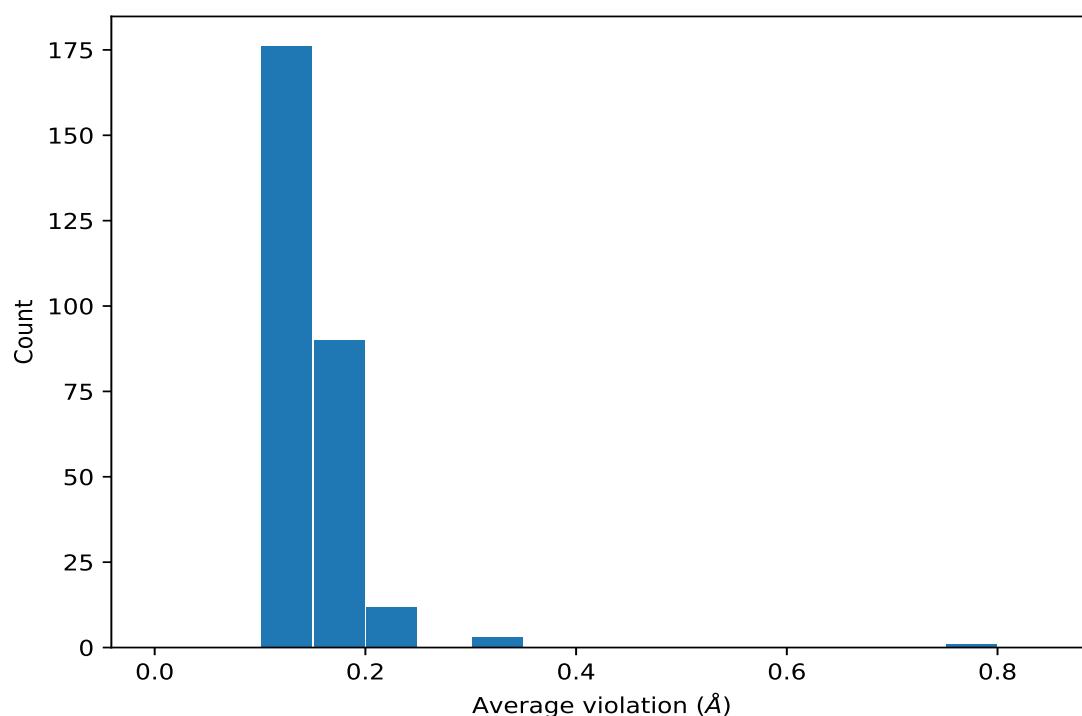
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1658)	1:423:A:GLY:HA2	1:424:A:ASN:H	25	0.19	0.03	0.19
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD11	25	0.14	0.01	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD12	25	0.14	0.01	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD13	25	0.14	0.01	0.14
(1,3070)	1:400:A:VAL:HG11	1:419:A:GLN:H	24	0.2	0.05	0.2
(1,3070)	1:400:A:VAL:HG12	1:419:A:GLN:H	24	0.2	0.05	0.2
(1,3070)	1:400:A:VAL:HG13	1:419:A:GLN:H	24	0.2	0.05	0.2
(1,3070)	1:400:A:VAL:HG21	1:419:A:GLN:H	24	0.2	0.05	0.2
(1,3070)	1:400:A:VAL:HG22	1:419:A:GLN:H	24	0.2	0.05	0.2
(1,3070)	1:400:A:VAL:HG23	1:419:A:GLN:H	24	0.2	0.05	0.2
(1,3153)	1:418:A:LEU:HD11	1:419:A:GLN:H	24	0.16	0.04	0.14
(1,3153)	1:418:A:LEU:HD12	1:419:A:GLN:H	24	0.16	0.04	0.14
(1,3153)	1:418:A:LEU:HD13	1:419:A:GLN:H	24	0.16	0.04	0.14
(1,3153)	1:418:A:LEU:HD21	1:419:A:GLN:H	24	0.16	0.04	0.14
(1,3153)	1:418:A:LEU:HD22	1:419:A:GLN:H	24	0.16	0.04	0.14
(1,3153)	1:418:A:LEU:HD23	1:419:A:GLN:H	24	0.16	0.04	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,57)	1:411:A:GLY:HA3	1:412:A:THR:HB	22	0.17	0.02	0.18
(1,1149)	1:406:A:VAL:HB	1:415:A:ASN:H	21	0.23	0.02	0.22
(1,2117)	1:423:A:GLY:HA2	1:450:A:ALA:H	21	0.15	0.02	0.15
(1,1809)	1:423:A:GLY:HA3	1:456:A:MET:H	21	0.12	0.01	0.12
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG2	19	0.14	0.03	0.13
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG3	19	0.14	0.03	0.13
(1,1660)	1:425:A:ASP:HB3	1:426:A:GLN:H	18	0.14	0.02	0.14
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD2	18	0.12	0.01	0.12
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD3	18	0.12	0.01	0.12
(1,463)	1:401:A:VAL:HG21	1:417:A:GLY:HA2	17	0.14	0.04	0.13
(1,463)	1:401:A:VAL:HG22	1:417:A:GLY:HA2	17	0.14	0.04	0.13
(1,463)	1:401:A:VAL:HG23	1:417:A:GLY:HA2	17	0.14	0.04	0.13
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD2	16	0.16	0.03	0.15
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD3	16	0.16	0.03	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD11	16	0.15	0.03	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD12	16	0.15	0.03	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD13	16	0.15	0.03	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD21	16	0.15	0.03	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD22	16	0.15	0.03	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD23	16	0.15	0.03	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD11	16	0.15	0.03	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD12	16	0.15	0.03	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD13	16	0.15	0.03	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD21	16	0.15	0.03	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD22	16	0.15	0.03	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD23	16	0.15	0.03	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD11	16	0.15	0.03	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD12	16	0.15	0.03	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD13	16	0.15	0.03	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD21	16	0.15	0.03	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD22	16	0.15	0.03	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD23	16	0.15	0.03	0.15
(1,1882)	1:423:A:GLY:HA3	1:447:A:TRP:HE1	16	0.12	0.02	0.12
(1,855)	1:399:A:GLY:HA3	1:418:A:LEU:HB3	16	0.12	0.01	0.12
(1,1661)	1:421:A:ARG:HD2	1:425:A:ASP:H	13	0.13	0.01	0.12
(1,1661)	1:421:A:ARG:HD3	1:425:A:ASP:H	13	0.13	0.01	0.12
(1,1644)	1:418:A:LEU:H	1:418:A:LEU:HG	12	0.17	0.01	0.18
(1,914)	1:460:A:THR:HA	1:461:A:LEU:HG	12	0.13	0.02	0.12
(1,719)	1:363:A:ARG:HA	1:363:A:ARG:HD2	11	0.15	0.02	0.16
(1,719)	1:363:A:ARG:HA	1:363:A:ARG:HD3	11	0.15	0.02	0.16
(1,1414)	1:419:A:GLN:HB3	1:419:A:GLN:HE22	11	0.13	0.01	0.13
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD11	10	0.18	0.05	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD12	10	0.18	0.05	0.19
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD13	10	0.18	0.05	0.19
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD21	10	0.18	0.05	0.19
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD22	10	0.18	0.05	0.19
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD23	10	0.18	0.05	0.19
(1,737)	1:345:A:VAL:HG21	1:459:A:PRO:HD3	10	0.15	0.02	0.16
(1,737)	1:345:A:VAL:HG22	1:459:A:PRO:HD3	10	0.15	0.02	0.16
(1,737)	1:345:A:VAL:HG23	1:459:A:PRO:HD3	10	0.15	0.02	0.16
(1,3184)	1:423:A:GLY:HA3	1:456:A:MET:HB2	10	0.12	0.01	0.12
(1,3184)	1:423:A:GLY:HA3	1:456:A:MET:HB3	10	0.12	0.01	0.12
(1,2250)	1:429:A:PHE:H	1:429:A:PHE:HD1	9	0.2	0.04	0.18
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG11	9	0.17	0.03	0.14
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG12	9	0.17	0.03	0.14
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG13	9	0.17	0.03	0.14
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE1	9	0.16	0.05	0.16
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE2	9	0.16	0.05	0.16
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE3	9	0.16	0.05	0.16
(1,2003)	1:348:A:PRO:HD3	1:444:A:PHE:H	8	0.11	0.01	0.12
(1,1935)	1:405:A:LYS:H	1:405:A:LYS:HE2	7	0.17	0.03	0.16
(1,1935)	1:405:A:LYS:H	1:405:A:LYS:HE3	7	0.17	0.03	0.16
(1,3358)	1:460:A:THR:H	1:463:A:GLU:HB2	7	0.13	0.02	0.13
(1,3358)	1:460:A:THR:H	1:463:A:GLU:HB3	7	0.13	0.02	0.13
(1,2852)	1:356:A:LEU:HD11	1:379:A:VAL:HB	7	0.13	0.01	0.13
(1,2852)	1:356:A:LEU:HD12	1:379:A:VAL:HB	7	0.13	0.01	0.13
(1,2852)	1:356:A:LEU:HD13	1:379:A:VAL:HB	7	0.13	0.01	0.13
(1,2852)	1:356:A:LEU:HD21	1:379:A:VAL:HB	7	0.13	0.01	0.13
(1,2852)	1:356:A:LEU:HD22	1:379:A:VAL:HB	7	0.13	0.01	0.13
(1,2852)	1:356:A:LEU:HD23	1:379:A:VAL:HB	7	0.13	0.01	0.13
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD11	7	0.12	0.01	0.12
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD12	7	0.12	0.01	0.12
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD13	7	0.12	0.01	0.12
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD21	7	0.12	0.01	0.12
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD22	7	0.12	0.01	0.12
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD23	7	0.12	0.01	0.12
(1,247)	1:440:A:THR:HG21	1:444:A:PHE:H	7	0.12	0.02	0.11
(1,247)	1:440:A:THR:HG22	1:444:A:PHE:H	7	0.12	0.02	0.11
(1,247)	1:440:A:THR:HG23	1:444:A:PHE:H	7	0.12	0.02	0.11
(1,78)	1:370:A:PHE:H	1:370:A:PHE:HB2	6	0.14	0.01	0.14
(1,178)	1:393:A:ARG:H	1:395:A:ALA:HB1	6	0.12	0.02	0.12
(1,178)	1:393:A:ARG:H	1:395:A:ALA:HB2	6	0.12	0.02	0.12
(1,178)	1:393:A:ARG:H	1:395:A:ALA:HB3	6	0.12	0.02	0.12
(1,1479)	1:347:A:LEU:HG	1:349:A:GLU:H	6	0.12	0.01	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1383)	1:470:A:SER:H	1:471:A:ILE:HD11	6	0.11	0.01	0.11
(1,1383)	1:470:A:SER:H	1:471:A:ILE:HD12	6	0.11	0.01	0.11
(1,1383)	1:470:A:SER:H	1:471:A:ILE:HD13	6	0.11	0.01	0.11
(1,212)	1:397:A:ILE:HD11	1:418:A:LEU:HD21	6	0.11	0.01	0.11
(1,212)	1:397:A:ILE:HD11	1:418:A:LEU:HD22	6	0.11	0.01	0.11
(1,212)	1:397:A:ILE:HD11	1:418:A:LEU:HD23	6	0.11	0.01	0.11
(1,212)	1:397:A:ILE:HD12	1:418:A:LEU:HD21	6	0.11	0.01	0.11
(1,212)	1:397:A:ILE:HD12	1:418:A:LEU:HD22	6	0.11	0.01	0.11
(1,212)	1:397:A:ILE:HD12	1:418:A:LEU:HD23	6	0.11	0.01	0.11
(1,212)	1:397:A:ILE:HD13	1:418:A:LEU:HD21	6	0.11	0.01	0.11
(1,212)	1:397:A:ILE:HD13	1:418:A:LEU:HD22	6	0.11	0.01	0.11
(1,212)	1:397:A:ILE:HD13	1:418:A:LEU:HD23	6	0.11	0.01	0.11
(1,3062)	1:400:A:VAL:HG11	1:416:A:LYS:H	6	0.11	0.0	0.11
(1,3062)	1:400:A:VAL:HG12	1:416:A:LYS:H	6	0.11	0.0	0.11
(1,3062)	1:400:A:VAL:HG13	1:416:A:LYS:H	6	0.11	0.0	0.11
(1,3062)	1:400:A:VAL:HG21	1:416:A:LYS:H	6	0.11	0.0	0.11
(1,3062)	1:400:A:VAL:HG22	1:416:A:LYS:H	6	0.11	0.0	0.11
(1,3062)	1:400:A:VAL:HG23	1:416:A:LYS:H	6	0.11	0.0	0.11
(1,2400)	1:407:A:TYR:HD1	1:408:A:GLN:H	5	0.79	0.31	0.89
(1,586)	1:466:A:LYS:HA	1:466:A:LYS:HD2	5	0.22	0.03	0.21
(1,586)	1:466:A:LYS:HA	1:466:A:LYS:HD3	5	0.22	0.03	0.21
(1,1814)	1:446:A:LYS:H	1:446:A:LYS:HG2	5	0.19	0.01	0.18
(1,2923)	1:364:A:TRP:HB3	1:367:A:MET:HB2	5	0.15	0.02	0.14
(1,2923)	1:364:A:TRP:HB3	1:367:A:MET:HB3	5	0.15	0.02	0.14
(1,2328)	1:-2:A:HIS:HA	1:-1:A:MET:H	5	0.14	0.01	0.13
(1,2678)	1:-1:A:MET:HE1	1:345:A:VAL:H	5	0.14	0.01	0.14
(1,2678)	1:-1:A:MET:HE2	1:345:A:VAL:H	5	0.14	0.01	0.14
(1,2678)	1:-1:A:MET:HE3	1:345:A:VAL:H	5	0.14	0.01	0.14
(1,2405)	1:446:A:LYS:H	1:446:A:LYS:HG2	5	0.13	0.0	0.13
(1,2405)	1:446:A:LYS:H	1:446:A:LYS:HG3	5	0.13	0.0	0.13
(1,1389)	1:435:A:SER:HA	1:437:A:GLN:HE22	5	0.13	0.02	0.12
(1,1940)	1:362:A:GLU:H	1:412:A:THR:HG21	5	0.12	0.02	0.12
(1,1940)	1:362:A:GLU:H	1:412:A:THR:HG22	5	0.12	0.02	0.12
(1,1940)	1:362:A:GLU:H	1:412:A:THR:HG23	5	0.12	0.02	0.12
(1,1153)	1:366:A:HIS:HE1	1:367:A:MET:H	5	0.12	0.02	0.11
(1,2739)	1:345:A:VAL:HG11	1:459:A:PRO:HA	5	0.11	0.01	0.11
(1,2739)	1:345:A:VAL:HG12	1:459:A:PRO:HA	5	0.11	0.01	0.11
(1,2739)	1:345:A:VAL:HG13	1:459:A:PRO:HA	5	0.11	0.01	0.11
(1,2739)	1:345:A:VAL:HG21	1:459:A:PRO:HA	5	0.11	0.01	0.11
(1,2739)	1:345:A:VAL:HG22	1:459:A:PRO:HA	5	0.11	0.01	0.11
(1,2739)	1:345:A:VAL:HG23	1:459:A:PRO:HA	5	0.11	0.01	0.11
(1,2360)	1:415:A:ASN:H	1:416:A:LYS:HB2	5	0.11	0.0	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2360)	1:415:A:ASN:H	1:416:A:LYS:HB3	5	0.11	0.0	0.11
(1,1286)	1:411:A:GLY:H	1:412:A:THR:HG21	4	0.33	0.08	0.36
(1,1286)	1:411:A:GLY:H	1:412:A:THR:HG22	4	0.33	0.08	0.36
(1,1286)	1:411:A:GLY:H	1:412:A:THR:HG23	4	0.33	0.08	0.36
(1,2000)	1:406:A:VAL:HG11	1:416:A:LYS:H	4	0.17	0.03	0.18
(1,2000)	1:406:A:VAL:HG12	1:416:A:LYS:H	4	0.17	0.03	0.18
(1,2000)	1:406:A:VAL:HG13	1:416:A:LYS:H	4	0.17	0.03	0.18
(1,1888)	1:380:A:ARG:HE	1:437:A:GLN:H	4	0.15	0.01	0.15
(1,2173)	1:423:A:GLY:H	1:454:A:ALA:HB1	4	0.13	0.01	0.12
(1,2173)	1:423:A:GLY:H	1:454:A:ALA:HB2	4	0.13	0.01	0.12
(1,2173)	1:423:A:GLY:H	1:454:A:ALA:HB3	4	0.13	0.01	0.12
(1,2601)	1:424:A:ASN:HD22	1:454:A:ALA:HB1	4	0.13	0.01	0.13
(1,2601)	1:424:A:ASN:HD22	1:454:A:ALA:HB2	4	0.13	0.01	0.13
(1,2601)	1:424:A:ASN:HD22	1:454:A:ALA:HB3	4	0.13	0.01	0.13
(1,535)	1:363:A:ARG:HD2	1:364:A:TRP:H	4	0.12	0.01	0.12
(1,535)	1:363:A:ARG:HD3	1:364:A:TRP:H	4	0.12	0.01	0.12
(1,279)	1:392:A:TYR:HE1	1:435:A:SER:HA	4	0.12	0.01	0.12
(1,279)	1:392:A:TYR:HE2	1:435:A:SER:HA	4	0.12	0.01	0.12
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD11	4	0.12	0.01	0.12
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD12	4	0.12	0.01	0.12
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD13	4	0.12	0.01	0.12
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD21	4	0.12	0.01	0.12
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD22	4	0.12	0.01	0.12
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD23	4	0.12	0.01	0.12
(1,2470)	1:400:A:VAL:HA	1:418:A:LEU:H	4	0.12	0.01	0.12
(1,2270)	1:369:A:PHE:HD2	1:370:A:PHE:H	4	0.11	0.01	0.11
(1,3332)	1:456:A:MET:H	1:456:A:MET:HG2	3	0.21	0.01	0.21
(1,3332)	1:456:A:MET:H	1:456:A:MET:HG3	3	0.21	0.01	0.21
(1,1030)	1:449:A:GLU:HG2	1:450:A:ALA:H	3	0.19	0.04	0.22
(1,3379)	1:466:A:LYS:H	1:466:A:LYS:HG2	3	0.17	0.01	0.17
(1,3379)	1:466:A:LYS:H	1:466:A:LYS:HG3	3	0.17	0.01	0.17
(1,2624)	1:455:A:GLY:H	1:456:A:MET:HG2	3	0.16	0.0	0.16
(1,2624)	1:455:A:GLY:H	1:456:A:MET:HG3	3	0.16	0.0	0.16
(1,2581)	1:-3:A:SER:H	1:-2:A:HIS:HB2	3	0.14	0.0	0.14
(1,2581)	1:-3:A:SER:H	1:-2:A:HIS:HB3	3	0.14	0.0	0.14
(1,3103)	1:407:A:TYR:HE1	1:416:A:LYS:HD2	3	0.14	0.02	0.13
(1,3103)	1:407:A:TYR:HE1	1:416:A:LYS:HD3	3	0.14	0.02	0.13
(1,3103)	1:407:A:TYR:HE2	1:416:A:LYS:HD2	3	0.14	0.02	0.13
(1,3103)	1:407:A:TYR:HE2	1:416:A:LYS:HD3	3	0.14	0.02	0.13
(1,907)	1:464:A:ILE:HA	1:467:A:LYS:HE2	3	0.12	0.02	0.12
(1,907)	1:464:A:ILE:HA	1:467:A:LYS:HE3	3	0.12	0.02	0.12
(1,909)	1:347:A:LEU:HB2	1:348:A:PRO:HD3	3	0.12	0.01	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,921)	1:351:A:LEU:HB2	1:444:A:PHE:HZ	3	0.12	0.0	0.12
(1,2327)	1:-8:A:LEU:H	1:-8:A:LEU:HG	3	0.12	0.0	0.12
(1,1789)	1:456:A:MET:H	1:456:A:MET:HG2	3	0.11	0.01	0.11
(1,1939)	1:442:A:SER:H	1:442:A:SER:HB3	3	0.11	0.01	0.11
(1,2148)	1:348:A:PRO:HD3	1:350:A:GLU:H	3	0.11	0.01	0.11
(1,83)	1:382:A:GLY:HA3	1:392:A:TYR:HB2	3	0.11	0.01	0.1
(1,2612)	1:399:A:GLY:H	1:418:A:LEU:HA	3	0.1	0.0	0.1
(1,1829)	1:438:A:GLU:H	1:438:A:GLU:HG2	2	0.18	0.02	0.18
(1,167)	1:355:A:ARG:HB3	1:439:A:PHE:HD1	2	0.17	0.02	0.17
(1,167)	1:355:A:ARG:HB3	1:439:A:PHE:HD2	2	0.17	0.02	0.17
(1,701)	1:369:A:PHE:HD1	1:370:A:PHE:HA	2	0.16	0.04	0.16
(1,701)	1:369:A:PHE:HD2	1:370:A:PHE:HA	2	0.16	0.04	0.16
(1,161)	1:370:A:PHE:HD1	1:371:A:ALA:HB1	2	0.16	0.02	0.16
(1,161)	1:370:A:PHE:HD1	1:371:A:ALA:HB2	2	0.16	0.02	0.16
(1,161)	1:370:A:PHE:HD1	1:371:A:ALA:HB3	2	0.16	0.02	0.16
(1,161)	1:370:A:PHE:HD2	1:371:A:ALA:HB1	2	0.16	0.02	0.16
(1,161)	1:370:A:PHE:HD2	1:371:A:ALA:HB2	2	0.16	0.02	0.16
(1,161)	1:370:A:PHE:HD2	1:371:A:ALA:HB3	2	0.16	0.02	0.16
(1,2949)	1:374:A:VAL:HG21	1:400:A:VAL:HG11	2	0.16	0.02	0.16
(1,2949)	1:374:A:VAL:HG21	1:400:A:VAL:HG12	2	0.16	0.02	0.16
(1,2949)	1:374:A:VAL:HG21	1:400:A:VAL:HG13	2	0.16	0.02	0.16
(1,2949)	1:374:A:VAL:HG21	1:400:A:VAL:HG21	2	0.16	0.02	0.16
(1,2949)	1:374:A:VAL:HG21	1:400:A:VAL:HG22	2	0.16	0.02	0.16
(1,2949)	1:374:A:VAL:HG21	1:400:A:VAL:HG23	2	0.16	0.02	0.16
(1,2949)	1:374:A:VAL:HG22	1:400:A:VAL:HG11	2	0.16	0.02	0.16
(1,2949)	1:374:A:VAL:HG22	1:400:A:VAL:HG12	2	0.16	0.02	0.16
(1,2949)	1:374:A:VAL:HG22	1:400:A:VAL:HG13	2	0.16	0.02	0.16
(1,2949)	1:374:A:VAL:HG22	1:400:A:VAL:HG21	2	0.16	0.02	0.16
(1,2949)	1:374:A:VAL:HG22	1:400:A:VAL:HG22	2	0.16	0.02	0.16
(1,2949)	1:374:A:VAL:HG22	1:400:A:VAL:HG23	2	0.16	0.02	0.16
(1,2949)	1:374:A:VAL:HG23	1:400:A:VAL:HG11	2	0.16	0.02	0.16
(1,2949)	1:374:A:VAL:HG23	1:400:A:VAL:HG12	2	0.16	0.02	0.16
(1,2949)	1:374:A:VAL:HG23	1:400:A:VAL:HG13	2	0.16	0.02	0.16
(1,2949)	1:374:A:VAL:HG23	1:400:A:VAL:HG21	2	0.16	0.02	0.16
(1,2949)	1:374:A:VAL:HG23	1:400:A:VAL:HG22	2	0.16	0.02	0.16
(1,2949)	1:374:A:VAL:HG23	1:400:A:VAL:HG23	2	0.16	0.02	0.16
(1,510)	1:440:A:THR:HA	1:441:A:GLU:HG2	2	0.14	0.01	0.14
(1,510)	1:440:A:THR:HA	1:441:A:GLU:HG3	2	0.14	0.01	0.14
(1,2025)	1:358:A:ARG:H	1:358:A:ARG:HG3	2	0.14	0.02	0.14
(1,1889)	1:392:A:TYR:HE1	1:437:A:GLN:H	2	0.13	0.03	0.13
(1,1889)	1:392:A:TYR:HE2	1:437:A:GLN:H	2	0.13	0.03	0.13
(1,3166)	1:419:A:GLN:HE21	1:428:A:VAL:HB	2	0.13	0.0	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3166)	1:419:A:GLN:HE22	1:428:A:VAL:HB	2	0.13	0.0	0.13
(1,3248)	1:435:A:SER:HA	1:437:A:GLN:HG2	2	0.13	0.01	0.13
(1,3248)	1:435:A:SER:HA	1:437:A:GLN:HG3	2	0.13	0.01	0.13
(1,3286)	1:446:A:LYS:HG2	1:449:A:GLU:H	2	0.13	0.02	0.13
(1,3286)	1:446:A:LYS:HG3	1:449:A:GLU:H	2	0.13	0.02	0.13
(1,487)	1:398:A:THR:HG21	1:419:A:GLN:HG3	2	0.12	0.02	0.12
(1,487)	1:398:A:THR:HG22	1:419:A:GLN:HG3	2	0.12	0.02	0.12
(1,487)	1:398:A:THR:HG23	1:419:A:GLN:HG3	2	0.12	0.02	0.12
(1,1471)	1:345:A:VAL:H	1:345:A:VAL:HB	2	0.12	0.01	0.12
(1,3012)	1:385:A:ASN:HD21	1:386:A:HIS:HA	2	0.12	0.01	0.12
(1,3012)	1:385:A:ASN:HD22	1:386:A:HIS:HA	2	0.12	0.01	0.12
(1,241)	1:421:A:ARG:H	1:421:A:ARG:HG2	2	0.12	0.0	0.12
(1,1084)	1:405:A:LYS:HG2	1:406:A:VAL:H	2	0.12	0.01	0.12
(1,1084)	1:405:A:LYS:HG3	1:406:A:VAL:H	2	0.12	0.01	0.12
(1,1145)	1:419:A:GLN:HG3	1:428:A:VAL:H	2	0.12	0.01	0.12
(1,1902)	1:423:A:GLY:HA2	1:425:A:ASP:H	2	0.12	0.01	0.12
(1,375)	1:395:A:ALA:HB1	1:420:A:LEU:HG	2	0.12	0.02	0.12
(1,375)	1:395:A:ALA:HB2	1:420:A:LEU:HG	2	0.12	0.02	0.12
(1,375)	1:395:A:ALA:HB3	1:420:A:LEU:HG	2	0.12	0.02	0.12
(1,790)	1:361:A:LEU:HA	1:370:A:PHE:HE1	2	0.12	0.02	0.12
(1,790)	1:361:A:LEU:HA	1:370:A:PHE:HE2	2	0.12	0.02	0.12
(1,922)	1:439:A:PHE:HD1	1:440:A:THR:HA	2	0.12	0.0	0.12
(1,922)	1:439:A:PHE:HD2	1:440:A:THR:HA	2	0.12	0.0	0.12
(1,2435)	1:370:A:PHE:HD1	1:371:A:ALA:H	2	0.12	0.0	0.12
(1,2708)	1:-3:A:SER:H	1:-3:A:SER:HB2	2	0.12	0.0	0.12
(1,2708)	1:-3:A:SER:H	1:-3:A:SER:HB3	2	0.12	0.0	0.12
(1,2725)	1:345:A:VAL:HG11	1:350:A:GLU:H	2	0.12	0.0	0.12
(1,2725)	1:345:A:VAL:HG12	1:350:A:GLU:H	2	0.12	0.0	0.12
(1,2725)	1:345:A:VAL:HG13	1:350:A:GLU:H	2	0.12	0.0	0.12
(1,2725)	1:345:A:VAL:HG21	1:350:A:GLU:H	2	0.12	0.0	0.12
(1,2725)	1:345:A:VAL:HG22	1:350:A:GLU:H	2	0.12	0.0	0.12
(1,2725)	1:345:A:VAL:HG23	1:350:A:GLU:H	2	0.12	0.0	0.12
(1,3179)	1:421:A:ARG:HE	1:426:A:GLN:HG2	2	0.12	0.0	0.12
(1,3179)	1:421:A:ARG:HE	1:426:A:GLN:HG3	2	0.12	0.0	0.12
(1,1633)	1:413:A:ARG:HG3	1:414:A:THR:H	2	0.11	0.01	0.11
(1,2695)	1:-7:A:VAL:HB	1:-6:A:PRO:HD2	2	0.11	0.0	0.11
(1,2695)	1:-7:A:VAL:HB	1:-6:A:PRO:HD3	2	0.11	0.0	0.11
(1,154)	1:397:A:ILE:HG12	1:418:A:LEU:HG	2	0.11	0.0	0.11
(1,154)	1:397:A:ILE:HG13	1:418:A:LEU:HG	2	0.11	0.0	0.11
(1,1659)	1:424:A:ASN:H	1:425:A:ASP:H	2	0.11	0.0	0.11
(1,3356)	1:459:A:PRO:HD2	1:461:A:LEU:HD11	2	0.11	0.0	0.11
(1,3356)	1:459:A:PRO:HD2	1:461:A:LEU:HD12	2	0.11	0.0	0.11

Continued on next page...

Continued from previous page...

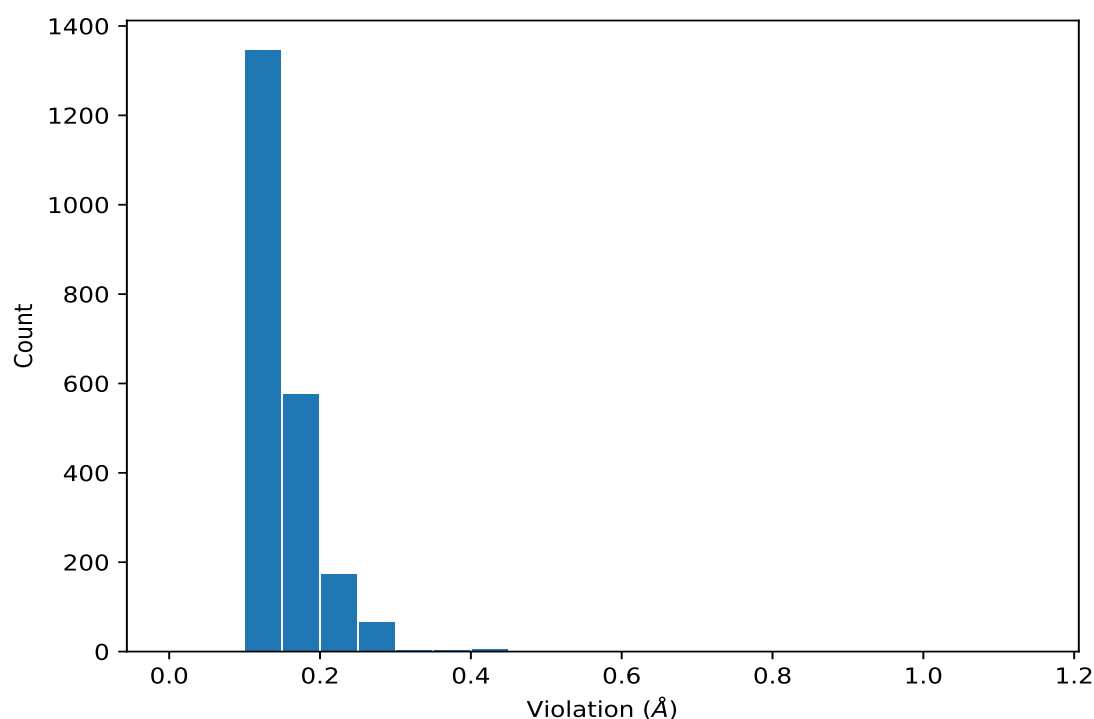
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,3356)	1:459:A:PRO:HD2	1:461:A:LEU:HD13	2	0.11	0.0	0.11
(1,3356)	1:459:A:PRO:HD2	1:461:A:LEU:HD21	2	0.11	0.0	0.11
(1,3356)	1:459:A:PRO:HD2	1:461:A:LEU:HD22	2	0.11	0.0	0.11
(1,3356)	1:459:A:PRO:HD2	1:461:A:LEU:HD23	2	0.11	0.0	0.11
(1,130)	1:380:A:ARG:HB2	1:435:A:SER:H	2	0.1	0.0	0.1
(1,892)	1:345:A:VAL:HG21	1:351:A:LEU:HD11	2	0.1	0.0	0.1
(1,892)	1:345:A:VAL:HG21	1:351:A:LEU:HD12	2	0.1	0.0	0.1
(1,892)	1:345:A:VAL:HG21	1:351:A:LEU:HD13	2	0.1	0.0	0.1
(1,892)	1:345:A:VAL:HG22	1:351:A:LEU:HD11	2	0.1	0.0	0.1
(1,892)	1:345:A:VAL:HG22	1:351:A:LEU:HD12	2	0.1	0.0	0.1
(1,892)	1:345:A:VAL:HG22	1:351:A:LEU:HD13	2	0.1	0.0	0.1
(1,892)	1:345:A:VAL:HG23	1:351:A:LEU:HD11	2	0.1	0.0	0.1
(1,892)	1:345:A:VAL:HG23	1:351:A:LEU:HD12	2	0.1	0.0	0.1
(1,892)	1:345:A:VAL:HG23	1:351:A:LEU:HD13	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2400)	1:407:A:TYR:HD1	1:408:A:GLN:H	5	1.15
(1,2400)	1:407:A:TYR:HD1	1:408:A:GLN:H	13	1.06
(1,2400)	1:407:A:TYR:HD1	1:408:A:GLN:H	6	0.89
(1,2400)	1:407:A:TYR:HD1	1:408:A:GLN:H	23	0.44
(1,2400)	1:407:A:TYR:HD1	1:408:A:GLN:H	7	0.41
(1,1286)	1:411:A:GLY:H	1:412:A:THR:HG21	15	0.4
(1,1286)	1:411:A:GLY:H	1:412:A:THR:HG22	15	0.4
(1,1286)	1:411:A:GLY:H	1:412:A:THR:HG23	15	0.4
(1,1286)	1:411:A:GLY:H	1:412:A:THR:HG21	16	0.39
(1,1286)	1:411:A:GLY:H	1:412:A:THR:HG22	16	0.39
(1,1286)	1:411:A:GLY:H	1:412:A:THR:HG23	16	0.39
(1,1286)	1:411:A:GLY:H	1:412:A:THR:HG21	9	0.34
(1,1286)	1:411:A:GLY:H	1:412:A:THR:HG22	9	0.34
(1,1286)	1:411:A:GLY:H	1:412:A:THR:HG23	9	0.34
(1,1149)	1:406:A:VAL:HB	1:415:A:ASN:H	22	0.3
(1,3070)	1:400:A:VAL:HG11	1:419:A:GLN:H	8	0.28
(1,3070)	1:400:A:VAL:HG12	1:419:A:GLN:H	8	0.28
(1,3070)	1:400:A:VAL:HG13	1:419:A:GLN:H	8	0.28
(1,3070)	1:400:A:VAL:HG21	1:419:A:GLN:H	8	0.28
(1,3070)	1:400:A:VAL:HG22	1:419:A:GLN:H	8	0.28
(1,3070)	1:400:A:VAL:HG23	1:419:A:GLN:H	8	0.28
(1,3070)	1:400:A:VAL:HG11	1:419:A:GLN:H	19	0.28
(1,3070)	1:400:A:VAL:HG12	1:419:A:GLN:H	19	0.28
(1,3070)	1:400:A:VAL:HG13	1:419:A:GLN:H	19	0.28
(1,3070)	1:400:A:VAL:HG21	1:419:A:GLN:H	19	0.28
(1,3070)	1:400:A:VAL:HG22	1:419:A:GLN:H	19	0.28
(1,3070)	1:400:A:VAL:HG23	1:419:A:GLN:H	19	0.28
(1,3070)	1:400:A:VAL:HG11	1:419:A:GLN:H	24	0.28
(1,3070)	1:400:A:VAL:HG12	1:419:A:GLN:H	24	0.28
(1,3070)	1:400:A:VAL:HG13	1:419:A:GLN:H	24	0.28
(1,3070)	1:400:A:VAL:HG21	1:419:A:GLN:H	24	0.28
(1,3070)	1:400:A:VAL:HG22	1:419:A:GLN:H	24	0.28
(1,3070)	1:400:A:VAL:HG23	1:419:A:GLN:H	24	0.28
(1,3153)	1:418:A:LEU:HD11	1:419:A:GLN:H	22	0.27
(1,3153)	1:418:A:LEU:HD12	1:419:A:GLN:H	22	0.27
(1,3153)	1:418:A:LEU:HD13	1:419:A:GLN:H	22	0.27
(1,3153)	1:418:A:LEU:HD21	1:419:A:GLN:H	22	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3153)	1:418:A:LEU:HD22	1:419:A:GLN:H	22	0.27
(1,3153)	1:418:A:LEU:HD23	1:419:A:GLN:H	22	0.27
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE1	9	0.27
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE2	9	0.27
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE3	9	0.27
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD11	24	0.26
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD12	24	0.26
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD13	24	0.26
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD21	24	0.26
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD22	24	0.26
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD23	24	0.26
(1,3070)	1:400:A:VAL:HG11	1:419:A:GLN:H	2	0.26
(1,3070)	1:400:A:VAL:HG12	1:419:A:GLN:H	2	0.26
(1,3070)	1:400:A:VAL:HG13	1:419:A:GLN:H	2	0.26
(1,3070)	1:400:A:VAL:HG21	1:419:A:GLN:H	2	0.26
(1,3070)	1:400:A:VAL:HG22	1:419:A:GLN:H	2	0.26
(1,3070)	1:400:A:VAL:HG23	1:419:A:GLN:H	2	0.26
(1,3070)	1:400:A:VAL:HG11	1:419:A:GLN:H	25	0.26
(1,3070)	1:400:A:VAL:HG12	1:419:A:GLN:H	25	0.26
(1,3070)	1:400:A:VAL:HG13	1:419:A:GLN:H	25	0.26
(1,3070)	1:400:A:VAL:HG21	1:419:A:GLN:H	25	0.26
(1,3070)	1:400:A:VAL:HG22	1:419:A:GLN:H	25	0.26
(1,3070)	1:400:A:VAL:HG23	1:419:A:GLN:H	25	0.26
(1,2250)	1:429:A:PHE:H	1:429:A:PHE:HD1	1	0.26
(1,1149)	1:406:A:VAL:HB	1:415:A:ASN:H	15	0.26
(1,586)	1:466:A:LYS:HA	1:466:A:LYS:HD2	21	0.26
(1,586)	1:466:A:LYS:HA	1:466:A:LYS:HD3	21	0.26
(1,3070)	1:400:A:VAL:HG11	1:419:A:GLN:H	7	0.25
(1,3070)	1:400:A:VAL:HG12	1:419:A:GLN:H	7	0.25
(1,3070)	1:400:A:VAL:HG13	1:419:A:GLN:H	7	0.25
(1,3070)	1:400:A:VAL:HG21	1:419:A:GLN:H	7	0.25
(1,3070)	1:400:A:VAL:HG22	1:419:A:GLN:H	7	0.25
(1,3070)	1:400:A:VAL:HG23	1:419:A:GLN:H	7	0.25
(1,3070)	1:400:A:VAL:HG11	1:419:A:GLN:H	20	0.25
(1,3070)	1:400:A:VAL:HG12	1:419:A:GLN:H	20	0.25
(1,3070)	1:400:A:VAL:HG13	1:419:A:GLN:H	20	0.25
(1,3070)	1:400:A:VAL:HG21	1:419:A:GLN:H	20	0.25
(1,3070)	1:400:A:VAL:HG22	1:419:A:GLN:H	20	0.25
(1,3070)	1:400:A:VAL:HG23	1:419:A:GLN:H	20	0.25
(1,2250)	1:429:A:PHE:H	1:429:A:PHE:HD1	15	0.25
(1,1658)	1:423:A:GLY:HA2	1:424:A:ASN:H	2	0.25
(1,1149)	1:406:A:VAL:HB	1:415:A:ASN:H	19	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,586)	1:466:A:LYS:HA	1:466:A:LYS:HD2	22	0.25
(1,586)	1:466:A:LYS:HA	1:466:A:LYS:HD3	22	0.25
(1,3153)	1:418:A:LEU:HD11	1:419:A:GLN:H	9	0.24
(1,3153)	1:418:A:LEU:HD12	1:419:A:GLN:H	9	0.24
(1,3153)	1:418:A:LEU:HD13	1:419:A:GLN:H	9	0.24
(1,3153)	1:418:A:LEU:HD21	1:419:A:GLN:H	9	0.24
(1,3153)	1:418:A:LEU:HD22	1:419:A:GLN:H	9	0.24
(1,3153)	1:418:A:LEU:HD23	1:419:A:GLN:H	9	0.24
(1,2250)	1:429:A:PHE:H	1:429:A:PHE:HD1	19	0.24
(1,1658)	1:423:A:GLY:HA2	1:424:A:ASN:H	7	0.24
(1,1149)	1:406:A:VAL:HB	1:415:A:ASN:H	4	0.24
(1,1149)	1:406:A:VAL:HB	1:415:A:ASN:H	7	0.24
(1,1149)	1:406:A:VAL:HB	1:415:A:ASN:H	11	0.24
(1,1149)	1:406:A:VAL:HB	1:415:A:ASN:H	21	0.24
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG11	22	0.24
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG12	22	0.24
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG13	22	0.24
(1,463)	1:401:A:VAL:HG21	1:417:A:GLY:HA2	18	0.24
(1,463)	1:401:A:VAL:HG22	1:417:A:GLY:HA2	18	0.24
(1,463)	1:401:A:VAL:HG23	1:417:A:GLY:HA2	18	0.24
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD2	6	0.24
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD3	6	0.24
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD11	11	0.23
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD12	11	0.23
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD13	11	0.23
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD21	11	0.23
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD22	11	0.23
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD23	11	0.23
(1,3070)	1:400:A:VAL:HG11	1:419:A:GLN:H	11	0.23
(1,3070)	1:400:A:VAL:HG12	1:419:A:GLN:H	11	0.23
(1,3070)	1:400:A:VAL:HG13	1:419:A:GLN:H	11	0.23
(1,3070)	1:400:A:VAL:HG21	1:419:A:GLN:H	11	0.23
(1,3070)	1:400:A:VAL:HG22	1:419:A:GLN:H	11	0.23
(1,3070)	1:400:A:VAL:HG23	1:419:A:GLN:H	11	0.23
(1,1848)	1:463:A:GLU:H	1:463:A:GLU:HG2	2	0.23
(1,1848)	1:463:A:GLU:H	1:463:A:GLU:HG3	2	0.23
(1,1658)	1:423:A:GLY:HA2	1:424:A:ASN:H	4	0.23
(1,1149)	1:406:A:VAL:HB	1:415:A:ASN:H	9	0.23
(1,1149)	1:406:A:VAL:HB	1:415:A:ASN:H	14	0.23
(1,1030)	1:449:A:GLU:HG2	1:450:A:ALA:H	10	0.23
(1,3332)	1:456:A:MET:H	1:456:A:MET:HG2	17	0.22
(1,3332)	1:456:A:MET:H	1:456:A:MET:HG3	17	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3153)	1:418:A:LEU:HD11	1:419:A:GLN:H	5	0.22
(1,3153)	1:418:A:LEU:HD12	1:419:A:GLN:H	5	0.22
(1,3153)	1:418:A:LEU:HD13	1:419:A:GLN:H	5	0.22
(1,3153)	1:418:A:LEU:HD21	1:419:A:GLN:H	5	0.22
(1,3153)	1:418:A:LEU:HD22	1:419:A:GLN:H	5	0.22
(1,3153)	1:418:A:LEU:HD23	1:419:A:GLN:H	5	0.22
(1,3153)	1:418:A:LEU:HD11	1:419:A:GLN:H	21	0.22
(1,3153)	1:418:A:LEU:HD12	1:419:A:GLN:H	21	0.22
(1,3153)	1:418:A:LEU:HD13	1:419:A:GLN:H	21	0.22
(1,3153)	1:418:A:LEU:HD21	1:419:A:GLN:H	21	0.22
(1,3153)	1:418:A:LEU:HD22	1:419:A:GLN:H	21	0.22
(1,3153)	1:418:A:LEU:HD23	1:419:A:GLN:H	21	0.22
(1,3070)	1:400:A:VAL:HG11	1:419:A:GLN:H	14	0.22
(1,3070)	1:400:A:VAL:HG12	1:419:A:GLN:H	14	0.22
(1,3070)	1:400:A:VAL:HG13	1:419:A:GLN:H	14	0.22
(1,3070)	1:400:A:VAL:HG21	1:419:A:GLN:H	14	0.22
(1,3070)	1:400:A:VAL:HG22	1:419:A:GLN:H	14	0.22
(1,3070)	1:400:A:VAL:HG23	1:419:A:GLN:H	14	0.22
(1,3070)	1:400:A:VAL:HG11	1:419:A:GLN:H	23	0.22
(1,3070)	1:400:A:VAL:HG12	1:419:A:GLN:H	23	0.22
(1,3070)	1:400:A:VAL:HG13	1:419:A:GLN:H	23	0.22
(1,3070)	1:400:A:VAL:HG21	1:419:A:GLN:H	23	0.22
(1,3070)	1:400:A:VAL:HG22	1:419:A:GLN:H	23	0.22
(1,3070)	1:400:A:VAL:HG23	1:419:A:GLN:H	23	0.22
(1,2250)	1:429:A:PHE:H	1:429:A:PHE:HD1	20	0.22
(1,1658)	1:423:A:GLY:HA2	1:424:A:ASN:H	1	0.22
(1,1658)	1:423:A:GLY:HA2	1:424:A:ASN:H	18	0.22
(1,1658)	1:423:A:GLY:HA2	1:424:A:ASN:H	20	0.22
(1,1149)	1:406:A:VAL:HB	1:415:A:ASN:H	5	0.22
(1,1149)	1:406:A:VAL:HB	1:415:A:ASN:H	8	0.22
(1,1149)	1:406:A:VAL:HB	1:415:A:ASN:H	10	0.22
(1,1149)	1:406:A:VAL:HB	1:415:A:ASN:H	17	0.22
(1,1149)	1:406:A:VAL:HB	1:415:A:ASN:H	23	0.22
(1,1149)	1:406:A:VAL:HB	1:415:A:ASN:H	25	0.22
(1,1030)	1:449:A:GLU:HG2	1:450:A:ALA:H	20	0.22
(1,463)	1:401:A:VAL:HG21	1:417:A:GLY:HA2	12	0.22
(1,463)	1:401:A:VAL:HG22	1:417:A:GLY:HA2	12	0.22
(1,463)	1:401:A:VAL:HG23	1:417:A:GLY:HA2	12	0.22
(1,3332)	1:456:A:MET:H	1:456:A:MET:HG2	11	0.21
(1,3332)	1:456:A:MET:H	1:456:A:MET:HG3	11	0.21
(1,3153)	1:418:A:LEU:HD11	1:419:A:GLN:H	1	0.21
(1,3153)	1:418:A:LEU:HD12	1:419:A:GLN:H	1	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3153)	1:418:A:LEU:HD13	1:419:A:GLN:H	1	0.21
(1,3153)	1:418:A:LEU:HD21	1:419:A:GLN:H	1	0.21
(1,3153)	1:418:A:LEU:HD22	1:419:A:GLN:H	1	0.21
(1,3153)	1:418:A:LEU:HD23	1:419:A:GLN:H	1	0.21
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD11	6	0.21
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD12	6	0.21
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD13	6	0.21
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD21	6	0.21
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD22	6	0.21
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD23	6	0.21
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD11	8	0.21
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD12	8	0.21
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD13	8	0.21
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD21	8	0.21
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD22	8	0.21
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD23	8	0.21
(1,3070)	1:400:A:VAL:HG11	1:419:A:GLN:H	6	0.21
(1,3070)	1:400:A:VAL:HG12	1:419:A:GLN:H	6	0.21
(1,3070)	1:400:A:VAL:HG13	1:419:A:GLN:H	6	0.21
(1,3070)	1:400:A:VAL:HG21	1:419:A:GLN:H	6	0.21
(1,3070)	1:400:A:VAL:HG22	1:419:A:GLN:H	6	0.21
(1,3070)	1:400:A:VAL:HG23	1:419:A:GLN:H	6	0.21
(1,3070)	1:400:A:VAL:HG11	1:419:A:GLN:H	12	0.21
(1,3070)	1:400:A:VAL:HG12	1:419:A:GLN:H	12	0.21
(1,3070)	1:400:A:VAL:HG13	1:419:A:GLN:H	12	0.21
(1,3070)	1:400:A:VAL:HG21	1:419:A:GLN:H	12	0.21
(1,3070)	1:400:A:VAL:HG22	1:419:A:GLN:H	12	0.21
(1,3070)	1:400:A:VAL:HG23	1:419:A:GLN:H	12	0.21
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE1	13	0.21
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE2	13	0.21
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE3	13	0.21
(1,1935)	1:405:A:LYS:H	1:405:A:LYS:HE2	1	0.21
(1,1935)	1:405:A:LYS:H	1:405:A:LYS:HE3	1	0.21
(1,1814)	1:446:A:LYS:H	1:446:A:LYS:HG2	18	0.21
(1,1658)	1:423:A:GLY:HA2	1:424:A:ASN:H	24	0.21
(1,1149)	1:406:A:VAL:HB	1:415:A:ASN:H	6	0.21
(1,1149)	1:406:A:VAL:HB	1:415:A:ASN:H	16	0.21
(1,1149)	1:406:A:VAL:HB	1:415:A:ASN:H	24	0.21
(1,586)	1:466:A:LYS:HA	1:466:A:LYS:HD2	23	0.21
(1,586)	1:466:A:LYS:HA	1:466:A:LYS:HD3	23	0.21
(1,463)	1:401:A:VAL:HG21	1:417:A:GLY:HA2	17	0.21
(1,463)	1:401:A:VAL:HG22	1:417:A:GLY:HA2	17	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,463)	1:401:A:VAL:HG23	1:417:A:GLY:HA2	17	0.21
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD2	2	0.21
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD3	2	0.21
(1,3332)	1:456:A:MET:H	1:456:A:MET:HG2	8	0.2
(1,3332)	1:456:A:MET:H	1:456:A:MET:HG3	8	0.2
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD11	7	0.2
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD12	7	0.2
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD13	7	0.2
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD21	7	0.2
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD22	7	0.2
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD23	7	0.2
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD11	11	0.2
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD12	11	0.2
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD13	11	0.2
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD21	11	0.2
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD22	11	0.2
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD23	11	0.2
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD11	11	0.2
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD12	11	0.2
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD13	11	0.2
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD21	11	0.2
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD22	11	0.2
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD23	11	0.2
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD11	11	0.2
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD12	11	0.2
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD13	11	0.2
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD21	11	0.2
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD22	11	0.2
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD23	11	0.2
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG2	1	0.2
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG3	1	0.2
(1,1814)	1:446:A:LYS:H	1:446:A:LYS:HG2	25	0.2
(1,1658)	1:423:A:GLY:HA2	1:424:A:ASN:H	19	0.2
(1,1658)	1:423:A:GLY:HA2	1:424:A:ASN:H	23	0.2
(1,1658)	1:423:A:GLY:HA2	1:424:A:ASN:H	25	0.2
(1,1286)	1:411:A:GLY:H	1:412:A:THR:HG21	3	0.2
(1,1286)	1:411:A:GLY:H	1:412:A:THR:HG22	3	0.2
(1,1286)	1:411:A:GLY:H	1:412:A:THR:HG23	3	0.2
(1,1149)	1:406:A:VAL:HB	1:415:A:ASN:H	2	0.2
(1,1103)	1:385:A:ASN:HA	1:391:A:VAL:H	23	0.2
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG11	16	0.2
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG12	16	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG13	16	0.2
(1,701)	1:369:A:PHE:HD1	1:370:A:PHE:HA	6	0.2
(1,701)	1:369:A:PHE:HD2	1:370:A:PHE:HA	6	0.2
(1,586)	1:466:A:LYS:HA	1:466:A:LYS:HD2	14	0.2
(1,586)	1:466:A:LYS:HA	1:466:A:LYS:HD3	14	0.2
(1,57)	1:411:A:GLY:HA3	1:412:A:THR:HB	17	0.2
(1,57)	1:411:A:GLY:HA3	1:412:A:THR:HB	18	0.2
(1,3153)	1:418:A:LEU:HD11	1:419:A:GLN:H	4	0.19
(1,3153)	1:418:A:LEU:HD12	1:419:A:GLN:H	4	0.19
(1,3153)	1:418:A:LEU:HD13	1:419:A:GLN:H	4	0.19
(1,3153)	1:418:A:LEU:HD21	1:419:A:GLN:H	4	0.19
(1,3153)	1:418:A:LEU:HD22	1:419:A:GLN:H	4	0.19
(1,3153)	1:418:A:LEU:HD23	1:419:A:GLN:H	4	0.19
(1,3070)	1:400:A:VAL:HG11	1:419:A:GLN:H	13	0.19
(1,3070)	1:400:A:VAL:HG12	1:419:A:GLN:H	13	0.19
(1,3070)	1:400:A:VAL:HG13	1:419:A:GLN:H	13	0.19
(1,3070)	1:400:A:VAL:HG21	1:419:A:GLN:H	13	0.19
(1,3070)	1:400:A:VAL:HG22	1:419:A:GLN:H	13	0.19
(1,3070)	1:400:A:VAL:HG23	1:419:A:GLN:H	13	0.19
(1,3070)	1:400:A:VAL:HG11	1:419:A:GLN:H	16	0.19
(1,3070)	1:400:A:VAL:HG12	1:419:A:GLN:H	16	0.19
(1,3070)	1:400:A:VAL:HG13	1:419:A:GLN:H	16	0.19
(1,3070)	1:400:A:VAL:HG21	1:419:A:GLN:H	16	0.19
(1,3070)	1:400:A:VAL:HG22	1:419:A:GLN:H	16	0.19
(1,3070)	1:400:A:VAL:HG23	1:419:A:GLN:H	16	0.19
(1,2665)	1:380:A:ARG:HE	1:443:A:GLU:HG2	15	0.19
(1,2665)	1:380:A:ARG:HE	1:443:A:GLU:HG3	15	0.19
(1,2000)	1:406:A:VAL:HG11	1:416:A:LYS:H	12	0.19
(1,2000)	1:406:A:VAL:HG12	1:416:A:LYS:H	12	0.19
(1,2000)	1:406:A:VAL:HG13	1:416:A:LYS:H	12	0.19
(1,2000)	1:406:A:VAL:HG11	1:416:A:LYS:H	20	0.19
(1,2000)	1:406:A:VAL:HG12	1:416:A:LYS:H	20	0.19
(1,2000)	1:406:A:VAL:HG13	1:416:A:LYS:H	20	0.19
(1,1935)	1:405:A:LYS:H	1:405:A:LYS:HE2	14	0.19
(1,1935)	1:405:A:LYS:H	1:405:A:LYS:HE3	14	0.19
(1,1829)	1:438:A:GLU:H	1:438:A:GLU:HG2	14	0.19
(1,1658)	1:423:A:GLY:HA2	1:424:A:ASN:H	8	0.19
(1,1658)	1:423:A:GLY:HA2	1:424:A:ASN:H	9	0.19
(1,1658)	1:423:A:GLY:HA2	1:424:A:ASN:H	14	0.19
(1,1658)	1:423:A:GLY:HA2	1:424:A:ASN:H	21	0.19
(1,1644)	1:418:A:LEU:H	1:418:A:LEU:HG	2	0.19
(1,1644)	1:418:A:LEU:H	1:418:A:LEU:HG	19	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1149)	1:406:A:VAL:HB	1:415:A:ASN:H	3	0.19
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG11	19	0.19
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG12	19	0.19
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG13	19	0.19
(1,167)	1:355:A:ARG:HB3	1:439:A:PHE:HD1	9	0.19
(1,167)	1:355:A:ARG:HB3	1:439:A:PHE:HD2	9	0.19
(1,57)	1:411:A:GLY:HA3	1:412:A:THR:HB	1	0.19
(1,57)	1:411:A:GLY:HA3	1:412:A:THR:HB	22	0.19
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD2	8	0.19
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD3	8	0.19
(1,3379)	1:466:A:LYS:H	1:466:A:LYS:HG2	6	0.18
(1,3379)	1:466:A:LYS:H	1:466:A:LYS:HG3	6	0.18
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD11	20	0.18
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD12	20	0.18
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD13	20	0.18
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD21	20	0.18
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD22	20	0.18
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD23	20	0.18
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD11	25	0.18
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD12	25	0.18
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD13	25	0.18
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD21	25	0.18
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD22	25	0.18
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD23	25	0.18
(1,3070)	1:400:A:VAL:HG11	1:419:A:GLN:H	4	0.18
(1,3070)	1:400:A:VAL:HG12	1:419:A:GLN:H	4	0.18
(1,3070)	1:400:A:VAL:HG13	1:419:A:GLN:H	4	0.18
(1,3070)	1:400:A:VAL:HG21	1:419:A:GLN:H	4	0.18
(1,3070)	1:400:A:VAL:HG22	1:419:A:GLN:H	4	0.18
(1,3070)	1:400:A:VAL:HG23	1:419:A:GLN:H	4	0.18
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD11	6	0.18
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD12	6	0.18
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD13	6	0.18
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD21	6	0.18
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD22	6	0.18
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD23	6	0.18
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD11	6	0.18
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD12	6	0.18
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD13	6	0.18
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD21	6	0.18
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD22	6	0.18
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD23	6	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD11	6	0.18
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD12	6	0.18
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD13	6	0.18
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD21	6	0.18
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD22	6	0.18
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD23	6	0.18
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD11	8	0.18
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD12	8	0.18
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD13	8	0.18
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD21	8	0.18
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD22	8	0.18
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD23	8	0.18
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD11	8	0.18
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD12	8	0.18
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD13	8	0.18
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD21	8	0.18
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD22	8	0.18
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD23	8	0.18
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD11	8	0.18
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD12	8	0.18
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD13	8	0.18
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD21	8	0.18
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD22	8	0.18
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD23	8	0.18
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD11	13	0.18
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD12	13	0.18
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD13	13	0.18
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD21	13	0.18
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD22	13	0.18
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD23	13	0.18
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD11	13	0.18
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD12	13	0.18
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD13	13	0.18
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD21	13	0.18
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD22	13	0.18
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD23	13	0.18
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD11	13	0.18
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD12	13	0.18
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD13	13	0.18
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD21	13	0.18
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD22	13	0.18
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD23	13	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2923)	1:364:A:TRP:HB3	1:367:A:MET:HB2	12	0.18
(1,2923)	1:364:A:TRP:HB3	1:367:A:MET:HB3	12	0.18
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG2	2	0.18
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG3	2	0.18
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE1	6	0.18
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE2	6	0.18
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE3	6	0.18
(1,2250)	1:429:A:PHE:H	1:429:A:PHE:HD1	14	0.18
(1,2117)	1:423:A:GLY:HA2	1:450:A:ALA:H	6	0.18
(1,2117)	1:423:A:GLY:HA2	1:450:A:ALA:H	23	0.18
(1,1935)	1:405:A:LYS:H	1:405:A:LYS:HE2	25	0.18
(1,1935)	1:405:A:LYS:H	1:405:A:LYS:HE3	25	0.18
(1,1882)	1:423:A:GLY:HA3	1:447:A:TRP:HE1	8	0.18
(1,1814)	1:446:A:LYS:H	1:446:A:LYS:HG2	1	0.18
(1,1814)	1:446:A:LYS:H	1:446:A:LYS:HG2	14	0.18
(1,1814)	1:446:A:LYS:H	1:446:A:LYS:HG2	17	0.18
(1,1660)	1:425:A:ASP:HB3	1:426:A:GLN:H	19	0.18
(1,1658)	1:423:A:GLY:HA2	1:424:A:ASN:H	22	0.18
(1,1644)	1:418:A:LEU:H	1:418:A:LEU:HG	3	0.18
(1,1644)	1:418:A:LEU:H	1:418:A:LEU:HG	10	0.18
(1,1644)	1:418:A:LEU:H	1:418:A:LEU:HG	15	0.18
(1,1644)	1:418:A:LEU:H	1:418:A:LEU:HG	23	0.18
(1,1149)	1:406:A:VAL:HB	1:415:A:ASN:H	18	0.18
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG11	11	0.18
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG12	11	0.18
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG13	11	0.18
(1,737)	1:345:A:VAL:HG21	1:459:A:PRO:HD3	10	0.18
(1,737)	1:345:A:VAL:HG22	1:459:A:PRO:HD3	10	0.18
(1,737)	1:345:A:VAL:HG23	1:459:A:PRO:HD3	10	0.18
(1,719)	1:363:A:ARG:HA	1:363:A:ARG:HD2	18	0.18
(1,719)	1:363:A:ARG:HA	1:363:A:ARG:HD3	18	0.18
(1,463)	1:401:A:VAL:HG21	1:417:A:GLY:HA2	3	0.18
(1,463)	1:401:A:VAL:HG22	1:417:A:GLY:HA2	3	0.18
(1,463)	1:401:A:VAL:HG23	1:417:A:GLY:HA2	3	0.18
(1,463)	1:401:A:VAL:HG21	1:417:A:GLY:HA2	23	0.18
(1,463)	1:401:A:VAL:HG22	1:417:A:GLY:HA2	23	0.18
(1,463)	1:401:A:VAL:HG23	1:417:A:GLY:HA2	23	0.18
(1,57)	1:411:A:GLY:HA3	1:412:A:THR:HB	5	0.18
(1,57)	1:411:A:GLY:HA3	1:412:A:THR:HB	11	0.18
(1,57)	1:411:A:GLY:HA3	1:412:A:THR:HB	12	0.18
(1,57)	1:411:A:GLY:HA3	1:412:A:THR:HB	13	0.18
(1,57)	1:411:A:GLY:HA3	1:412:A:THR:HB	21	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,57)	1:411:A:GLY:HA3	1:412:A:THR:HB	23	0.18
(1,57)	1:411:A:GLY:HA3	1:412:A:THR:HB	24	0.18
(1,57)	1:411:A:GLY:HA3	1:412:A:THR:HB	25	0.18
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD2	10	0.18
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD3	10	0.18
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD2	24	0.18
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD3	24	0.18
(1,3379)	1:466:A:LYS:H	1:466:A:LYS:HG2	11	0.17
(1,3379)	1:466:A:LYS:H	1:466:A:LYS:HG3	11	0.17
(1,3153)	1:418:A:LEU:HD11	1:419:A:GLN:H	11	0.17
(1,3153)	1:418:A:LEU:HD12	1:419:A:GLN:H	11	0.17
(1,3153)	1:418:A:LEU:HD13	1:419:A:GLN:H	11	0.17
(1,3153)	1:418:A:LEU:HD21	1:419:A:GLN:H	11	0.17
(1,3153)	1:418:A:LEU:HD22	1:419:A:GLN:H	11	0.17
(1,3153)	1:418:A:LEU:HD23	1:419:A:GLN:H	11	0.17
(1,3103)	1:407:A:TYR:HE1	1:416:A:LYS:HD2	13	0.17
(1,3103)	1:407:A:TYR:HE1	1:416:A:LYS:HD3	13	0.17
(1,3103)	1:407:A:TYR:HE2	1:416:A:LYS:HD2	13	0.17
(1,3103)	1:407:A:TYR:HE2	1:416:A:LYS:HD3	13	0.17
(1,3070)	1:400:A:VAL:HG11	1:419:A:GLN:H	3	0.17
(1,3070)	1:400:A:VAL:HG12	1:419:A:GLN:H	3	0.17
(1,3070)	1:400:A:VAL:HG13	1:419:A:GLN:H	3	0.17
(1,3070)	1:400:A:VAL:HG21	1:419:A:GLN:H	3	0.17
(1,3070)	1:400:A:VAL:HG22	1:419:A:GLN:H	3	0.17
(1,3070)	1:400:A:VAL:HG23	1:419:A:GLN:H	3	0.17
(1,3070)	1:400:A:VAL:HG11	1:419:A:GLN:H	10	0.17
(1,3070)	1:400:A:VAL:HG12	1:419:A:GLN:H	10	0.17
(1,3070)	1:400:A:VAL:HG13	1:419:A:GLN:H	10	0.17
(1,3070)	1:400:A:VAL:HG21	1:419:A:GLN:H	10	0.17
(1,3070)	1:400:A:VAL:HG22	1:419:A:GLN:H	10	0.17
(1,3070)	1:400:A:VAL:HG23	1:419:A:GLN:H	10	0.17
(1,3070)	1:400:A:VAL:HG11	1:419:A:GLN:H	15	0.17
(1,3070)	1:400:A:VAL:HG12	1:419:A:GLN:H	15	0.17
(1,3070)	1:400:A:VAL:HG13	1:419:A:GLN:H	15	0.17
(1,3070)	1:400:A:VAL:HG21	1:419:A:GLN:H	15	0.17
(1,3070)	1:400:A:VAL:HG22	1:419:A:GLN:H	15	0.17
(1,3070)	1:400:A:VAL:HG23	1:419:A:GLN:H	15	0.17
(1,2949)	1:374:A:VAL:HG21	1:400:A:VAL:HG11	18	0.17
(1,2949)	1:374:A:VAL:HG21	1:400:A:VAL:HG12	18	0.17
(1,2949)	1:374:A:VAL:HG21	1:400:A:VAL:HG13	18	0.17
(1,2949)	1:374:A:VAL:HG21	1:400:A:VAL:HG21	18	0.17
(1,2949)	1:374:A:VAL:HG21	1:400:A:VAL:HG22	18	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2949)	1:374:A:VAL:HG21	1:400:A:VAL:HG23	18	0.17
(1,2949)	1:374:A:VAL:HG22	1:400:A:VAL:HG11	18	0.17
(1,2949)	1:374:A:VAL:HG22	1:400:A:VAL:HG12	18	0.17
(1,2949)	1:374:A:VAL:HG22	1:400:A:VAL:HG13	18	0.17
(1,2949)	1:374:A:VAL:HG22	1:400:A:VAL:HG21	18	0.17
(1,2949)	1:374:A:VAL:HG22	1:400:A:VAL:HG22	18	0.17
(1,2949)	1:374:A:VAL:HG22	1:400:A:VAL:HG23	18	0.17
(1,2949)	1:374:A:VAL:HG23	1:400:A:VAL:HG11	18	0.17
(1,2949)	1:374:A:VAL:HG23	1:400:A:VAL:HG12	18	0.17
(1,2949)	1:374:A:VAL:HG23	1:400:A:VAL:HG13	18	0.17
(1,2949)	1:374:A:VAL:HG23	1:400:A:VAL:HG21	18	0.17
(1,2949)	1:374:A:VAL:HG23	1:400:A:VAL:HG22	18	0.17
(1,2949)	1:374:A:VAL:HG23	1:400:A:VAL:HG23	18	0.17
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD11	22	0.17
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD12	22	0.17
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD13	22	0.17
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD21	22	0.17
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD22	22	0.17
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD23	22	0.17
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD11	22	0.17
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD12	22	0.17
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD13	22	0.17
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD21	22	0.17
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD22	22	0.17
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD23	22	0.17
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD11	22	0.17
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD12	22	0.17
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD13	22	0.17
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD21	22	0.17
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD22	22	0.17
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD23	22	0.17
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD11	24	0.17
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD12	24	0.17
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD13	24	0.17
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD21	24	0.17
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD22	24	0.17
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD23	24	0.17
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD11	24	0.17
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD12	24	0.17
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD13	24	0.17
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD21	24	0.17
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD22	24	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD23	24	0.17
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD11	24	0.17
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD12	24	0.17
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD13	24	0.17
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD21	24	0.17
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD22	24	0.17
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD23	24	0.17
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG2	6	0.17
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG3	6	0.17
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG2	12	0.17
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG3	12	0.17
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG2	15	0.17
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG3	15	0.17
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG2	21	0.17
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG3	21	0.17
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG2	24	0.17
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG3	24	0.17
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE1	16	0.17
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE2	16	0.17
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE3	16	0.17
(1,2250)	1:429:A:PHE:H	1:429:A:PHE:HD1	6	0.17
(1,2117)	1:423:A:GLY:HA2	1:450:A:ALA:H	2	0.17
(1,2117)	1:423:A:GLY:HA2	1:450:A:ALA:H	3	0.17
(1,2117)	1:423:A:GLY:HA2	1:450:A:ALA:H	15	0.17
(1,2086)	1:-1:A:MET:H	1:461:A:LEU:HG	16	0.17
(1,2000)	1:406:A:VAL:HG11	1:416:A:LYS:H	1	0.17
(1,2000)	1:406:A:VAL:HG12	1:416:A:LYS:H	1	0.17
(1,2000)	1:406:A:VAL:HG13	1:416:A:LYS:H	1	0.17
(1,1660)	1:425:A:ASP:HB3	1:426:A:GLN:H	3	0.17
(1,1660)	1:425:A:ASP:HB3	1:426:A:GLN:H	6	0.17
(1,1660)	1:425:A:ASP:HB3	1:426:A:GLN:H	10	0.17
(1,1658)	1:423:A:GLY:HA2	1:424:A:ASN:H	3	0.17
(1,1658)	1:423:A:GLY:HA2	1:424:A:ASN:H	5	0.17
(1,1658)	1:423:A:GLY:HA2	1:424:A:ASN:H	10	0.17
(1,1644)	1:418:A:LEU:H	1:418:A:LEU:HG	13	0.17
(1,1644)	1:418:A:LEU:H	1:418:A:LEU:HG	14	0.17
(1,1644)	1:418:A:LEU:H	1:418:A:LEU:HG	16	0.17
(1,1389)	1:435:A:SER:HA	1:437:A:GLN:HE22	23	0.17
(1,737)	1:345:A:VAL:HG21	1:459:A:PRO:HD3	1	0.17
(1,737)	1:345:A:VAL:HG22	1:459:A:PRO:HD3	1	0.17
(1,737)	1:345:A:VAL:HG23	1:459:A:PRO:HD3	1	0.17
(1,737)	1:345:A:VAL:HG21	1:459:A:PRO:HD3	20	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,737)	1:345:A:VAL:HG22	1:459:A:PRO:HD3	20	0.17
(1,737)	1:345:A:VAL:HG23	1:459:A:PRO:HD3	20	0.17
(1,719)	1:363:A:ARG:HA	1:363:A:ARG:HD2	1	0.17
(1,719)	1:363:A:ARG:HA	1:363:A:ARG:HD3	1	0.17
(1,719)	1:363:A:ARG:HA	1:363:A:ARG:HD2	3	0.17
(1,719)	1:363:A:ARG:HA	1:363:A:ARG:HD3	3	0.17
(1,719)	1:363:A:ARG:HA	1:363:A:ARG:HD2	13	0.17
(1,719)	1:363:A:ARG:HA	1:363:A:ARG:HD3	13	0.17
(1,586)	1:466:A:LYS:HA	1:466:A:LYS:HD2	20	0.17
(1,586)	1:466:A:LYS:HA	1:466:A:LYS:HD3	20	0.17
(1,161)	1:370:A:PHE:HD1	1:371:A:ALA:HB1	20	0.17
(1,161)	1:370:A:PHE:HD1	1:371:A:ALA:HB2	20	0.17
(1,161)	1:370:A:PHE:HD1	1:371:A:ALA:HB3	20	0.17
(1,161)	1:370:A:PHE:HD2	1:371:A:ALA:HB1	20	0.17
(1,161)	1:370:A:PHE:HD2	1:371:A:ALA:HB2	20	0.17
(1,161)	1:370:A:PHE:HD2	1:371:A:ALA:HB3	20	0.17
(1,57)	1:411:A:GLY:HA3	1:412:A:THR:HB	4	0.17
(1,57)	1:411:A:GLY:HA3	1:412:A:THR:HB	8	0.17
(1,57)	1:411:A:GLY:HA3	1:412:A:THR:HB	10	0.17
(1,57)	1:411:A:GLY:HA3	1:412:A:THR:HB	14	0.17
(1,57)	1:411:A:GLY:HA3	1:412:A:THR:HB	20	0.17
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD2	21	0.17
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD3	21	0.17
(1,3379)	1:466:A:LYS:H	1:466:A:LYS:HG2	16	0.16
(1,3379)	1:466:A:LYS:H	1:466:A:LYS:HG3	16	0.16
(1,3153)	1:418:A:LEU:HD11	1:419:A:GLN:H	6	0.16
(1,3153)	1:418:A:LEU:HD12	1:419:A:GLN:H	6	0.16
(1,3153)	1:418:A:LEU:HD13	1:419:A:GLN:H	6	0.16
(1,3153)	1:418:A:LEU:HD21	1:419:A:GLN:H	6	0.16
(1,3153)	1:418:A:LEU:HD22	1:419:A:GLN:H	6	0.16
(1,3153)	1:418:A:LEU:HD23	1:419:A:GLN:H	6	0.16
(1,3153)	1:418:A:LEU:HD11	1:419:A:GLN:H	20	0.16
(1,3153)	1:418:A:LEU:HD12	1:419:A:GLN:H	20	0.16
(1,3153)	1:418:A:LEU:HD13	1:419:A:GLN:H	20	0.16
(1,3153)	1:418:A:LEU:HD21	1:419:A:GLN:H	20	0.16
(1,3153)	1:418:A:LEU:HD22	1:419:A:GLN:H	20	0.16
(1,3153)	1:418:A:LEU:HD23	1:419:A:GLN:H	20	0.16
(1,3070)	1:400:A:VAL:HG11	1:419:A:GLN:H	18	0.16
(1,3070)	1:400:A:VAL:HG12	1:419:A:GLN:H	18	0.16
(1,3070)	1:400:A:VAL:HG13	1:419:A:GLN:H	18	0.16
(1,3070)	1:400:A:VAL:HG21	1:419:A:GLN:H	18	0.16
(1,3070)	1:400:A:VAL:HG22	1:419:A:GLN:H	18	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3070)	1:400:A:VAL:HG23	1:419:A:GLN:H	18	0.16
(1,2923)	1:364:A:TRP:HB3	1:367:A:MET:HB2	23	0.16
(1,2923)	1:364:A:TRP:HB3	1:367:A:MET:HB3	23	0.16
(1,2624)	1:455:A:GLY:H	1:456:A:MET:HG2	11	0.16
(1,2624)	1:455:A:GLY:H	1:456:A:MET:HG3	11	0.16
(1,2624)	1:455:A:GLY:H	1:456:A:MET:HG2	17	0.16
(1,2624)	1:455:A:GLY:H	1:456:A:MET:HG3	17	0.16
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE1	12	0.16
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE2	12	0.16
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE3	12	0.16
(1,2328)	1:-2:A:HIS:HA	1:-1:A:MET:H	19	0.16
(1,2250)	1:429:A:PHE:H	1:429:A:PHE:HD1	3	0.16
(1,2250)	1:429:A:PHE:H	1:429:A:PHE:HD1	4	0.16
(1,2250)	1:429:A:PHE:H	1:429:A:PHE:HD1	22	0.16
(1,2117)	1:423:A:GLY:HA2	1:450:A:ALA:H	4	0.16
(1,2117)	1:423:A:GLY:HA2	1:450:A:ALA:H	20	0.16
(1,2117)	1:423:A:GLY:HA2	1:450:A:ALA:H	21	0.16
(1,2117)	1:423:A:GLY:HA2	1:450:A:ALA:H	22	0.16
(1,1935)	1:405:A:LYS:H	1:405:A:LYS:HE2	19	0.16
(1,1935)	1:405:A:LYS:H	1:405:A:LYS:HE3	19	0.16
(1,1889)	1:392:A:TYR:HE1	1:437:A:GLN:H	24	0.16
(1,1889)	1:392:A:TYR:HE2	1:437:A:GLN:H	24	0.16
(1,1888)	1:380:A:ARG:HE	1:437:A:GLN:H	3	0.16
(1,1829)	1:438:A:GLU:H	1:438:A:GLU:HG2	20	0.16
(1,1809)	1:423:A:GLY:HA3	1:456:A:MET:H	12	0.16
(1,1660)	1:425:A:ASP:HB3	1:426:A:GLN:H	8	0.16
(1,1660)	1:425:A:ASP:HB3	1:426:A:GLN:H	11	0.16
(1,1658)	1:423:A:GLY:HA2	1:424:A:ASN:H	6	0.16
(1,1658)	1:423:A:GLY:HA2	1:424:A:ASN:H	11	0.16
(1,1658)	1:423:A:GLY:HA2	1:424:A:ASN:H	12	0.16
(1,1658)	1:423:A:GLY:HA2	1:424:A:ASN:H	13	0.16
(1,1658)	1:423:A:GLY:HA2	1:424:A:ASN:H	15	0.16
(1,1644)	1:418:A:LEU:H	1:418:A:LEU:HG	12	0.16
(1,1644)	1:418:A:LEU:H	1:418:A:LEU:HG	18	0.16
(1,914)	1:460:A:THR:HA	1:461:A:LEU:HG	1	0.16
(1,737)	1:345:A:VAL:HG21	1:459:A:PRO:HD3	4	0.16
(1,737)	1:345:A:VAL:HG22	1:459:A:PRO:HD3	4	0.16
(1,737)	1:345:A:VAL:HG23	1:459:A:PRO:HD3	4	0.16
(1,737)	1:345:A:VAL:HG21	1:459:A:PRO:HD3	5	0.16
(1,737)	1:345:A:VAL:HG22	1:459:A:PRO:HD3	5	0.16
(1,737)	1:345:A:VAL:HG23	1:459:A:PRO:HD3	5	0.16
(1,737)	1:345:A:VAL:HG21	1:459:A:PRO:HD3	18	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,737)	1:345:A:VAL:HG22	1:459:A:PRO:HD3	18	0.16
(1,737)	1:345:A:VAL:HG23	1:459:A:PRO:HD3	18	0.16
(1,719)	1:363:A:ARG:HA	1:363:A:ARG:HD2	19	0.16
(1,719)	1:363:A:ARG:HA	1:363:A:ARG:HD3	19	0.16
(1,719)	1:363:A:ARG:HA	1:363:A:ARG:HD2	24	0.16
(1,719)	1:363:A:ARG:HA	1:363:A:ARG:HD3	24	0.16
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD11	13	0.16
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD12	13	0.16
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD13	13	0.16
(1,57)	1:411:A:GLY:HA3	1:412:A:THR:HB	2	0.16
(1,57)	1:411:A:GLY:HA3	1:412:A:THR:HB	6	0.16
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD2	20	0.16
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD3	20	0.16
(1,3358)	1:460:A:THR:H	1:463:A:GLU:HB2	8	0.15
(1,3358)	1:460:A:THR:H	1:463:A:GLU:HB3	8	0.15
(1,3358)	1:460:A:THR:H	1:463:A:GLU:HB2	10	0.15
(1,3358)	1:460:A:THR:H	1:463:A:GLU:HB3	10	0.15
(1,3286)	1:446:A:LYS:HG2	1:449:A:GLU:H	3	0.15
(1,3286)	1:446:A:LYS:HG3	1:449:A:GLU:H	3	0.15
(1,3184)	1:423:A:GLY:HA3	1:456:A:MET:HB2	2	0.15
(1,3184)	1:423:A:GLY:HA3	1:456:A:MET:HB3	2	0.15
(1,3153)	1:418:A:LEU:HD11	1:419:A:GLN:H	8	0.15
(1,3153)	1:418:A:LEU:HD12	1:419:A:GLN:H	8	0.15
(1,3153)	1:418:A:LEU:HD13	1:419:A:GLN:H	8	0.15
(1,3153)	1:418:A:LEU:HD21	1:419:A:GLN:H	8	0.15
(1,3153)	1:418:A:LEU:HD22	1:419:A:GLN:H	8	0.15
(1,3153)	1:418:A:LEU:HD23	1:419:A:GLN:H	8	0.15
(1,3153)	1:418:A:LEU:HD11	1:419:A:GLN:H	25	0.15
(1,3153)	1:418:A:LEU:HD12	1:419:A:GLN:H	25	0.15
(1,3153)	1:418:A:LEU:HD13	1:419:A:GLN:H	25	0.15
(1,3153)	1:418:A:LEU:HD21	1:419:A:GLN:H	25	0.15
(1,3153)	1:418:A:LEU:HD22	1:419:A:GLN:H	25	0.15
(1,3153)	1:418:A:LEU:HD23	1:419:A:GLN:H	25	0.15
(1,3070)	1:400:A:VAL:HG11	1:419:A:GLN:H	17	0.15
(1,3070)	1:400:A:VAL:HG12	1:419:A:GLN:H	17	0.15
(1,3070)	1:400:A:VAL:HG13	1:419:A:GLN:H	17	0.15
(1,3070)	1:400:A:VAL:HG21	1:419:A:GLN:H	17	0.15
(1,3070)	1:400:A:VAL:HG22	1:419:A:GLN:H	17	0.15
(1,3070)	1:400:A:VAL:HG23	1:419:A:GLN:H	17	0.15
(1,3070)	1:400:A:VAL:HG11	1:419:A:GLN:H	21	0.15
(1,3070)	1:400:A:VAL:HG12	1:419:A:GLN:H	21	0.15
(1,3070)	1:400:A:VAL:HG13	1:419:A:GLN:H	21	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3070)	1:400:A:VAL:HG21	1:419:A:GLN:H	21	0.15
(1,3070)	1:400:A:VAL:HG22	1:419:A:GLN:H	21	0.15
(1,3070)	1:400:A:VAL:HG23	1:419:A:GLN:H	21	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD11	2	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD12	2	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD13	2	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD21	2	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD22	2	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD23	2	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD11	2	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD12	2	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD13	2	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD21	2	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD22	2	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD23	2	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD11	2	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD12	2	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD13	2	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD21	2	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD22	2	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD23	2	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD11	12	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD12	12	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD13	12	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD21	12	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD22	12	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD23	12	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD11	12	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD12	12	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD13	12	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD21	12	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD22	12	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD23	12	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD11	12	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD12	12	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD13	12	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD21	12	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD22	12	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD23	12	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD11	15	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD12	15	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD13	15	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD21	15	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD22	15	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD23	15	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD11	15	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD12	15	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD13	15	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD21	15	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD22	15	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD23	15	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD11	15	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD12	15	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD13	15	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD21	15	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD22	15	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD23	15	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD11	23	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD12	23	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD13	23	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD21	23	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD22	23	0.15
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD23	23	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD11	23	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD12	23	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD13	23	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD21	23	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD22	23	0.15
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD23	23	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD11	23	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD12	23	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD13	23	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD21	23	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD22	23	0.15
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD23	23	0.15
(1,2678)	1:-1:A:MET:HE1	1:345:A:VAL:H	22	0.15
(1,2678)	1:-1:A:MET:HE2	1:345:A:VAL:H	22	0.15
(1,2678)	1:-1:A:MET:HE3	1:345:A:VAL:H	22	0.15
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG2	18	0.15
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG3	18	0.15
(1,2624)	1:455:A:GLY:H	1:456:A:MET:HG2	8	0.15
(1,2624)	1:455:A:GLY:H	1:456:A:MET:HG3	8	0.15
(1,2328)	1:-2:A:HIS:HA	1:-1:A:MET:H	4	0.15
(1,2180)	1:382:A:GLY:HA3	1:393:A:ARG:H	13	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2173)	1:423:A:GLY:H	1:454:A:ALA:HB1	13	0.15
(1,2173)	1:423:A:GLY:H	1:454:A:ALA:HB2	13	0.15
(1,2173)	1:423:A:GLY:H	1:454:A:ALA:HB3	13	0.15
(1,2117)	1:423:A:GLY:HA2	1:450:A:ALA:H	10	0.15
(1,2117)	1:423:A:GLY:HA2	1:450:A:ALA:H	14	0.15
(1,2117)	1:423:A:GLY:HA2	1:450:A:ALA:H	19	0.15
(1,2025)	1:358:A:ARG:H	1:358:A:ARG:HG3	2	0.15
(1,1940)	1:362:A:GLU:H	1:412:A:THR:HG21	17	0.15
(1,1940)	1:362:A:GLU:H	1:412:A:THR:HG22	17	0.15
(1,1940)	1:362:A:GLU:H	1:412:A:THR:HG23	17	0.15
(1,1935)	1:405:A:LYS:H	1:405:A:LYS:HE2	8	0.15
(1,1935)	1:405:A:LYS:H	1:405:A:LYS:HE3	8	0.15
(1,1935)	1:405:A:LYS:H	1:405:A:LYS:HE2	10	0.15
(1,1935)	1:405:A:LYS:H	1:405:A:LYS:HE3	10	0.15
(1,1888)	1:380:A:ARG:HE	1:437:A:GLN:H	18	0.15
(1,1661)	1:421:A:ARG:HD2	1:425:A:ASP:H	9	0.15
(1,1661)	1:421:A:ARG:HD3	1:425:A:ASP:H	9	0.15
(1,1661)	1:421:A:ARG:HD2	1:425:A:ASP:H	22	0.15
(1,1661)	1:421:A:ARG:HD3	1:425:A:ASP:H	22	0.15
(1,1660)	1:425:A:ASP:HB3	1:426:A:GLN:H	2	0.15
(1,1660)	1:425:A:ASP:HB3	1:426:A:GLN:H	4	0.15
(1,1658)	1:423:A:GLY:HA2	1:424:A:ASN:H	17	0.15
(1,1644)	1:418:A:LEU:H	1:418:A:LEU:HG	17	0.15
(1,1389)	1:435:A:SER:HA	1:437:A:GLN:HE22	9	0.15
(1,1153)	1:366:A:HIS:HE1	1:367:A:MET:H	17	0.15
(1,914)	1:460:A:THR:HA	1:461:A:LEU:HG	13	0.15
(1,737)	1:345:A:VAL:HG21	1:459:A:PRO:HD3	13	0.15
(1,737)	1:345:A:VAL:HG22	1:459:A:PRO:HD3	13	0.15
(1,737)	1:345:A:VAL:HG23	1:459:A:PRO:HD3	13	0.15
(1,719)	1:363:A:ARG:HA	1:363:A:ARG:HD2	9	0.15
(1,719)	1:363:A:ARG:HA	1:363:A:ARG:HD3	9	0.15
(1,662)	1:438:A:GLU:HA	1:438:A:GLU:HG3	16	0.15
(1,535)	1:363:A:ARG:HD2	1:364:A:TRP:H	10	0.15
(1,535)	1:363:A:ARG:HD3	1:364:A:TRP:H	10	0.15
(1,510)	1:440:A:THR:HA	1:441:A:GLU:HG2	25	0.15
(1,510)	1:440:A:THR:HA	1:441:A:GLU:HG3	25	0.15
(1,463)	1:401:A:VAL:HG21	1:417:A:GLY:HA2	9	0.15
(1,463)	1:401:A:VAL:HG22	1:417:A:GLY:HA2	9	0.15
(1,463)	1:401:A:VAL:HG23	1:417:A:GLY:HA2	9	0.15
(1,463)	1:401:A:VAL:HG21	1:417:A:GLY:HA2	22	0.15
(1,463)	1:401:A:VAL:HG22	1:417:A:GLY:HA2	22	0.15
(1,463)	1:401:A:VAL:HG23	1:417:A:GLY:HA2	22	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD11	3	0.15
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD12	3	0.15
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD13	3	0.15
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD11	6	0.15
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD12	6	0.15
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD13	6	0.15
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD11	11	0.15
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD12	11	0.15
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD13	11	0.15
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD11	18	0.15
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD12	18	0.15
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD13	18	0.15
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD11	21	0.15
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD12	21	0.15
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD13	21	0.15
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD11	23	0.15
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD12	23	0.15
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD13	23	0.15
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD11	24	0.15
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD12	24	0.15
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD13	24	0.15
(1,247)	1:440:A:THR:HG21	1:444:A:PHE:H	1	0.15
(1,247)	1:440:A:THR:HG22	1:444:A:PHE:H	1	0.15
(1,247)	1:440:A:THR:HG23	1:444:A:PHE:H	1	0.15
(1,178)	1:393:A:ARG:H	1:395:A:ALA:HB1	17	0.15
(1,178)	1:393:A:ARG:H	1:395:A:ALA:HB2	17	0.15
(1,178)	1:393:A:ARG:H	1:395:A:ALA:HB3	17	0.15
(1,167)	1:355:A:ARG:HB3	1:439:A:PHE:HD1	22	0.15
(1,167)	1:355:A:ARG:HB3	1:439:A:PHE:HD2	22	0.15
(1,78)	1:370:A:PHE:H	1:370:A:PHE:HB2	23	0.15
(1,57)	1:411:A:GLY:HA3	1:412:A:THR:HB	19	0.15
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD2	11	0.15
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD3	11	0.15
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD2	22	0.15
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD3	22	0.15
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD2	23	0.15
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD3	23	0.15
(1,3410)	1:470:A:SER:HA	1:472:A:LYS:HG2	8	0.14
(1,3410)	1:470:A:SER:HA	1:472:A:LYS:HG3	8	0.14
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD11	5	0.14
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD12	5	0.14
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD13	5	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD21	5	0.14
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD22	5	0.14
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD23	5	0.14
(1,3248)	1:435:A:SER:HA	1:437:A:GLN:HG2	6	0.14
(1,3248)	1:435:A:SER:HA	1:437:A:GLN:HG3	6	0.14
(1,3153)	1:418:A:LEU:HD11	1:419:A:GLN:H	3	0.14
(1,3153)	1:418:A:LEU:HD12	1:419:A:GLN:H	3	0.14
(1,3153)	1:418:A:LEU:HD13	1:419:A:GLN:H	3	0.14
(1,3153)	1:418:A:LEU:HD21	1:419:A:GLN:H	3	0.14
(1,3153)	1:418:A:LEU:HD22	1:419:A:GLN:H	3	0.14
(1,3153)	1:418:A:LEU:HD23	1:419:A:GLN:H	3	0.14
(1,3153)	1:418:A:LEU:HD11	1:419:A:GLN:H	7	0.14
(1,3153)	1:418:A:LEU:HD12	1:419:A:GLN:H	7	0.14
(1,3153)	1:418:A:LEU:HD13	1:419:A:GLN:H	7	0.14
(1,3153)	1:418:A:LEU:HD21	1:419:A:GLN:H	7	0.14
(1,3153)	1:418:A:LEU:HD22	1:419:A:GLN:H	7	0.14
(1,3153)	1:418:A:LEU:HD23	1:419:A:GLN:H	7	0.14
(1,3153)	1:418:A:LEU:HD11	1:419:A:GLN:H	14	0.14
(1,3153)	1:418:A:LEU:HD12	1:419:A:GLN:H	14	0.14
(1,3153)	1:418:A:LEU:HD13	1:419:A:GLN:H	14	0.14
(1,3153)	1:418:A:LEU:HD21	1:419:A:GLN:H	14	0.14
(1,3153)	1:418:A:LEU:HD22	1:419:A:GLN:H	14	0.14
(1,3153)	1:418:A:LEU:HD23	1:419:A:GLN:H	14	0.14
(1,3153)	1:418:A:LEU:HD11	1:419:A:GLN:H	23	0.14
(1,3153)	1:418:A:LEU:HD12	1:419:A:GLN:H	23	0.14
(1,3153)	1:418:A:LEU:HD13	1:419:A:GLN:H	23	0.14
(1,3153)	1:418:A:LEU:HD21	1:419:A:GLN:H	23	0.14
(1,3153)	1:418:A:LEU:HD22	1:419:A:GLN:H	23	0.14
(1,3153)	1:418:A:LEU:HD23	1:419:A:GLN:H	23	0.14
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD11	4	0.14
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD12	4	0.14
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD13	4	0.14
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD21	4	0.14
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD22	4	0.14
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD23	4	0.14
(1,3070)	1:400:A:VAL:HG11	1:419:A:GLN:H	1	0.14
(1,3070)	1:400:A:VAL:HG12	1:419:A:GLN:H	1	0.14
(1,3070)	1:400:A:VAL:HG13	1:419:A:GLN:H	1	0.14
(1,3070)	1:400:A:VAL:HG21	1:419:A:GLN:H	1	0.14
(1,3070)	1:400:A:VAL:HG22	1:419:A:GLN:H	1	0.14
(1,3070)	1:400:A:VAL:HG23	1:419:A:GLN:H	1	0.14
(1,3007)	1:384:A:GLY:H	1:391:A:VAL:HG11	23	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3007)	1:384:A:GLY:H	1:391:A:VAL:HG12	23	0.14
(1,3007)	1:384:A:GLY:H	1:391:A:VAL:HG13	23	0.14
(1,3007)	1:384:A:GLY:H	1:391:A:VAL:HG21	23	0.14
(1,3007)	1:384:A:GLY:H	1:391:A:VAL:HG22	23	0.14
(1,3007)	1:384:A:GLY:H	1:391:A:VAL:HG23	23	0.14
(1,2949)	1:374:A:VAL:HG21	1:400:A:VAL:HG11	17	0.14
(1,2949)	1:374:A:VAL:HG21	1:400:A:VAL:HG12	17	0.14
(1,2949)	1:374:A:VAL:HG21	1:400:A:VAL:HG13	17	0.14
(1,2949)	1:374:A:VAL:HG21	1:400:A:VAL:HG21	17	0.14
(1,2949)	1:374:A:VAL:HG21	1:400:A:VAL:HG22	17	0.14
(1,2949)	1:374:A:VAL:HG21	1:400:A:VAL:HG23	17	0.14
(1,2949)	1:374:A:VAL:HG22	1:400:A:VAL:HG11	17	0.14
(1,2949)	1:374:A:VAL:HG22	1:400:A:VAL:HG12	17	0.14
(1,2949)	1:374:A:VAL:HG22	1:400:A:VAL:HG13	17	0.14
(1,2949)	1:374:A:VAL:HG22	1:400:A:VAL:HG21	17	0.14
(1,2949)	1:374:A:VAL:HG22	1:400:A:VAL:HG22	17	0.14
(1,2949)	1:374:A:VAL:HG22	1:400:A:VAL:HG23	17	0.14
(1,2949)	1:374:A:VAL:HG23	1:400:A:VAL:HG11	17	0.14
(1,2949)	1:374:A:VAL:HG23	1:400:A:VAL:HG12	17	0.14
(1,2949)	1:374:A:VAL:HG23	1:400:A:VAL:HG13	17	0.14
(1,2949)	1:374:A:VAL:HG23	1:400:A:VAL:HG21	17	0.14
(1,2949)	1:374:A:VAL:HG23	1:400:A:VAL:HG22	17	0.14
(1,2949)	1:374:A:VAL:HG23	1:400:A:VAL:HG23	17	0.14
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD11	10	0.14
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD12	10	0.14
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD13	10	0.14
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD21	10	0.14
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD22	10	0.14
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD23	10	0.14
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD11	10	0.14
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD12	10	0.14
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD13	10	0.14
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD21	10	0.14
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD22	10	0.14
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD23	10	0.14
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD11	10	0.14
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD12	10	0.14
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD13	10	0.14
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD21	10	0.14
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD22	10	0.14
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD23	10	0.14
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD11	20	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD12	20	0.14
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD13	20	0.14
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD21	20	0.14
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD22	20	0.14
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD23	20	0.14
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD11	20	0.14
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD12	20	0.14
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD13	20	0.14
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD21	20	0.14
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD22	20	0.14
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD23	20	0.14
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD11	20	0.14
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD12	20	0.14
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD13	20	0.14
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD21	20	0.14
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD22	20	0.14
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD23	20	0.14
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD11	25	0.14
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD12	25	0.14
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD13	25	0.14
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD21	25	0.14
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD22	25	0.14
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD23	25	0.14
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD11	25	0.14
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD12	25	0.14
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD13	25	0.14
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD21	25	0.14
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD22	25	0.14
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD23	25	0.14
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD11	25	0.14
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD12	25	0.14
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD13	25	0.14
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD21	25	0.14
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD22	25	0.14
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD23	25	0.14
(1,2923)	1:364:A:TRP:HB3	1:367:A:MET:HB2	17	0.14
(1,2923)	1:364:A:TRP:HB3	1:367:A:MET:HB3	17	0.14
(1,2852)	1:356:A:LEU:HD11	1:379:A:VAL:HB	9	0.14
(1,2852)	1:356:A:LEU:HD12	1:379:A:VAL:HB	9	0.14
(1,2852)	1:356:A:LEU:HD13	1:379:A:VAL:HB	9	0.14
(1,2852)	1:356:A:LEU:HD21	1:379:A:VAL:HB	9	0.14
(1,2852)	1:356:A:LEU:HD22	1:379:A:VAL:HB	9	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2852)	1:356:A:LEU:HD23	1:379:A:VAL:HB	9	0.14
(1,2852)	1:356:A:LEU:HD11	1:379:A:VAL:HB	20	0.14
(1,2852)	1:356:A:LEU:HD12	1:379:A:VAL:HB	20	0.14
(1,2852)	1:356:A:LEU:HD13	1:379:A:VAL:HB	20	0.14
(1,2852)	1:356:A:LEU:HD21	1:379:A:VAL:HB	20	0.14
(1,2852)	1:356:A:LEU:HD22	1:379:A:VAL:HB	20	0.14
(1,2852)	1:356:A:LEU:HD23	1:379:A:VAL:HB	20	0.14
(1,2678)	1:-1:A:MET:HE1	1:345:A:VAL:H	1	0.14
(1,2678)	1:-1:A:MET:HE2	1:345:A:VAL:H	1	0.14
(1,2678)	1:-1:A:MET:HE3	1:345:A:VAL:H	1	0.14
(1,2678)	1:-1:A:MET:HE1	1:345:A:VAL:H	20	0.14
(1,2678)	1:-1:A:MET:HE2	1:345:A:VAL:H	20	0.14
(1,2678)	1:-1:A:MET:HE3	1:345:A:VAL:H	20	0.14
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG2	7	0.14
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG3	7	0.14
(1,2601)	1:424:A:ASN:HD22	1:454:A:ALA:HB1	5	0.14
(1,2601)	1:424:A:ASN:HD22	1:454:A:ALA:HB2	5	0.14
(1,2601)	1:424:A:ASN:HD22	1:454:A:ALA:HB3	5	0.14
(1,2599)	1:424:A:ASN:HD22	1:454:A:ALA:HA	16	0.14
(1,2581)	1:-3:A:SER:H	1:-2:A:HIS:HB2	3	0.14
(1,2581)	1:-3:A:SER:H	1:-2:A:HIS:HB3	3	0.14
(1,2581)	1:-3:A:SER:H	1:-2:A:HIS:HB2	11	0.14
(1,2581)	1:-3:A:SER:H	1:-2:A:HIS:HB3	11	0.14
(1,2581)	1:-3:A:SER:H	1:-2:A:HIS:HB2	18	0.14
(1,2581)	1:-3:A:SER:H	1:-2:A:HIS:HB3	18	0.14
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE1	5	0.14
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE2	5	0.14
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE3	5	0.14
(1,2405)	1:446:A:LYS:H	1:446:A:LYS:HG2	1	0.14
(1,2405)	1:446:A:LYS:H	1:446:A:LYS:HG3	1	0.14
(1,2405)	1:446:A:LYS:H	1:446:A:LYS:HG2	18	0.14
(1,2405)	1:446:A:LYS:H	1:446:A:LYS:HG3	18	0.14
(1,2182)	1:407:A:TYR:HD1	1:414:A:THR:H	20	0.14
(1,2182)	1:407:A:TYR:HD2	1:414:A:THR:H	20	0.14
(1,2117)	1:423:A:GLY:HA2	1:450:A:ALA:H	1	0.14
(1,2117)	1:423:A:GLY:HA2	1:450:A:ALA:H	8	0.14
(1,2117)	1:423:A:GLY:HA2	1:450:A:ALA:H	24	0.14
(1,1940)	1:362:A:GLU:H	1:412:A:THR:HG21	10	0.14
(1,1940)	1:362:A:GLU:H	1:412:A:THR:HG22	10	0.14
(1,1940)	1:362:A:GLU:H	1:412:A:THR:HG23	10	0.14
(1,1888)	1:380:A:ARG:HE	1:437:A:GLN:H	10	0.14
(1,1888)	1:380:A:ARG:HE	1:437:A:GLN:H	20	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1882)	1:423:A:GLY:HA3	1:447:A:TRP:HE1	9	0.14
(1,1809)	1:423:A:GLY:HA3	1:456:A:MET:H	11	0.14
(1,1809)	1:423:A:GLY:HA3	1:456:A:MET:H	22	0.14
(1,1661)	1:421:A:ARG:HD2	1:425:A:ASP:H	2	0.14
(1,1661)	1:421:A:ARG:HD3	1:425:A:ASP:H	2	0.14
(1,1660)	1:425:A:ASP:HB3	1:426:A:GLN:H	1	0.14
(1,1660)	1:425:A:ASP:HB3	1:426:A:GLN:H	18	0.14
(1,1660)	1:425:A:ASP:HB3	1:426:A:GLN:H	22	0.14
(1,1414)	1:419:A:GLN:HB3	1:419:A:GLN:HE22	5	0.14
(1,1414)	1:419:A:GLN:HB3	1:419:A:GLN:HE22	9	0.14
(1,1414)	1:419:A:GLN:HB3	1:419:A:GLN:HE22	14	0.14
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG11	2	0.14
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG12	2	0.14
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG13	2	0.14
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG11	9	0.14
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG12	9	0.14
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG13	9	0.14
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG11	12	0.14
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG12	12	0.14
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG13	12	0.14
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG11	17	0.14
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG12	17	0.14
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG13	17	0.14
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG11	18	0.14
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG12	18	0.14
(1,1017)	1:420:A:LEU:H	1:428:A:VAL:HG13	18	0.14
(1,914)	1:460:A:THR:HA	1:461:A:LEU:HG	4	0.14
(1,914)	1:460:A:THR:HA	1:461:A:LEU:HG	10	0.14
(1,907)	1:464:A:ILE:HA	1:467:A:LYS:HE2	22	0.14
(1,907)	1:464:A:ILE:HA	1:467:A:LYS:HE3	22	0.14
(1,896)	1:407:A:TYR:HD1	1:412:A:THR:HG21	7	0.14
(1,896)	1:407:A:TYR:HD1	1:412:A:THR:HG22	7	0.14
(1,896)	1:407:A:TYR:HD1	1:412:A:THR:HG23	7	0.14
(1,896)	1:407:A:TYR:HD2	1:412:A:THR:HG21	7	0.14
(1,896)	1:407:A:TYR:HD2	1:412:A:THR:HG22	7	0.14
(1,896)	1:407:A:TYR:HD2	1:412:A:THR:HG23	7	0.14
(1,855)	1:399:A:GLY:HA3	1:418:A:LEU:HB3	6	0.14
(1,855)	1:399:A:GLY:HA3	1:418:A:LEU:HB3	11	0.14
(1,855)	1:399:A:GLY:HA3	1:418:A:LEU:HB3	13	0.14
(1,719)	1:363:A:ARG:HA	1:363:A:ARG:HD2	21	0.14
(1,719)	1:363:A:ARG:HA	1:363:A:ARG:HD3	21	0.14
(1,719)	1:363:A:ARG:HA	1:363:A:ARG:HD2	23	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,719)	1:363:A:ARG:HA	1:363:A:ARG:HD3	23	0.14
(1,487)	1:398:A:THR:HG21	1:419:A:GLN:HG3	22	0.14
(1,487)	1:398:A:THR:HG22	1:419:A:GLN:HG3	22	0.14
(1,487)	1:398:A:THR:HG23	1:419:A:GLN:HG3	22	0.14
(1,463)	1:401:A:VAL:HG21	1:417:A:GLY:HA2	16	0.14
(1,463)	1:401:A:VAL:HG22	1:417:A:GLY:HA2	16	0.14
(1,463)	1:401:A:VAL:HG23	1:417:A:GLY:HA2	16	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD11	1	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD12	1	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD13	1	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD11	2	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD12	2	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD13	2	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD11	4	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD12	4	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD13	4	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD11	5	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD12	5	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD13	5	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD11	7	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD12	7	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD13	7	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD11	8	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD12	8	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD13	8	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD11	10	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD12	10	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD13	10	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD11	14	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD12	14	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD13	14	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD11	15	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD12	15	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD13	15	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD11	19	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD12	19	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD13	19	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD11	20	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD12	20	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD13	20	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD11	22	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD12	22	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD13	22	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD11	25	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD12	25	0.14
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD13	25	0.14
(1,279)	1:392:A:TYR:HE1	1:435:A:SER:HA	19	0.14
(1,279)	1:392:A:TYR:HE2	1:435:A:SER:HA	19	0.14
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD2	5	0.14
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD3	5	0.14
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD2	7	0.14
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD3	7	0.14
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD2	24	0.14
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD3	24	0.14
(1,161)	1:370:A:PHE:HD1	1:371:A:ALA:HB1	3	0.14
(1,161)	1:370:A:PHE:HD1	1:371:A:ALA:HB2	3	0.14
(1,161)	1:370:A:PHE:HD1	1:371:A:ALA:HB3	3	0.14
(1,161)	1:370:A:PHE:HD2	1:371:A:ALA:HB1	3	0.14
(1,161)	1:370:A:PHE:HD2	1:371:A:ALA:HB2	3	0.14
(1,161)	1:370:A:PHE:HD2	1:371:A:ALA:HB3	3	0.14
(1,78)	1:370:A:PHE:H	1:370:A:PHE:HB2	13	0.14
(1,78)	1:370:A:PHE:H	1:370:A:PHE:HB2	17	0.14
(1,57)	1:411:A:GLY:HA3	1:412:A:THR:HB	7	0.14
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD2	4	0.14
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD3	4	0.14
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD2	9	0.14
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD3	9	0.14
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD2	12	0.14
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD3	12	0.14
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD2	16	0.14
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD3	16	0.14
(1,3369)	1:461:A:LEU:HD11	1:464:A:ILE:HB	16	0.13
(1,3369)	1:461:A:LEU:HD12	1:464:A:ILE:HB	16	0.13
(1,3369)	1:461:A:LEU:HD13	1:464:A:ILE:HB	16	0.13
(1,3369)	1:461:A:LEU:HD21	1:464:A:ILE:HB	16	0.13
(1,3369)	1:461:A:LEU:HD22	1:464:A:ILE:HB	16	0.13
(1,3369)	1:461:A:LEU:HD23	1:464:A:ILE:HB	16	0.13
(1,3358)	1:460:A:THR:H	1:463:A:GLU:HB2	11	0.13
(1,3358)	1:460:A:THR:H	1:463:A:GLU:HB3	11	0.13
(1,3358)	1:460:A:THR:H	1:463:A:GLU:HB2	23	0.13
(1,3358)	1:460:A:THR:H	1:463:A:GLU:HB3	23	0.13
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD11	6	0.13
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD12	6	0.13
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD13	6	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD21	6	0.13
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD22	6	0.13
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD23	6	0.13
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD11	10	0.13
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD12	10	0.13
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD13	10	0.13
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD21	10	0.13
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD22	10	0.13
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD23	10	0.13
(1,3184)	1:423:A:GLY:HA3	1:456:A:MET:HB2	18	0.13
(1,3184)	1:423:A:GLY:HA3	1:456:A:MET:HB3	18	0.13
(1,3166)	1:419:A:GLN:HE21	1:428:A:VAL:HB	6	0.13
(1,3166)	1:419:A:GLN:HE22	1:428:A:VAL:HB	6	0.13
(1,3166)	1:419:A:GLN:HE21	1:428:A:VAL:HB	20	0.13
(1,3166)	1:419:A:GLN:HE22	1:428:A:VAL:HB	20	0.13
(1,3153)	1:418:A:LEU:HD11	1:419:A:GLN:H	10	0.13
(1,3153)	1:418:A:LEU:HD12	1:419:A:GLN:H	10	0.13
(1,3153)	1:418:A:LEU:HD13	1:419:A:GLN:H	10	0.13
(1,3153)	1:418:A:LEU:HD21	1:419:A:GLN:H	10	0.13
(1,3153)	1:418:A:LEU:HD22	1:419:A:GLN:H	10	0.13
(1,3153)	1:418:A:LEU:HD23	1:419:A:GLN:H	10	0.13
(1,3153)	1:418:A:LEU:HD11	1:419:A:GLN:H	12	0.13
(1,3153)	1:418:A:LEU:HD12	1:419:A:GLN:H	12	0.13
(1,3153)	1:418:A:LEU:HD13	1:419:A:GLN:H	12	0.13
(1,3153)	1:418:A:LEU:HD21	1:419:A:GLN:H	12	0.13
(1,3153)	1:418:A:LEU:HD22	1:419:A:GLN:H	12	0.13
(1,3153)	1:418:A:LEU:HD23	1:419:A:GLN:H	12	0.13
(1,3153)	1:418:A:LEU:HD11	1:419:A:GLN:H	13	0.13
(1,3153)	1:418:A:LEU:HD12	1:419:A:GLN:H	13	0.13
(1,3153)	1:418:A:LEU:HD13	1:419:A:GLN:H	13	0.13
(1,3153)	1:418:A:LEU:HD21	1:419:A:GLN:H	13	0.13
(1,3153)	1:418:A:LEU:HD22	1:419:A:GLN:H	13	0.13
(1,3153)	1:418:A:LEU:HD23	1:419:A:GLN:H	13	0.13
(1,3153)	1:418:A:LEU:HD11	1:419:A:GLN:H	15	0.13
(1,3153)	1:418:A:LEU:HD12	1:419:A:GLN:H	15	0.13
(1,3153)	1:418:A:LEU:HD13	1:419:A:GLN:H	15	0.13
(1,3153)	1:418:A:LEU:HD21	1:419:A:GLN:H	15	0.13
(1,3153)	1:418:A:LEU:HD22	1:419:A:GLN:H	15	0.13
(1,3153)	1:418:A:LEU:HD23	1:419:A:GLN:H	15	0.13
(1,3153)	1:418:A:LEU:HD11	1:419:A:GLN:H	16	0.13
(1,3153)	1:418:A:LEU:HD12	1:419:A:GLN:H	16	0.13
(1,3153)	1:418:A:LEU:HD13	1:419:A:GLN:H	16	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3153)	1:418:A:LEU:HD21	1:419:A:GLN:H	16	0.13
(1,3153)	1:418:A:LEU:HD22	1:419:A:GLN:H	16	0.13
(1,3153)	1:418:A:LEU:HD23	1:419:A:GLN:H	16	0.13
(1,3103)	1:407:A:TYR:HE1	1:416:A:LYS:HD2	22	0.13
(1,3103)	1:407:A:TYR:HE1	1:416:A:LYS:HD3	22	0.13
(1,3103)	1:407:A:TYR:HE2	1:416:A:LYS:HD2	22	0.13
(1,3103)	1:407:A:TYR:HE2	1:416:A:LYS:HD3	22	0.13
(1,3070)	1:400:A:VAL:HG11	1:419:A:GLN:H	9	0.13
(1,3070)	1:400:A:VAL:HG12	1:419:A:GLN:H	9	0.13
(1,3070)	1:400:A:VAL:HG13	1:419:A:GLN:H	9	0.13
(1,3070)	1:400:A:VAL:HG21	1:419:A:GLN:H	9	0.13
(1,3070)	1:400:A:VAL:HG22	1:419:A:GLN:H	9	0.13
(1,3070)	1:400:A:VAL:HG23	1:419:A:GLN:H	9	0.13
(1,3012)	1:385:A:ASN:HD21	1:386:A:HIS:HA	23	0.13
(1,3012)	1:385:A:ASN:HD22	1:386:A:HIS:HA	23	0.13
(1,2923)	1:364:A:TRP:HB3	1:367:A:MET:HB2	13	0.13
(1,2923)	1:364:A:TRP:HB3	1:367:A:MET:HB3	13	0.13
(1,2852)	1:356:A:LEU:HD11	1:379:A:VAL:HB	13	0.13
(1,2852)	1:356:A:LEU:HD12	1:379:A:VAL:HB	13	0.13
(1,2852)	1:356:A:LEU:HD13	1:379:A:VAL:HB	13	0.13
(1,2852)	1:356:A:LEU:HD21	1:379:A:VAL:HB	13	0.13
(1,2852)	1:356:A:LEU:HD22	1:379:A:VAL:HB	13	0.13
(1,2852)	1:356:A:LEU:HD23	1:379:A:VAL:HB	13	0.13
(1,2852)	1:356:A:LEU:HD11	1:379:A:VAL:HB	14	0.13
(1,2852)	1:356:A:LEU:HD12	1:379:A:VAL:HB	14	0.13
(1,2852)	1:356:A:LEU:HD13	1:379:A:VAL:HB	14	0.13
(1,2852)	1:356:A:LEU:HD21	1:379:A:VAL:HB	14	0.13
(1,2852)	1:356:A:LEU:HD22	1:379:A:VAL:HB	14	0.13
(1,2852)	1:356:A:LEU:HD23	1:379:A:VAL:HB	14	0.13
(1,2678)	1:-1:A:MET:HE1	1:345:A:VAL:H	4	0.13
(1,2678)	1:-1:A:MET:HE2	1:345:A:VAL:H	4	0.13
(1,2678)	1:-1:A:MET:HE3	1:345:A:VAL:H	4	0.13
(1,2678)	1:-1:A:MET:HE1	1:345:A:VAL:H	8	0.13
(1,2678)	1:-1:A:MET:HE2	1:345:A:VAL:H	8	0.13
(1,2678)	1:-1:A:MET:HE3	1:345:A:VAL:H	8	0.13
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG2	5	0.13
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG3	5	0.13
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG2	14	0.13
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG3	14	0.13
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG2	17	0.13
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG3	17	0.13
(1,2601)	1:424:A:ASN:HD22	1:454:A:ALA:HB1	10	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2601)	1:424:A:ASN:HD22	1:454:A:ALA:HB2	10	0.13
(1,2601)	1:424:A:ASN:HD22	1:454:A:ALA:HB3	10	0.13
(1,2601)	1:424:A:ASN:HD22	1:454:A:ALA:HB1	13	0.13
(1,2601)	1:424:A:ASN:HD22	1:454:A:ALA:HB2	13	0.13
(1,2601)	1:424:A:ASN:HD22	1:454:A:ALA:HB3	13	0.13
(1,2470)	1:400:A:VAL:HA	1:418:A:LEU:H	24	0.13
(1,2405)	1:446:A:LYS:H	1:446:A:LYS:HG2	14	0.13
(1,2405)	1:446:A:LYS:H	1:446:A:LYS:HG3	14	0.13
(1,2405)	1:446:A:LYS:H	1:446:A:LYS:HG2	17	0.13
(1,2405)	1:446:A:LYS:H	1:446:A:LYS:HG3	17	0.13
(1,2405)	1:446:A:LYS:H	1:446:A:LYS:HG2	25	0.13
(1,2405)	1:446:A:LYS:H	1:446:A:LYS:HG3	25	0.13
(1,2328)	1:-2:A:HIS:HA	1:-1:A:MET:H	11	0.13
(1,2328)	1:-2:A:HIS:HA	1:-1:A:MET:H	12	0.13
(1,2173)	1:423:A:GLY:H	1:454:A:ALA:HB1	17	0.13
(1,2173)	1:423:A:GLY:H	1:454:A:ALA:HB2	17	0.13
(1,2173)	1:423:A:GLY:H	1:454:A:ALA:HB3	17	0.13
(1,2117)	1:423:A:GLY:HA2	1:450:A:ALA:H	7	0.13
(1,2117)	1:423:A:GLY:HA2	1:450:A:ALA:H	11	0.13
(1,2117)	1:423:A:GLY:HA2	1:450:A:ALA:H	12	0.13
(1,2117)	1:423:A:GLY:HA2	1:450:A:ALA:H	25	0.13
(1,1935)	1:405:A:LYS:H	1:405:A:LYS:HE2	11	0.13
(1,1935)	1:405:A:LYS:H	1:405:A:LYS:HE3	11	0.13
(1,1914)	1:371:A:ALA:H	1:400:A:VAL:HG21	17	0.13
(1,1914)	1:371:A:ALA:H	1:400:A:VAL:HG22	17	0.13
(1,1914)	1:371:A:ALA:H	1:400:A:VAL:HG23	17	0.13
(1,1908)	1:421:A:ARG:H	1:421:A:ARG:HE	24	0.13
(1,1902)	1:423:A:GLY:HA2	1:425:A:ASP:H	17	0.13
(1,1882)	1:423:A:GLY:HA3	1:447:A:TRP:HE1	6	0.13
(1,1882)	1:423:A:GLY:HA3	1:447:A:TRP:HE1	11	0.13
(1,1818)	1:365:A:CYS:HA	1:367:A:MET:H	17	0.13
(1,1809)	1:423:A:GLY:HA3	1:456:A:MET:H	4	0.13
(1,1809)	1:423:A:GLY:HA3	1:456:A:MET:H	9	0.13
(1,1809)	1:423:A:GLY:HA3	1:456:A:MET:H	10	0.13
(1,1809)	1:423:A:GLY:HA3	1:456:A:MET:H	13	0.13
(1,1809)	1:423:A:GLY:HA3	1:456:A:MET:H	14	0.13
(1,1809)	1:423:A:GLY:HA3	1:456:A:MET:H	15	0.13
(1,1809)	1:423:A:GLY:HA3	1:456:A:MET:H	24	0.13
(1,1690)	1:438:A:GLU:H	1:438:A:GLU:HG3	16	0.13
(1,1661)	1:421:A:ARG:HD2	1:425:A:ASP:H	7	0.13
(1,1661)	1:421:A:ARG:HD3	1:425:A:ASP:H	7	0.13
(1,1661)	1:421:A:ARG:HD2	1:425:A:ASP:H	12	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1661)	1:421:A:ARG:HD3	1:425:A:ASP:H	12	0.13
(1,1661)	1:421:A:ARG:HD2	1:425:A:ASP:H	20	0.13
(1,1661)	1:421:A:ARG:HD3	1:425:A:ASP:H	20	0.13
(1,1660)	1:425:A:ASP:HB3	1:426:A:GLN:H	9	0.13
(1,1660)	1:425:A:ASP:HB3	1:426:A:GLN:H	20	0.13
(1,1660)	1:425:A:ASP:HB3	1:426:A:GLN:H	23	0.13
(1,1479)	1:347:A:LEU:HG	1:349:A:GLU:H	24	0.13
(1,1471)	1:345:A:VAL:H	1:345:A:VAL:HB	11	0.13
(1,1414)	1:419:A:GLN:HB3	1:419:A:GLN:HE22	8	0.13
(1,1414)	1:419:A:GLN:HB3	1:419:A:GLN:HE22	15	0.13
(1,1414)	1:419:A:GLN:HB3	1:419:A:GLN:HE22	16	0.13
(1,1414)	1:419:A:GLN:HB3	1:419:A:GLN:HE22	17	0.13
(1,1414)	1:419:A:GLN:HB3	1:419:A:GLN:HE22	19	0.13
(1,1414)	1:419:A:GLN:HB3	1:419:A:GLN:HE22	25	0.13
(1,1383)	1:470:A:SER:H	1:471:A:ILE:HD11	22	0.13
(1,1383)	1:470:A:SER:H	1:471:A:ILE:HD12	22	0.13
(1,1383)	1:470:A:SER:H	1:471:A:ILE:HD13	22	0.13
(1,1145)	1:419:A:GLN:HG3	1:428:A:VAL:H	14	0.13
(1,1084)	1:405:A:LYS:HG2	1:406:A:VAL:H	16	0.13
(1,1084)	1:405:A:LYS:HG3	1:406:A:VAL:H	16	0.13
(1,1030)	1:449:A:GLU:HG2	1:450:A:ALA:H	2	0.13
(1,914)	1:460:A:THR:HA	1:461:A:LEU:HG	12	0.13
(1,909)	1:347:A:LEU:HB2	1:348:A:PRO:HD3	23	0.13
(1,855)	1:399:A:GLY:HA3	1:418:A:LEU:HB3	20	0.13
(1,855)	1:399:A:GLY:HA3	1:418:A:LEU:HB3	25	0.13
(1,790)	1:361:A:LEU:HA	1:370:A:PHE:HE1	17	0.13
(1,790)	1:361:A:LEU:HA	1:370:A:PHE:HE2	17	0.13
(1,729)	1:385:A:ASN:HA	1:390:A:PRO:HA	23	0.13
(1,719)	1:363:A:ARG:HA	1:363:A:ARG:HD2	4	0.13
(1,719)	1:363:A:ARG:HA	1:363:A:ARG:HD3	4	0.13
(1,719)	1:363:A:ARG:HA	1:363:A:ARG:HD2	12	0.13
(1,719)	1:363:A:ARG:HA	1:363:A:ARG:HD3	12	0.13
(1,510)	1:440:A:THR:HA	1:441:A:GLU:HG2	8	0.13
(1,510)	1:440:A:THR:HA	1:441:A:GLU:HG3	8	0.13
(1,463)	1:401:A:VAL:HG21	1:417:A:GLY:HA2	15	0.13
(1,463)	1:401:A:VAL:HG22	1:417:A:GLY:HA2	15	0.13
(1,463)	1:401:A:VAL:HG23	1:417:A:GLY:HA2	15	0.13
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD11	9	0.13
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD12	9	0.13
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD13	9	0.13
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD11	12	0.13
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD12	12	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD13	12	0.13
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD11	16	0.13
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD12	16	0.13
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD13	16	0.13
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD11	17	0.13
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD12	17	0.13
(1,393)	1:475:A:LEU:HA	1:475:A:LEU:HD13	17	0.13
(1,375)	1:395:A:ALA:HB1	1:420:A:LEU:HG	8	0.13
(1,375)	1:395:A:ALA:HB2	1:420:A:LEU:HG	8	0.13
(1,375)	1:395:A:ALA:HB3	1:420:A:LEU:HG	8	0.13
(1,279)	1:392:A:TYR:HE1	1:435:A:SER:HA	14	0.13
(1,279)	1:392:A:TYR:HE2	1:435:A:SER:HA	14	0.13
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD2	2	0.13
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD3	2	0.13
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD2	4	0.13
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD3	4	0.13
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD2	16	0.13
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD3	16	0.13
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD2	18	0.13
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD3	18	0.13
(1,247)	1:440:A:THR:HG21	1:444:A:PHE:H	10	0.13
(1,247)	1:440:A:THR:HG22	1:444:A:PHE:H	10	0.13
(1,247)	1:440:A:THR:HG23	1:444:A:PHE:H	10	0.13
(1,212)	1:397:A:ILE:HD11	1:418:A:LEU:HD21	11	0.13
(1,212)	1:397:A:ILE:HD11	1:418:A:LEU:HD22	11	0.13
(1,212)	1:397:A:ILE:HD11	1:418:A:LEU:HD23	11	0.13
(1,212)	1:397:A:ILE:HD12	1:418:A:LEU:HD21	11	0.13
(1,212)	1:397:A:ILE:HD12	1:418:A:LEU:HD22	11	0.13
(1,212)	1:397:A:ILE:HD12	1:418:A:LEU:HD23	11	0.13
(1,212)	1:397:A:ILE:HD13	1:418:A:LEU:HD21	11	0.13
(1,212)	1:397:A:ILE:HD13	1:418:A:LEU:HD22	11	0.13
(1,212)	1:397:A:ILE:HD13	1:418:A:LEU:HD23	11	0.13
(1,200)	1:448:A:LYS:HG3	1:449:A:GLU:HB2	10	0.13
(1,200)	1:448:A:LYS:HG3	1:449:A:GLU:HB3	10	0.13
(1,78)	1:370:A:PHE:H	1:370:A:PHE:HB2	12	0.13
(1,78)	1:370:A:PHE:H	1:370:A:PHE:HB2	24	0.13
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD2	15	0.13
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD3	15	0.13
(1,3358)	1:460:A:THR:H	1:463:A:GLU:HB2	7	0.12
(1,3358)	1:460:A:THR:H	1:463:A:GLU:HB3	7	0.12
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD11	2	0.12
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD12	2	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD13	2	0.12
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD21	2	0.12
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD22	2	0.12
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD23	2	0.12
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD11	22	0.12
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD12	22	0.12
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD13	22	0.12
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD21	22	0.12
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD22	22	0.12
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD23	22	0.12
(1,3337)	1:456:A:MET:HG2	1:457:A:GLN:H	9	0.12
(1,3337)	1:456:A:MET:HG3	1:457:A:GLN:H	9	0.12
(1,3319)	1:451:A:MET:HE1	1:456:A:MET:HB2	8	0.12
(1,3319)	1:451:A:MET:HE1	1:456:A:MET:HB3	8	0.12
(1,3319)	1:451:A:MET:HE2	1:456:A:MET:HB2	8	0.12
(1,3319)	1:451:A:MET:HE2	1:456:A:MET:HB3	8	0.12
(1,3319)	1:451:A:MET:HE3	1:456:A:MET:HB2	8	0.12
(1,3319)	1:451:A:MET:HE3	1:456:A:MET:HB3	8	0.12
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD11	8	0.12
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD12	8	0.12
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD13	8	0.12
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD21	8	0.12
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD22	8	0.12
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD23	8	0.12
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD11	9	0.12
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD12	9	0.12
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD13	9	0.12
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD21	9	0.12
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD22	9	0.12
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD23	9	0.12
(1,3248)	1:435:A:SER:HA	1:437:A:GLN:HG2	1	0.12
(1,3248)	1:435:A:SER:HA	1:437:A:GLN:HG3	1	0.12
(1,3184)	1:423:A:GLY:HA3	1:456:A:MET:HB2	7	0.12
(1,3184)	1:423:A:GLY:HA3	1:456:A:MET:HB3	7	0.12
(1,3184)	1:423:A:GLY:HA3	1:456:A:MET:HB2	15	0.12
(1,3184)	1:423:A:GLY:HA3	1:456:A:MET:HB3	15	0.12
(1,3184)	1:423:A:GLY:HA3	1:456:A:MET:HB2	20	0.12
(1,3184)	1:423:A:GLY:HA3	1:456:A:MET:HB3	20	0.12
(1,3179)	1:421:A:ARG:HE	1:426:A:GLN:HG2	10	0.12
(1,3179)	1:421:A:ARG:HE	1:426:A:GLN:HG3	10	0.12
(1,3153)	1:418:A:LEU:HD11	1:419:A:GLN:H	19	0.12
(1,3153)	1:418:A:LEU:HD12	1:419:A:GLN:H	19	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3153)	1:418:A:LEU:HD13	1:419:A:GLN:H	19	0.12
(1,3153)	1:418:A:LEU:HD21	1:419:A:GLN:H	19	0.12
(1,3153)	1:418:A:LEU:HD22	1:419:A:GLN:H	19	0.12
(1,3153)	1:418:A:LEU:HD23	1:419:A:GLN:H	19	0.12
(1,3103)	1:407:A:TYR:HE1	1:416:A:LYS:HD2	1	0.12
(1,3103)	1:407:A:TYR:HE1	1:416:A:LYS:HD3	1	0.12
(1,3103)	1:407:A:TYR:HE2	1:416:A:LYS:HD2	1	0.12
(1,3103)	1:407:A:TYR:HE2	1:416:A:LYS:HD3	1	0.12
(1,3070)	1:400:A:VAL:HG11	1:419:A:GLN:H	22	0.12
(1,3070)	1:400:A:VAL:HG12	1:419:A:GLN:H	22	0.12
(1,3070)	1:400:A:VAL:HG13	1:419:A:GLN:H	22	0.12
(1,3070)	1:400:A:VAL:HG21	1:419:A:GLN:H	22	0.12
(1,3070)	1:400:A:VAL:HG22	1:419:A:GLN:H	22	0.12
(1,3070)	1:400:A:VAL:HG23	1:419:A:GLN:H	22	0.12
(1,3012)	1:385:A:ASN:HD21	1:386:A:HIS:HA	22	0.12
(1,3012)	1:385:A:ASN:HD22	1:386:A:HIS:HA	22	0.12
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD11	7	0.12
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD12	7	0.12
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD13	7	0.12
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD21	7	0.12
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD22	7	0.12
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD23	7	0.12
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD11	7	0.12
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD12	7	0.12
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD13	7	0.12
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD21	7	0.12
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD22	7	0.12
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD23	7	0.12
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD11	7	0.12
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD12	7	0.12
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD13	7	0.12
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD21	7	0.12
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD22	7	0.12
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD23	7	0.12
(1,2933)	1:369:A:PHE:HB2	1:372:A:LYS:H	17	0.12
(1,2933)	1:369:A:PHE:HB3	1:372:A:LYS:H	17	0.12
(1,2923)	1:364:A:TRP:HB3	1:367:A:MET:HB2	24	0.12
(1,2923)	1:364:A:TRP:HB3	1:367:A:MET:HB3	24	0.12
(1,2855)	1:358:A:ARG:H	1:358:A:ARG:HG2	20	0.12
(1,2855)	1:358:A:ARG:H	1:358:A:ARG:HG3	20	0.12
(1,2852)	1:356:A:LEU:HD11	1:379:A:VAL:HB	15	0.12
(1,2852)	1:356:A:LEU:HD12	1:379:A:VAL:HB	15	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2852)	1:356:A:LEU:HD13	1:379:A:VAL:HB	15	0.12
(1,2852)	1:356:A:LEU:HD21	1:379:A:VAL:HB	15	0.12
(1,2852)	1:356:A:LEU:HD22	1:379:A:VAL:HB	15	0.12
(1,2852)	1:356:A:LEU:HD23	1:379:A:VAL:HB	15	0.12
(1,2746)	1:345:A:VAL:HG11	1:464:A:ILE:H	25	0.12
(1,2746)	1:345:A:VAL:HG12	1:464:A:ILE:H	25	0.12
(1,2746)	1:345:A:VAL:HG13	1:464:A:ILE:H	25	0.12
(1,2746)	1:345:A:VAL:HG21	1:464:A:ILE:H	25	0.12
(1,2746)	1:345:A:VAL:HG22	1:464:A:ILE:H	25	0.12
(1,2746)	1:345:A:VAL:HG23	1:464:A:ILE:H	25	0.12
(1,2739)	1:345:A:VAL:HG11	1:459:A:PRO:HA	5	0.12
(1,2739)	1:345:A:VAL:HG12	1:459:A:PRO:HA	5	0.12
(1,2739)	1:345:A:VAL:HG13	1:459:A:PRO:HA	5	0.12
(1,2739)	1:345:A:VAL:HG21	1:459:A:PRO:HA	5	0.12
(1,2739)	1:345:A:VAL:HG22	1:459:A:PRO:HA	5	0.12
(1,2739)	1:345:A:VAL:HG23	1:459:A:PRO:HA	5	0.12
(1,2739)	1:345:A:VAL:HG11	1:459:A:PRO:HA	20	0.12
(1,2739)	1:345:A:VAL:HG12	1:459:A:PRO:HA	20	0.12
(1,2739)	1:345:A:VAL:HG13	1:459:A:PRO:HA	20	0.12
(1,2739)	1:345:A:VAL:HG21	1:459:A:PRO:HA	20	0.12
(1,2739)	1:345:A:VAL:HG22	1:459:A:PRO:HA	20	0.12
(1,2739)	1:345:A:VAL:HG23	1:459:A:PRO:HA	20	0.12
(1,2725)	1:345:A:VAL:HG11	1:350:A:GLU:H	14	0.12
(1,2725)	1:345:A:VAL:HG12	1:350:A:GLU:H	14	0.12
(1,2725)	1:345:A:VAL:HG13	1:350:A:GLU:H	14	0.12
(1,2725)	1:345:A:VAL:HG21	1:350:A:GLU:H	14	0.12
(1,2725)	1:345:A:VAL:HG22	1:350:A:GLU:H	14	0.12
(1,2725)	1:345:A:VAL:HG23	1:350:A:GLU:H	14	0.12
(1,2708)	1:-3:A:SER:H	1:-3:A:SER:HB2	6	0.12
(1,2708)	1:-3:A:SER:H	1:-3:A:SER:HB3	6	0.12
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG2	10	0.12
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG3	10	0.12
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG2	20	0.12
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG3	20	0.12
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG2	22	0.12
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG3	22	0.12
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG2	25	0.12
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG3	25	0.12
(1,2562)	1:467:A:LYS:HE2	1:470:A:SER:H	15	0.12
(1,2562)	1:467:A:LYS:HE3	1:470:A:SER:H	15	0.12
(1,2470)	1:400:A:VAL:HA	1:418:A:LEU:H	19	0.12
(1,2435)	1:370:A:PHE:HD1	1:371:A:ALA:H	17	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2333)	1:456:A:MET:HG2	1:457:A:GLN:H	9	0.12
(1,2333)	1:456:A:MET:HG3	1:457:A:GLN:H	9	0.12
(1,2330)	1:-1:A:MET:H	1:461:A:LEU:HD11	18	0.12
(1,2330)	1:-1:A:MET:H	1:461:A:LEU:HD12	18	0.12
(1,2330)	1:-1:A:MET:H	1:461:A:LEU:HD13	18	0.12
(1,2328)	1:-2:A:HIS:HA	1:-1:A:MET:H	5	0.12
(1,2327)	1:-8:A:LEU:H	1:-8:A:LEU:HG	13	0.12
(1,2327)	1:-8:A:LEU:H	1:-8:A:LEU:HG	25	0.12
(1,2270)	1:369:A:PHE:HD2	1:370:A:PHE:H	14	0.12
(1,2206)	1:424:A:ASN:H	1:424:A:ASN:HB2	25	0.12
(1,2173)	1:423:A:GLY:H	1:454:A:ALA:HB1	16	0.12
(1,2173)	1:423:A:GLY:H	1:454:A:ALA:HB2	16	0.12
(1,2173)	1:423:A:GLY:H	1:454:A:ALA:HB3	16	0.12
(1,2148)	1:348:A:PRO:HD3	1:350:A:GLU:H	21	0.12
(1,2117)	1:423:A:GLY:HA2	1:450:A:ALA:H	9	0.12
(1,2025)	1:358:A:ARG:H	1:358:A:ARG:HG3	20	0.12
(1,2003)	1:348:A:PRO:HD3	1:444:A:PHE:H	11	0.12
(1,2003)	1:348:A:PRO:HD3	1:444:A:PHE:H	15	0.12
(1,2003)	1:348:A:PRO:HD3	1:444:A:PHE:H	18	0.12
(1,2003)	1:348:A:PRO:HD3	1:444:A:PHE:H	21	0.12
(1,2003)	1:348:A:PRO:HD3	1:444:A:PHE:H	24	0.12
(1,2000)	1:406:A:VAL:HG11	1:416:A:LYS:H	13	0.12
(1,2000)	1:406:A:VAL:HG12	1:416:A:LYS:H	13	0.12
(1,2000)	1:406:A:VAL:HG13	1:416:A:LYS:H	13	0.12
(1,1940)	1:362:A:GLU:H	1:412:A:THR:HG21	14	0.12
(1,1940)	1:362:A:GLU:H	1:412:A:THR:HG22	14	0.12
(1,1940)	1:362:A:GLU:H	1:412:A:THR:HG23	14	0.12
(1,1939)	1:442:A:SER:H	1:442:A:SER:HB3	25	0.12
(1,1897)	1:370:A:PHE:H	1:372:A:LYS:H	19	0.12
(1,1882)	1:423:A:GLY:HA3	1:447:A:TRP:HE1	1	0.12
(1,1882)	1:423:A:GLY:HA3	1:447:A:TRP:HE1	2	0.12
(1,1882)	1:423:A:GLY:HA3	1:447:A:TRP:HE1	14	0.12
(1,1882)	1:423:A:GLY:HA3	1:447:A:TRP:HE1	21	0.12
(1,1882)	1:423:A:GLY:HA3	1:447:A:TRP:HE1	23	0.12
(1,1882)	1:423:A:GLY:HA3	1:447:A:TRP:HE1	25	0.12
(1,1809)	1:423:A:GLY:HA3	1:456:A:MET:H	6	0.12
(1,1809)	1:423:A:GLY:HA3	1:456:A:MET:H	8	0.12
(1,1809)	1:423:A:GLY:HA3	1:456:A:MET:H	16	0.12
(1,1809)	1:423:A:GLY:HA3	1:456:A:MET:H	20	0.12
(1,1809)	1:423:A:GLY:HA3	1:456:A:MET:H	25	0.12
(1,1789)	1:456:A:MET:H	1:456:A:MET:HG2	8	0.12
(1,1661)	1:421:A:ARG:HD2	1:425:A:ASP:H	3	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1661)	1:421:A:ARG:HD3	1:425:A:ASP:H	3	0.12
(1,1661)	1:421:A:ARG:HD2	1:425:A:ASP:H	5	0.12
(1,1661)	1:421:A:ARG:HD3	1:425:A:ASP:H	5	0.12
(1,1661)	1:421:A:ARG:HD2	1:425:A:ASP:H	8	0.12
(1,1661)	1:421:A:ARG:HD3	1:425:A:ASP:H	8	0.12
(1,1661)	1:421:A:ARG:HD2	1:425:A:ASP:H	23	0.12
(1,1661)	1:421:A:ARG:HD3	1:425:A:ASP:H	23	0.12
(1,1660)	1:425:A:ASP:HB3	1:426:A:GLN:H	5	0.12
(1,1633)	1:413:A:ARG:HG3	1:414:A:THR:H	22	0.12
(1,1479)	1:347:A:LEU:HG	1:349:A:GLU:H	5	0.12
(1,1479)	1:347:A:LEU:HG	1:349:A:GLU:H	9	0.12
(1,1479)	1:347:A:LEU:HG	1:349:A:GLU:H	18	0.12
(1,1471)	1:345:A:VAL:H	1:345:A:VAL:HB	14	0.12
(1,1393)	1:435:A:SER:HA	1:437:A:GLN:HE21	8	0.12
(1,1389)	1:435:A:SER:HA	1:437:A:GLN:HE22	22	0.12
(1,1383)	1:470:A:SER:H	1:471:A:ILE:HD11	3	0.12
(1,1383)	1:470:A:SER:H	1:471:A:ILE:HD12	3	0.12
(1,1383)	1:470:A:SER:H	1:471:A:ILE:HD13	3	0.12
(1,1307)	1:363:A:ARG:H	1:364:A:TRP:HD1	14	0.12
(1,922)	1:439:A:PHE:HD1	1:440:A:THR:HA	8	0.12
(1,922)	1:439:A:PHE:HD2	1:440:A:THR:HA	8	0.12
(1,921)	1:351:A:LEU:HB2	1:444:A:PHE:HZ	12	0.12
(1,921)	1:351:A:LEU:HB2	1:444:A:PHE:HZ	16	0.12
(1,914)	1:460:A:THR:HA	1:461:A:LEU:HG	19	0.12
(1,914)	1:460:A:THR:HA	1:461:A:LEU:HG	21	0.12
(1,909)	1:347:A:LEU:HB2	1:348:A:PRO:HD3	16	0.12
(1,907)	1:464:A:ILE:HA	1:467:A:LYS:HE2	12	0.12
(1,907)	1:464:A:ILE:HA	1:467:A:LYS:HE3	12	0.12
(1,855)	1:399:A:GLY:HA3	1:418:A:LEU:HB3	7	0.12
(1,855)	1:399:A:GLY:HA3	1:418:A:LEU:HB3	15	0.12
(1,855)	1:399:A:GLY:HA3	1:418:A:LEU:HB3	18	0.12
(1,737)	1:345:A:VAL:HG21	1:459:A:PRO:HD3	2	0.12
(1,737)	1:345:A:VAL:HG22	1:459:A:PRO:HD3	2	0.12
(1,737)	1:345:A:VAL:HG23	1:459:A:PRO:HD3	2	0.12
(1,737)	1:345:A:VAL:HG21	1:459:A:PRO:HD3	22	0.12
(1,737)	1:345:A:VAL:HG22	1:459:A:PRO:HD3	22	0.12
(1,737)	1:345:A:VAL:HG23	1:459:A:PRO:HD3	22	0.12
(1,701)	1:369:A:PHE:HD1	1:370:A:PHE:HA	5	0.12
(1,701)	1:369:A:PHE:HD2	1:370:A:PHE:HA	5	0.12
(1,632)	1:402:A:GLU:HA	1:416:A:LYS:HG2	13	0.12
(1,632)	1:402:A:GLU:HA	1:416:A:LYS:HG3	13	0.12
(1,535)	1:363:A:ARG:HD2	1:364:A:TRP:H	1	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,535)	1:363:A:ARG:HD3	1:364:A:TRP:H	1	0.12
(1,535)	1:363:A:ARG:HD2	1:364:A:TRP:H	3	0.12
(1,535)	1:363:A:ARG:HD3	1:364:A:TRP:H	3	0.12
(1,463)	1:401:A:VAL:HG21	1:417:A:GLY:HA2	10	0.12
(1,463)	1:401:A:VAL:HG22	1:417:A:GLY:HA2	10	0.12
(1,463)	1:401:A:VAL:HG23	1:417:A:GLY:HA2	10	0.12
(1,300)	1:451:A:MET:HB3	1:456:A:MET:HE1	17	0.12
(1,300)	1:451:A:MET:HB3	1:456:A:MET:HE2	17	0.12
(1,300)	1:451:A:MET:HB3	1:456:A:MET:HE3	17	0.12
(1,279)	1:392:A:TYR:HE1	1:435:A:SER:HA	22	0.12
(1,279)	1:392:A:TYR:HE2	1:435:A:SER:HA	22	0.12
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD2	3	0.12
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD3	3	0.12
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD2	13	0.12
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD3	13	0.12
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD2	17	0.12
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD3	17	0.12
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD2	19	0.12
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD3	19	0.12
(1,241)	1:421:A:ARG:H	1:421:A:ARG:HG2	16	0.12
(1,241)	1:421:A:ARG:H	1:421:A:ARG:HG2	18	0.12
(1,217)	1:381:A:ILE:HG21	1:429:A:PHE:HE1	8	0.12
(1,217)	1:381:A:ILE:HG21	1:429:A:PHE:HE2	8	0.12
(1,217)	1:381:A:ILE:HG22	1:429:A:PHE:HE1	8	0.12
(1,217)	1:381:A:ILE:HG22	1:429:A:PHE:HE2	8	0.12
(1,217)	1:381:A:ILE:HG23	1:429:A:PHE:HE1	8	0.12
(1,217)	1:381:A:ILE:HG23	1:429:A:PHE:HE2	8	0.12
(1,212)	1:397:A:ILE:HD11	1:418:A:LEU:HD21	24	0.12
(1,212)	1:397:A:ILE:HD11	1:418:A:LEU:HD22	24	0.12
(1,212)	1:397:A:ILE:HD11	1:418:A:LEU:HD23	24	0.12
(1,212)	1:397:A:ILE:HD12	1:418:A:LEU:HD21	24	0.12
(1,212)	1:397:A:ILE:HD12	1:418:A:LEU:HD22	24	0.12
(1,212)	1:397:A:ILE:HD12	1:418:A:LEU:HD23	24	0.12
(1,212)	1:397:A:ILE:HD13	1:418:A:LEU:HD21	24	0.12
(1,212)	1:397:A:ILE:HD13	1:418:A:LEU:HD22	24	0.12
(1,212)	1:397:A:ILE:HD13	1:418:A:LEU:HD23	24	0.12
(1,178)	1:393:A:ARG:H	1:395:A:ALA:HB1	5	0.12
(1,178)	1:393:A:ARG:H	1:395:A:ALA:HB2	5	0.12
(1,178)	1:393:A:ARG:H	1:395:A:ALA:HB3	5	0.12
(1,178)	1:393:A:ARG:H	1:395:A:ALA:HB1	24	0.12
(1,178)	1:393:A:ARG:H	1:395:A:ALA:HB2	24	0.12
(1,178)	1:393:A:ARG:H	1:395:A:ALA:HB3	24	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,83)	1:382:A:GLY:HA3	1:392:A:TYR:HB2	3	0.12
(1,78)	1:370:A:PHE:H	1:370:A:PHE:HB2	21	0.12
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD2	7	0.12
(1,52)	1:446:A:LYS:HA	1:446:A:LYS:HD3	7	0.12
(1,12)	1:421:A:ARG:HB2	1:425:A:ASP:H	25	0.12
(1,12)	1:421:A:ARG:HB3	1:425:A:ASP:H	25	0.12
(1,3405)	1:469:A:LEU:HD11	1:473:A:GLU:HB2	8	0.11
(1,3405)	1:469:A:LEU:HD11	1:473:A:GLU:HB3	8	0.11
(1,3405)	1:469:A:LEU:HD12	1:473:A:GLU:HB2	8	0.11
(1,3405)	1:469:A:LEU:HD12	1:473:A:GLU:HB3	8	0.11
(1,3405)	1:469:A:LEU:HD13	1:473:A:GLU:HB2	8	0.11
(1,3405)	1:469:A:LEU:HD13	1:473:A:GLU:HB3	8	0.11
(1,3405)	1:469:A:LEU:HD21	1:473:A:GLU:HB2	8	0.11
(1,3405)	1:469:A:LEU:HD21	1:473:A:GLU:HB3	8	0.11
(1,3405)	1:469:A:LEU:HD22	1:473:A:GLU:HB2	8	0.11
(1,3405)	1:469:A:LEU:HD22	1:473:A:GLU:HB3	8	0.11
(1,3405)	1:469:A:LEU:HD23	1:473:A:GLU:HB2	8	0.11
(1,3405)	1:469:A:LEU:HD23	1:473:A:GLU:HB3	8	0.11
(1,3358)	1:460:A:THR:H	1:463:A:GLU:HB2	15	0.11
(1,3358)	1:460:A:THR:H	1:463:A:GLU:HB3	15	0.11
(1,3358)	1:460:A:THR:H	1:463:A:GLU:HB2	18	0.11
(1,3358)	1:460:A:THR:H	1:463:A:GLU:HB3	18	0.11
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD11	25	0.11
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD12	25	0.11
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD13	25	0.11
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD21	25	0.11
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD22	25	0.11
(1,3357)	1:460:A:THR:H	1:461:A:LEU:HD23	25	0.11
(1,3356)	1:459:A:PRO:HD2	1:461:A:LEU:HD11	14	0.11
(1,3356)	1:459:A:PRO:HD2	1:461:A:LEU:HD12	14	0.11
(1,3356)	1:459:A:PRO:HD2	1:461:A:LEU:HD13	14	0.11
(1,3356)	1:459:A:PRO:HD2	1:461:A:LEU:HD21	14	0.11
(1,3356)	1:459:A:PRO:HD2	1:461:A:LEU:HD22	14	0.11
(1,3356)	1:459:A:PRO:HD2	1:461:A:LEU:HD23	14	0.11
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD11	2	0.11
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD12	2	0.11
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD13	2	0.11
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD21	2	0.11
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD22	2	0.11
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD23	2	0.11
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD11	4	0.11
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD12	4	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD13	4	0.11
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD21	4	0.11
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD22	4	0.11
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD23	4	0.11
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD11	16	0.11
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD12	16	0.11
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD13	16	0.11
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD21	16	0.11
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD22	16	0.11
(1,3299)	1:448:A:LYS:HB3	1:458:A:LEU:HD23	16	0.11
(1,3286)	1:446:A:LYS:HG2	1:449:A:GLU:H	12	0.11
(1,3286)	1:446:A:LYS:HG3	1:449:A:GLU:H	12	0.11
(1,3249)	1:435:A:SER:HA	1:437:A:GLN:HE21	3	0.11
(1,3249)	1:435:A:SER:HA	1:437:A:GLN:HE22	3	0.11
(1,3184)	1:423:A:GLY:HA3	1:456:A:MET:HB2	1	0.11
(1,3184)	1:423:A:GLY:HA3	1:456:A:MET:HB3	1	0.11
(1,3184)	1:423:A:GLY:HA3	1:456:A:MET:HB2	4	0.11
(1,3184)	1:423:A:GLY:HA3	1:456:A:MET:HB3	4	0.11
(1,3184)	1:423:A:GLY:HA3	1:456:A:MET:HB2	10	0.11
(1,3184)	1:423:A:GLY:HA3	1:456:A:MET:HB3	10	0.11
(1,3184)	1:423:A:GLY:HA3	1:456:A:MET:HB2	21	0.11
(1,3184)	1:423:A:GLY:HA3	1:456:A:MET:HB3	21	0.11
(1,3179)	1:421:A:ARG:HE	1:426:A:GLN:HG2	19	0.11
(1,3179)	1:421:A:ARG:HE	1:426:A:GLN:HG3	19	0.11
(1,3169)	1:420:A:LEU:H	1:428:A:VAL:HG11	24	0.11
(1,3169)	1:420:A:LEU:H	1:428:A:VAL:HG12	24	0.11
(1,3169)	1:420:A:LEU:H	1:428:A:VAL:HG13	24	0.11
(1,3169)	1:420:A:LEU:H	1:428:A:VAL:HG21	24	0.11
(1,3169)	1:420:A:LEU:H	1:428:A:VAL:HG22	24	0.11
(1,3169)	1:420:A:LEU:H	1:428:A:VAL:HG23	24	0.11
(1,3153)	1:418:A:LEU:HD11	1:419:A:GLN:H	2	0.11
(1,3153)	1:418:A:LEU:HD12	1:419:A:GLN:H	2	0.11
(1,3153)	1:418:A:LEU:HD13	1:419:A:GLN:H	2	0.11
(1,3153)	1:418:A:LEU:HD21	1:419:A:GLN:H	2	0.11
(1,3153)	1:418:A:LEU:HD22	1:419:A:GLN:H	2	0.11
(1,3153)	1:418:A:LEU:HD23	1:419:A:GLN:H	2	0.11
(1,3153)	1:418:A:LEU:HD11	1:419:A:GLN:H	18	0.11
(1,3153)	1:418:A:LEU:HD12	1:419:A:GLN:H	18	0.11
(1,3153)	1:418:A:LEU:HD13	1:419:A:GLN:H	18	0.11
(1,3153)	1:418:A:LEU:HD21	1:419:A:GLN:H	18	0.11
(1,3153)	1:418:A:LEU:HD22	1:419:A:GLN:H	18	0.11
(1,3153)	1:418:A:LEU:HD23	1:419:A:GLN:H	18	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3153)	1:418:A:LEU:HD11	1:419:A:GLN:H	24	0.11
(1,3153)	1:418:A:LEU:HD12	1:419:A:GLN:H	24	0.11
(1,3153)	1:418:A:LEU:HD13	1:419:A:GLN:H	24	0.11
(1,3153)	1:418:A:LEU:HD21	1:419:A:GLN:H	24	0.11
(1,3153)	1:418:A:LEU:HD22	1:419:A:GLN:H	24	0.11
(1,3153)	1:418:A:LEU:HD23	1:419:A:GLN:H	24	0.11
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD11	9	0.11
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD12	9	0.11
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD13	9	0.11
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD21	9	0.11
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD22	9	0.11
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD23	9	0.11
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD11	22	0.11
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD12	22	0.11
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD13	22	0.11
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD21	22	0.11
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD22	22	0.11
(1,3143)	1:417:A:GLY:HA3	1:418:A:LEU:HD23	22	0.11
(1,3137)	1:415:A:ASN:H	1:416:A:LYS:HD2	22	0.11
(1,3137)	1:415:A:ASN:H	1:416:A:LYS:HD3	22	0.11
(1,3062)	1:400:A:VAL:HG11	1:416:A:LYS:H	7	0.11
(1,3062)	1:400:A:VAL:HG12	1:416:A:LYS:H	7	0.11
(1,3062)	1:400:A:VAL:HG13	1:416:A:LYS:H	7	0.11
(1,3062)	1:400:A:VAL:HG21	1:416:A:LYS:H	7	0.11
(1,3062)	1:400:A:VAL:HG22	1:416:A:LYS:H	7	0.11
(1,3062)	1:400:A:VAL:HG23	1:416:A:LYS:H	7	0.11
(1,3062)	1:400:A:VAL:HG11	1:416:A:LYS:H	8	0.11
(1,3062)	1:400:A:VAL:HG12	1:416:A:LYS:H	8	0.11
(1,3062)	1:400:A:VAL:HG13	1:416:A:LYS:H	8	0.11
(1,3062)	1:400:A:VAL:HG21	1:416:A:LYS:H	8	0.11
(1,3062)	1:400:A:VAL:HG22	1:416:A:LYS:H	8	0.11
(1,3062)	1:400:A:VAL:HG23	1:416:A:LYS:H	8	0.11
(1,3062)	1:400:A:VAL:HG11	1:416:A:LYS:H	12	0.11
(1,3062)	1:400:A:VAL:HG12	1:416:A:LYS:H	12	0.11
(1,3062)	1:400:A:VAL:HG13	1:416:A:LYS:H	12	0.11
(1,3062)	1:400:A:VAL:HG21	1:416:A:LYS:H	12	0.11
(1,3062)	1:400:A:VAL:HG22	1:416:A:LYS:H	12	0.11
(1,3062)	1:400:A:VAL:HG23	1:416:A:LYS:H	12	0.11
(1,3062)	1:400:A:VAL:HG11	1:416:A:LYS:H	17	0.11
(1,3062)	1:400:A:VAL:HG12	1:416:A:LYS:H	17	0.11
(1,3062)	1:400:A:VAL:HG13	1:416:A:LYS:H	17	0.11
(1,3062)	1:400:A:VAL:HG21	1:416:A:LYS:H	17	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3062)	1:400:A:VAL:HG22	1:416:A:LYS:H	17	0.11
(1,3062)	1:400:A:VAL:HG23	1:416:A:LYS:H	17	0.11
(1,3054)	1:399:A:GLY:H	1:400:A:VAL:HG11	17	0.11
(1,3054)	1:399:A:GLY:H	1:400:A:VAL:HG12	17	0.11
(1,3054)	1:399:A:GLY:H	1:400:A:VAL:HG13	17	0.11
(1,3054)	1:399:A:GLY:H	1:400:A:VAL:HG21	17	0.11
(1,3054)	1:399:A:GLY:H	1:400:A:VAL:HG22	17	0.11
(1,3054)	1:399:A:GLY:H	1:400:A:VAL:HG23	17	0.11
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD11	14	0.11
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD12	14	0.11
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD13	14	0.11
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD21	14	0.11
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD22	14	0.11
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD23	14	0.11
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD11	14	0.11
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD12	14	0.11
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD13	14	0.11
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD21	14	0.11
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD22	14	0.11
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD23	14	0.11
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD11	14	0.11
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD12	14	0.11
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD13	14	0.11
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD21	14	0.11
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD22	14	0.11
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD23	14	0.11
(1,2930)	1:367:A:MET:HG2	1:368:A:PRO:HD3	17	0.11
(1,2930)	1:367:A:MET:HG3	1:368:A:PRO:HD3	17	0.11
(1,2896)	1:361:A:LEU:HD11	1:432:A:GLU:H	2	0.11
(1,2896)	1:361:A:LEU:HD12	1:432:A:GLU:H	2	0.11
(1,2896)	1:361:A:LEU:HD13	1:432:A:GLU:H	2	0.11
(1,2896)	1:361:A:LEU:HD21	1:432:A:GLU:H	2	0.11
(1,2896)	1:361:A:LEU:HD22	1:432:A:GLU:H	2	0.11
(1,2896)	1:361:A:LEU:HD23	1:432:A:GLU:H	2	0.11
(1,2852)	1:356:A:LEU:HD11	1:379:A:VAL:HB	18	0.11
(1,2852)	1:356:A:LEU:HD12	1:379:A:VAL:HB	18	0.11
(1,2852)	1:356:A:LEU:HD13	1:379:A:VAL:HB	18	0.11
(1,2852)	1:356:A:LEU:HD21	1:379:A:VAL:HB	18	0.11
(1,2852)	1:356:A:LEU:HD22	1:379:A:VAL:HB	18	0.11
(1,2852)	1:356:A:LEU:HD23	1:379:A:VAL:HB	18	0.11
(1,2852)	1:356:A:LEU:HD11	1:379:A:VAL:HB	21	0.11
(1,2852)	1:356:A:LEU:HD12	1:379:A:VAL:HB	21	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2852)	1:356:A:LEU:HD13	1:379:A:VAL:HB	21	0.11
(1,2852)	1:356:A:LEU:HD21	1:379:A:VAL:HB	21	0.11
(1,2852)	1:356:A:LEU:HD22	1:379:A:VAL:HB	21	0.11
(1,2852)	1:356:A:LEU:HD23	1:379:A:VAL:HB	21	0.11
(1,2848)	1:356:A:LEU:HD11	1:377:A:CYS:H	23	0.11
(1,2848)	1:356:A:LEU:HD12	1:377:A:CYS:H	23	0.11
(1,2848)	1:356:A:LEU:HD13	1:377:A:CYS:H	23	0.11
(1,2848)	1:356:A:LEU:HD21	1:377:A:CYS:H	23	0.11
(1,2848)	1:356:A:LEU:HD22	1:377:A:CYS:H	23	0.11
(1,2848)	1:356:A:LEU:HD23	1:377:A:CYS:H	23	0.11
(1,2739)	1:345:A:VAL:HG11	1:459:A:PRO:HA	25	0.11
(1,2739)	1:345:A:VAL:HG12	1:459:A:PRO:HA	25	0.11
(1,2739)	1:345:A:VAL:HG13	1:459:A:PRO:HA	25	0.11
(1,2739)	1:345:A:VAL:HG21	1:459:A:PRO:HA	25	0.11
(1,2739)	1:345:A:VAL:HG22	1:459:A:PRO:HA	25	0.11
(1,2739)	1:345:A:VAL:HG23	1:459:A:PRO:HA	25	0.11
(1,2725)	1:345:A:VAL:HG11	1:350:A:GLU:H	11	0.11
(1,2725)	1:345:A:VAL:HG12	1:350:A:GLU:H	11	0.11
(1,2725)	1:345:A:VAL:HG13	1:350:A:GLU:H	11	0.11
(1,2725)	1:345:A:VAL:HG21	1:350:A:GLU:H	11	0.11
(1,2725)	1:345:A:VAL:HG22	1:350:A:GLU:H	11	0.11
(1,2725)	1:345:A:VAL:HG23	1:350:A:GLU:H	11	0.11
(1,2708)	1:-3:A:SER:H	1:-3:A:SER:HB2	8	0.11
(1,2708)	1:-3:A:SER:H	1:-3:A:SER:HB3	8	0.11
(1,2695)	1:-7:A:VAL:HB	1:-6:A:PRO:HD2	19	0.11
(1,2695)	1:-7:A:VAL:HB	1:-6:A:PRO:HD3	19	0.11
(1,2695)	1:-7:A:VAL:HB	1:-6:A:PRO:HD2	25	0.11
(1,2695)	1:-7:A:VAL:HB	1:-6:A:PRO:HD3	25	0.11
(1,2670)	1:345:A:VAL:HB	1:347:A:LEU:H	25	0.11
(1,2656)	1:380:A:ARG:HE	1:440:A:THR:HG21	22	0.11
(1,2656)	1:380:A:ARG:HE	1:440:A:THR:HG22	22	0.11
(1,2656)	1:380:A:ARG:HE	1:440:A:THR:HG23	22	0.11
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG2	3	0.11
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG3	3	0.11
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG2	13	0.11
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG3	13	0.11
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG2	16	0.11
(1,2637)	1:353:A:ARG:HE	1:468:A:GLU:HG3	16	0.11
(1,2635)	1:353:A:ARG:HA	1:353:A:ARG:HE	3	0.11
(1,2612)	1:399:A:GLY:H	1:418:A:LEU:HA	21	0.11
(1,2601)	1:424:A:ASN:HD22	1:454:A:ALA:HB1	16	0.11
(1,2601)	1:424:A:ASN:HD22	1:454:A:ALA:HB2	16	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2601)	1:424:A:ASN:HD22	1:454:A:ALA:HB3	16	0.11
(1,2515)	1:409:A:LEU:HB2	1:414:A:THR:H	23	0.11
(1,2515)	1:409:A:LEU:HB3	1:414:A:THR:H	23	0.11
(1,2470)	1:400:A:VAL:HA	1:418:A:LEU:H	7	0.11
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE1	14	0.11
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE2	14	0.11
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE3	14	0.11
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE1	20	0.11
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE2	20	0.11
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE3	20	0.11
(1,2435)	1:370:A:PHE:HD1	1:371:A:ALA:H	12	0.11
(1,2360)	1:415:A:ASN:H	1:416:A:LYS:HB2	6	0.11
(1,2360)	1:415:A:ASN:H	1:416:A:LYS:HB3	6	0.11
(1,2360)	1:415:A:ASN:H	1:416:A:LYS:HB2	7	0.11
(1,2360)	1:415:A:ASN:H	1:416:A:LYS:HB3	7	0.11
(1,2360)	1:415:A:ASN:H	1:416:A:LYS:HB2	8	0.11
(1,2360)	1:415:A:ASN:H	1:416:A:LYS:HB3	8	0.11
(1,2360)	1:415:A:ASN:H	1:416:A:LYS:HB2	15	0.11
(1,2360)	1:415:A:ASN:H	1:416:A:LYS:HB3	15	0.11
(1,2355)	1:427:A:ARG:HD2	1:428:A:VAL:H	18	0.11
(1,2355)	1:427:A:ARG:HD3	1:428:A:VAL:H	18	0.11
(1,2327)	1:-8:A:LEU:H	1:-8:A:LEU:HG	6	0.11
(1,2297)	1:406:A:VAL:H	1:406:A:VAL:HB	1	0.11
(1,2270)	1:369:A:PHE:HD2	1:370:A:PHE:H	3	0.11
(1,2270)	1:369:A:PHE:HD2	1:370:A:PHE:H	4	0.11
(1,2173)	1:423:A:GLY:H	1:454:A:ALA:HB1	5	0.11
(1,2173)	1:423:A:GLY:H	1:454:A:ALA:HB2	5	0.11
(1,2173)	1:423:A:GLY:H	1:454:A:ALA:HB3	5	0.11
(1,2148)	1:348:A:PRO:HD3	1:350:A:GLU:H	24	0.11
(1,2117)	1:423:A:GLY:HA2	1:450:A:ALA:H	17	0.11
(1,2003)	1:348:A:PRO:HD3	1:444:A:PHE:H	10	0.11
(1,1940)	1:362:A:GLU:H	1:412:A:THR:HG21	25	0.11
(1,1940)	1:362:A:GLU:H	1:412:A:THR:HG22	25	0.11
(1,1940)	1:362:A:GLU:H	1:412:A:THR:HG23	25	0.11
(1,1939)	1:442:A:SER:H	1:442:A:SER:HB3	8	0.11
(1,1931)	1:364:A:TRP:H	1:365:A:CYS:HA	19	0.11
(1,1902)	1:423:A:GLY:HA2	1:425:A:ASP:H	9	0.11
(1,1886)	1:440:A:THR:H	1:443:A:GLU:HA	16	0.11
(1,1882)	1:423:A:GLY:HA3	1:447:A:TRP:HE1	12	0.11
(1,1882)	1:423:A:GLY:HA3	1:447:A:TRP:HE1	17	0.11
(1,1882)	1:423:A:GLY:HA3	1:447:A:TRP:HE1	19	0.11
(1,1882)	1:423:A:GLY:HA3	1:447:A:TRP:HE1	22	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1882)	1:423:A:GLY:HA3	1:447:A:TRP:HE1	24	0.11
(1,1809)	1:423:A:GLY:HA3	1:456:A:MET:H	2	0.11
(1,1809)	1:423:A:GLY:HA3	1:456:A:MET:H	5	0.11
(1,1809)	1:423:A:GLY:HA3	1:456:A:MET:H	7	0.11
(1,1809)	1:423:A:GLY:HA3	1:456:A:MET:H	19	0.11
(1,1809)	1:423:A:GLY:HA3	1:456:A:MET:H	23	0.11
(1,1804)	1:359:A:HIS:H	1:359:A:HIS:HB3	19	0.11
(1,1789)	1:456:A:MET:H	1:456:A:MET:HG2	17	0.11
(1,1744)	1:461:A:LEU:HD11	1:462:A:ASP:H	2	0.11
(1,1744)	1:461:A:LEU:HD12	1:462:A:ASP:H	2	0.11
(1,1744)	1:461:A:LEU:HD13	1:462:A:ASP:H	2	0.11
(1,1708)	1:446:A:LYS:H	1:446:A:LYS:HG3	1	0.11
(1,1661)	1:421:A:ARG:HD2	1:425:A:ASP:H	1	0.11
(1,1661)	1:421:A:ARG:HD3	1:425:A:ASP:H	1	0.11
(1,1661)	1:421:A:ARG:HD2	1:425:A:ASP:H	4	0.11
(1,1661)	1:421:A:ARG:HD3	1:425:A:ASP:H	4	0.11
(1,1661)	1:421:A:ARG:HD2	1:425:A:ASP:H	6	0.11
(1,1661)	1:421:A:ARG:HD3	1:425:A:ASP:H	6	0.11
(1,1660)	1:425:A:ASP:HB3	1:426:A:GLN:H	16	0.11
(1,1659)	1:424:A:ASN:H	1:425:A:ASP:H	22	0.11
(1,1658)	1:423:A:GLY:HA2	1:424:A:ASN:H	16	0.11
(1,1628)	1:412:A:THR:HG21	1:413:A:ARG:H	25	0.11
(1,1628)	1:412:A:THR:HG22	1:413:A:ARG:H	25	0.11
(1,1628)	1:412:A:THR:HG23	1:413:A:ARG:H	25	0.11
(1,1479)	1:347:A:LEU:HG	1:349:A:GLU:H	20	0.11
(1,1414)	1:419:A:GLN:HB3	1:419:A:GLN:HE22	4	0.11
(1,1389)	1:435:A:SER:HA	1:437:A:GLN:HE22	5	0.11
(1,1389)	1:435:A:SER:HA	1:437:A:GLN:HE22	15	0.11
(1,1383)	1:470:A:SER:H	1:471:A:ILE:HD11	2	0.11
(1,1383)	1:470:A:SER:H	1:471:A:ILE:HD12	2	0.11
(1,1383)	1:470:A:SER:H	1:471:A:ILE:HD13	2	0.11
(1,1383)	1:470:A:SER:H	1:471:A:ILE:HD11	20	0.11
(1,1383)	1:470:A:SER:H	1:471:A:ILE:HD12	20	0.11
(1,1383)	1:470:A:SER:H	1:471:A:ILE:HD13	20	0.11
(1,1153)	1:366:A:HIS:HE1	1:367:A:MET:H	8	0.11
(1,1153)	1:366:A:HIS:HE1	1:367:A:MET:H	14	0.11
(1,1153)	1:366:A:HIS:HE1	1:367:A:MET:H	21	0.11
(1,1145)	1:419:A:GLN:HG3	1:428:A:VAL:H	25	0.11
(1,1084)	1:405:A:LYS:HG2	1:406:A:VAL:H	3	0.11
(1,1084)	1:405:A:LYS:HG3	1:406:A:VAL:H	3	0.11
(1,1060)	1:368:A:PRO:HD2	1:370:A:PHE:H	17	0.11
(1,922)	1:439:A:PHE:HD1	1:440:A:THR:HA	6	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,922)	1:439:A:PHE:HD2	1:440:A:THR:HA	6	0.11
(1,921)	1:351:A:LEU:HB2	1:444:A:PHE:HZ	3	0.11
(1,914)	1:460:A:THR:HA	1:461:A:LEU:HG	6	0.11
(1,914)	1:460:A:THR:HA	1:461:A:LEU:HG	7	0.11
(1,914)	1:460:A:THR:HA	1:461:A:LEU:HG	8	0.11
(1,914)	1:460:A:THR:HA	1:461:A:LEU:HG	18	0.11
(1,909)	1:347:A:LEU:HB2	1:348:A:PRO:HD3	15	0.11
(1,855)	1:399:A:GLY:HA3	1:418:A:LEU:HB3	3	0.11
(1,855)	1:399:A:GLY:HA3	1:418:A:LEU:HB3	14	0.11
(1,855)	1:399:A:GLY:HA3	1:418:A:LEU:HB3	17	0.11
(1,855)	1:399:A:GLY:HA3	1:418:A:LEU:HB3	23	0.11
(1,855)	1:399:A:GLY:HA3	1:418:A:LEU:HB3	24	0.11
(1,737)	1:345:A:VAL:HG21	1:459:A:PRO:HD3	17	0.11
(1,737)	1:345:A:VAL:HG22	1:459:A:PRO:HD3	17	0.11
(1,737)	1:345:A:VAL:HG23	1:459:A:PRO:HD3	17	0.11
(1,535)	1:363:A:ARG:HD2	1:364:A:TRP:H	24	0.11
(1,535)	1:363:A:ARG:HD3	1:364:A:TRP:H	24	0.11
(1,487)	1:398:A:THR:HG21	1:419:A:GLN:HG3	3	0.11
(1,487)	1:398:A:THR:HG22	1:419:A:GLN:HG3	3	0.11
(1,487)	1:398:A:THR:HG23	1:419:A:GLN:HG3	3	0.11
(1,463)	1:401:A:VAL:HG21	1:417:A:GLY:HA2	2	0.11
(1,463)	1:401:A:VAL:HG22	1:417:A:GLY:HA2	2	0.11
(1,463)	1:401:A:VAL:HG23	1:417:A:GLY:HA2	2	0.11
(1,463)	1:401:A:VAL:HG21	1:417:A:GLY:HA2	5	0.11
(1,463)	1:401:A:VAL:HG22	1:417:A:GLY:HA2	5	0.11
(1,463)	1:401:A:VAL:HG23	1:417:A:GLY:HA2	5	0.11
(1,463)	1:401:A:VAL:HG21	1:417:A:GLY:HA2	7	0.11
(1,463)	1:401:A:VAL:HG22	1:417:A:GLY:HA2	7	0.11
(1,463)	1:401:A:VAL:HG23	1:417:A:GLY:HA2	7	0.11
(1,463)	1:401:A:VAL:HG21	1:417:A:GLY:HA2	11	0.11
(1,463)	1:401:A:VAL:HG22	1:417:A:GLY:HA2	11	0.11
(1,463)	1:401:A:VAL:HG23	1:417:A:GLY:HA2	11	0.11
(1,377)	1:395:A:ALA:HB1	1:420:A:LEU:HB2	14	0.11
(1,377)	1:395:A:ALA:HB2	1:420:A:LEU:HB2	14	0.11
(1,377)	1:395:A:ALA:HB3	1:420:A:LEU:HB2	14	0.11
(1,343)	1:447:A:TRP:HZ3	1:458:A:LEU:HD21	20	0.11
(1,343)	1:447:A:TRP:HZ3	1:458:A:LEU:HD22	20	0.11
(1,343)	1:447:A:TRP:HZ3	1:458:A:LEU:HD23	20	0.11
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD2	1	0.11
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD3	1	0.11
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD2	9	0.11
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD3	9	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD2	21	0.11
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD3	21	0.11
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD2	23	0.11
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD3	23	0.11
(1,247)	1:440:A:THR:HG21	1:444:A:PHE:H	3	0.11
(1,247)	1:440:A:THR:HG22	1:444:A:PHE:H	3	0.11
(1,247)	1:440:A:THR:HG23	1:444:A:PHE:H	3	0.11
(1,247)	1:440:A:THR:HG21	1:444:A:PHE:H	19	0.11
(1,247)	1:440:A:THR:HG22	1:444:A:PHE:H	19	0.11
(1,247)	1:440:A:THR:HG23	1:444:A:PHE:H	19	0.11
(1,247)	1:440:A:THR:HG21	1:444:A:PHE:H	23	0.11
(1,247)	1:440:A:THR:HG22	1:444:A:PHE:H	23	0.11
(1,247)	1:440:A:THR:HG23	1:444:A:PHE:H	23	0.11
(1,212)	1:397:A:ILE:HD11	1:418:A:LEU:HD21	7	0.11
(1,212)	1:397:A:ILE:HD11	1:418:A:LEU:HD22	7	0.11
(1,212)	1:397:A:ILE:HD11	1:418:A:LEU:HD23	7	0.11
(1,212)	1:397:A:ILE:HD12	1:418:A:LEU:HD21	7	0.11
(1,212)	1:397:A:ILE:HD12	1:418:A:LEU:HD22	7	0.11
(1,212)	1:397:A:ILE:HD12	1:418:A:LEU:HD23	7	0.11
(1,212)	1:397:A:ILE:HD13	1:418:A:LEU:HD21	7	0.11
(1,212)	1:397:A:ILE:HD13	1:418:A:LEU:HD22	7	0.11
(1,212)	1:397:A:ILE:HD13	1:418:A:LEU:HD23	7	0.11
(1,203)	1:347:A:LEU:HD11	1:349:A:GLU:HG2	2	0.11
(1,203)	1:347:A:LEU:HD11	1:349:A:GLU:HG3	2	0.11
(1,203)	1:347:A:LEU:HD12	1:349:A:GLU:HG2	2	0.11
(1,203)	1:347:A:LEU:HD12	1:349:A:GLU:HG3	2	0.11
(1,203)	1:347:A:LEU:HD13	1:349:A:GLU:HG2	2	0.11
(1,203)	1:347:A:LEU:HD13	1:349:A:GLU:HG3	2	0.11
(1,178)	1:393:A:ARG:H	1:395:A:ALA:HB1	13	0.11
(1,178)	1:393:A:ARG:H	1:395:A:ALA:HB2	13	0.11
(1,178)	1:393:A:ARG:H	1:395:A:ALA:HB3	13	0.11
(1,154)	1:397:A:ILE:HG12	1:418:A:LEU:HG	1	0.11
(1,154)	1:397:A:ILE:HG13	1:418:A:LEU:HG	1	0.11
(1,57)	1:411:A:GLY:HA3	1:412:A:THR:HB	15	0.11
(1,3385)	1:467:A:LYS:HA	1:470:A:SER:HB2	16	0.1
(1,3385)	1:467:A:LYS:HA	1:470:A:SER:HB3	16	0.1
(1,3356)	1:459:A:PRO:HD2	1:461:A:LEU:HD11	11	0.1
(1,3356)	1:459:A:PRO:HD2	1:461:A:LEU:HD12	11	0.1
(1,3356)	1:459:A:PRO:HD2	1:461:A:LEU:HD13	11	0.1
(1,3356)	1:459:A:PRO:HD2	1:461:A:LEU:HD21	11	0.1
(1,3356)	1:459:A:PRO:HD2	1:461:A:LEU:HD22	11	0.1
(1,3356)	1:459:A:PRO:HD2	1:461:A:LEU:HD23	11	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3184)	1:423:A:GLY:HA3	1:456:A:MET:HB2	22	0.1
(1,3184)	1:423:A:GLY:HA3	1:456:A:MET:HB3	22	0.1
(1,3062)	1:400:A:VAL:HG11	1:416:A:LYS:H	2	0.1
(1,3062)	1:400:A:VAL:HG12	1:416:A:LYS:H	2	0.1
(1,3062)	1:400:A:VAL:HG13	1:416:A:LYS:H	2	0.1
(1,3062)	1:400:A:VAL:HG21	1:416:A:LYS:H	2	0.1
(1,3062)	1:400:A:VAL:HG22	1:416:A:LYS:H	2	0.1
(1,3062)	1:400:A:VAL:HG23	1:416:A:LYS:H	2	0.1
(1,3062)	1:400:A:VAL:HG11	1:416:A:LYS:H	19	0.1
(1,3062)	1:400:A:VAL:HG12	1:416:A:LYS:H	19	0.1
(1,3062)	1:400:A:VAL:HG13	1:416:A:LYS:H	19	0.1
(1,3062)	1:400:A:VAL:HG21	1:416:A:LYS:H	19	0.1
(1,3062)	1:400:A:VAL:HG22	1:416:A:LYS:H	19	0.1
(1,3062)	1:400:A:VAL:HG23	1:416:A:LYS:H	19	0.1
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD11	19	0.1
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD12	19	0.1
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD13	19	0.1
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD21	19	0.1
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD22	19	0.1
(1,2944)	1:371:A:ALA:HB1	1:418:A:LEU:HD23	19	0.1
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD11	19	0.1
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD12	19	0.1
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD13	19	0.1
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD21	19	0.1
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD22	19	0.1
(1,2944)	1:371:A:ALA:HB2	1:418:A:LEU:HD23	19	0.1
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD11	19	0.1
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD12	19	0.1
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD13	19	0.1
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD21	19	0.1
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD22	19	0.1
(1,2944)	1:371:A:ALA:HB3	1:418:A:LEU:HD23	19	0.1
(1,2876)	1:358:A:ARG:HE	1:436:A:ASN:HD21	12	0.1
(1,2876)	1:358:A:ARG:HE	1:436:A:ASN:HD22	12	0.1
(1,2763)	1:347:A:LEU:HD11	1:349:A:GLU:HB2	24	0.1
(1,2763)	1:347:A:LEU:HD11	1:349:A:GLU:HB3	24	0.1
(1,2763)	1:347:A:LEU:HD12	1:349:A:GLU:HB2	24	0.1
(1,2763)	1:347:A:LEU:HD12	1:349:A:GLU:HB3	24	0.1
(1,2763)	1:347:A:LEU:HD13	1:349:A:GLU:HB2	24	0.1
(1,2763)	1:347:A:LEU:HD13	1:349:A:GLU:HB3	24	0.1
(1,2763)	1:347:A:LEU:HD21	1:349:A:GLU:HB2	24	0.1
(1,2763)	1:347:A:LEU:HD21	1:349:A:GLU:HB3	24	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2763)	1:347:A:LEU:HD22	1:349:A:GLU:HB2	24	0.1
(1,2763)	1:347:A:LEU:HD22	1:349:A:GLU:HB3	24	0.1
(1,2763)	1:347:A:LEU:HD23	1:349:A:GLU:HB2	24	0.1
(1,2763)	1:347:A:LEU:HD23	1:349:A:GLU:HB3	24	0.1
(1,2739)	1:345:A:VAL:HG11	1:459:A:PRO:HA	14	0.1
(1,2739)	1:345:A:VAL:HG12	1:459:A:PRO:HA	14	0.1
(1,2739)	1:345:A:VAL:HG13	1:459:A:PRO:HA	14	0.1
(1,2739)	1:345:A:VAL:HG21	1:459:A:PRO:HA	14	0.1
(1,2739)	1:345:A:VAL:HG22	1:459:A:PRO:HA	14	0.1
(1,2739)	1:345:A:VAL:HG23	1:459:A:PRO:HA	14	0.1
(1,2739)	1:345:A:VAL:HG11	1:459:A:PRO:HA	16	0.1
(1,2739)	1:345:A:VAL:HG12	1:459:A:PRO:HA	16	0.1
(1,2739)	1:345:A:VAL:HG13	1:459:A:PRO:HA	16	0.1
(1,2739)	1:345:A:VAL:HG21	1:459:A:PRO:HA	16	0.1
(1,2739)	1:345:A:VAL:HG22	1:459:A:PRO:HA	16	0.1
(1,2739)	1:345:A:VAL:HG23	1:459:A:PRO:HA	16	0.1
(1,2612)	1:399:A:GLY:H	1:418:A:LEU:HA	1	0.1
(1,2612)	1:399:A:GLY:H	1:418:A:LEU:HA	5	0.1
(1,2470)	1:400:A:VAL:HA	1:418:A:LEU:H	20	0.1
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE1	24	0.1
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE2	24	0.1
(1,2447)	1:456:A:MET:H	1:456:A:MET:HE3	24	0.1
(1,2437)	1:371:A:ALA:H	1:400:A:VAL:HG11	15	0.1
(1,2437)	1:371:A:ALA:H	1:400:A:VAL:HG12	15	0.1
(1,2437)	1:371:A:ALA:H	1:400:A:VAL:HG13	15	0.1
(1,2360)	1:415:A:ASN:H	1:416:A:LYS:HB2	19	0.1
(1,2360)	1:415:A:ASN:H	1:416:A:LYS:HB3	19	0.1
(1,2313)	1:-6:A:PRO:HB2	1:-5:A:ARG:H	5	0.1
(1,2313)	1:-6:A:PRO:HB3	1:-5:A:ARG:H	5	0.1
(1,2270)	1:369:A:PHE:HD2	1:370:A:PHE:H	10	0.1
(1,2148)	1:348:A:PRO:HD3	1:350:A:GLU:H	15	0.1
(1,2138)	1:350:A:GLU:HB3	1:354:A:VAL:H	7	0.1
(1,2003)	1:348:A:PRO:HD3	1:444:A:PHE:H	22	0.1
(1,2003)	1:348:A:PRO:HD3	1:444:A:PHE:H	23	0.1
(1,1940)	1:362:A:GLU:H	1:412:A:THR:HG21	12	0.1
(1,1940)	1:362:A:GLU:H	1:412:A:THR:HG22	12	0.1
(1,1940)	1:362:A:GLU:H	1:412:A:THR:HG23	12	0.1
(1,1939)	1:442:A:SER:H	1:442:A:SER:HB3	13	0.1
(1,1901)	1:367:A:MET:H	1:368:A:PRO:HD2	2	0.1
(1,1889)	1:392:A:TYR:HE1	1:437:A:GLN:H	8	0.1
(1,1889)	1:392:A:TYR:HE2	1:437:A:GLN:H	8	0.1
(1,1882)	1:423:A:GLY:HA3	1:447:A:TRP:HE1	4	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1809)	1:423:A:GLY:HA3	1:456:A:MET:H	18	0.1
(1,1789)	1:456:A:MET:H	1:456:A:MET:HG2	12	0.1
(1,1660)	1:425:A:ASP:HB3	1:426:A:GLN:H	7	0.1
(1,1660)	1:425:A:ASP:HB3	1:426:A:GLN:H	14	0.1
(1,1659)	1:424:A:ASN:H	1:425:A:ASP:H	12	0.1
(1,1633)	1:413:A:ARG:HG3	1:414:A:THR:H	17	0.1
(1,1479)	1:347:A:LEU:HG	1:349:A:GLU:H	25	0.1
(1,1414)	1:419:A:GLN:HB3	1:419:A:GLN:HE22	2	0.1
(1,1383)	1:470:A:SER:H	1:471:A:ILE:HD11	7	0.1
(1,1383)	1:470:A:SER:H	1:471:A:ILE:HD12	7	0.1
(1,1383)	1:470:A:SER:H	1:471:A:ILE:HD13	7	0.1
(1,1383)	1:470:A:SER:H	1:471:A:ILE:HD11	11	0.1
(1,1383)	1:470:A:SER:H	1:471:A:ILE:HD12	11	0.1
(1,1383)	1:470:A:SER:H	1:471:A:ILE:HD13	11	0.1
(1,1153)	1:366:A:HIS:HE1	1:367:A:MET:H	15	0.1
(1,914)	1:460:A:THR:HA	1:461:A:LEU:HG	14	0.1
(1,907)	1:464:A:ILE:HA	1:467:A:LYS:HE2	19	0.1
(1,907)	1:464:A:ILE:HA	1:467:A:LYS:HE3	19	0.1
(1,892)	1:345:A:VAL:HG21	1:351:A:LEU:HD11	8	0.1
(1,892)	1:345:A:VAL:HG21	1:351:A:LEU:HD12	8	0.1
(1,892)	1:345:A:VAL:HG21	1:351:A:LEU:HD13	8	0.1
(1,892)	1:345:A:VAL:HG22	1:351:A:LEU:HD11	8	0.1
(1,892)	1:345:A:VAL:HG22	1:351:A:LEU:HD12	8	0.1
(1,892)	1:345:A:VAL:HG22	1:351:A:LEU:HD13	8	0.1
(1,892)	1:345:A:VAL:HG23	1:351:A:LEU:HD11	8	0.1
(1,892)	1:345:A:VAL:HG23	1:351:A:LEU:HD12	8	0.1
(1,892)	1:345:A:VAL:HG23	1:351:A:LEU:HD13	8	0.1
(1,892)	1:345:A:VAL:HG21	1:351:A:LEU:HD11	23	0.1
(1,892)	1:345:A:VAL:HG21	1:351:A:LEU:HD12	23	0.1
(1,892)	1:345:A:VAL:HG21	1:351:A:LEU:HD13	23	0.1
(1,892)	1:345:A:VAL:HG22	1:351:A:LEU:HD11	23	0.1
(1,892)	1:345:A:VAL:HG22	1:351:A:LEU:HD12	23	0.1
(1,892)	1:345:A:VAL:HG22	1:351:A:LEU:HD13	23	0.1
(1,892)	1:345:A:VAL:HG23	1:351:A:LEU:HD11	23	0.1
(1,892)	1:345:A:VAL:HG23	1:351:A:LEU:HD12	23	0.1
(1,892)	1:345:A:VAL:HG23	1:351:A:LEU:HD13	23	0.1
(1,855)	1:399:A:GLY:HA3	1:418:A:LEU:HB3	8	0.1
(1,855)	1:399:A:GLY:HA3	1:418:A:LEU:HB3	10	0.1
(1,855)	1:399:A:GLY:HA3	1:418:A:LEU:HB3	16	0.1
(1,797)	1:370:A:PHE:HE1	1:371:A:ALA:HB1	2	0.1
(1,797)	1:370:A:PHE:HE1	1:371:A:ALA:HB2	2	0.1
(1,797)	1:370:A:PHE:HE1	1:371:A:ALA:HB3	2	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,797)	1:370:A:PHE:HE2	1:371:A:ALA:HB1	2	0.1
(1,797)	1:370:A:PHE:HE2	1:371:A:ALA:HB2	2	0.1
(1,797)	1:370:A:PHE:HE2	1:371:A:ALA:HB3	2	0.1
(1,790)	1:361:A:LEU:HA	1:370:A:PHE:HE1	12	0.1
(1,790)	1:361:A:LEU:HA	1:370:A:PHE:HE2	12	0.1
(1,700)	1:380:A:ARG:HA	1:439:A:PHE:HD1	11	0.1
(1,700)	1:380:A:ARG:HA	1:439:A:PHE:HD2	11	0.1
(1,463)	1:401:A:VAL:HG21	1:417:A:GLY:HA2	1	0.1
(1,463)	1:401:A:VAL:HG22	1:417:A:GLY:HA2	1	0.1
(1,463)	1:401:A:VAL:HG23	1:417:A:GLY:HA2	1	0.1
(1,463)	1:401:A:VAL:HG21	1:417:A:GLY:HA2	4	0.1
(1,463)	1:401:A:VAL:HG22	1:417:A:GLY:HA2	4	0.1
(1,463)	1:401:A:VAL:HG23	1:417:A:GLY:HA2	4	0.1
(1,463)	1:401:A:VAL:HG21	1:417:A:GLY:HA2	21	0.1
(1,463)	1:401:A:VAL:HG22	1:417:A:GLY:HA2	21	0.1
(1,463)	1:401:A:VAL:HG23	1:417:A:GLY:HA2	21	0.1
(1,375)	1:395:A:ALA:HB1	1:420:A:LEU:HG	11	0.1
(1,375)	1:395:A:ALA:HB2	1:420:A:LEU:HG	11	0.1
(1,375)	1:395:A:ALA:HB3	1:420:A:LEU:HG	11	0.1
(1,338)	1:407:A:TYR:HE1	1:431:A:LEU:HD21	4	0.1
(1,338)	1:407:A:TYR:HE1	1:431:A:LEU:HD22	4	0.1
(1,338)	1:407:A:TYR:HE1	1:431:A:LEU:HD23	4	0.1
(1,338)	1:407:A:TYR:HE2	1:431:A:LEU:HD21	4	0.1
(1,338)	1:407:A:TYR:HE2	1:431:A:LEU:HD22	4	0.1
(1,338)	1:407:A:TYR:HE2	1:431:A:LEU:HD23	4	0.1
(1,279)	1:392:A:TYR:HE1	1:435:A:SER:HA	12	0.1
(1,279)	1:392:A:TYR:HE2	1:435:A:SER:HA	12	0.1
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD2	8	0.1
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD3	8	0.1
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD2	20	0.1
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD3	20	0.1
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD2	22	0.1
(1,268)	1:350:A:GLU:H	1:353:A:ARG:HD3	22	0.1
(1,258)	1:352:A:ASN:HD21	1:439:A:PHE:HB3	22	0.1
(1,247)	1:440:A:THR:HG21	1:444:A:PHE:H	4	0.1
(1,247)	1:440:A:THR:HG22	1:444:A:PHE:H	4	0.1
(1,247)	1:440:A:THR:HG23	1:444:A:PHE:H	4	0.1
(1,247)	1:440:A:THR:HG21	1:444:A:PHE:H	13	0.1
(1,247)	1:440:A:THR:HG22	1:444:A:PHE:H	13	0.1
(1,247)	1:440:A:THR:HG23	1:444:A:PHE:H	13	0.1
(1,212)	1:397:A:ILE:HD11	1:418:A:LEU:HD21	6	0.1
(1,212)	1:397:A:ILE:HD11	1:418:A:LEU:HD22	6	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,212)	1:397:A:ILE:HD11	1:418:A:LEU:HD23	6	0.1
(1,212)	1:397:A:ILE:HD12	1:418:A:LEU:HD21	6	0.1
(1,212)	1:397:A:ILE:HD12	1:418:A:LEU:HD22	6	0.1
(1,212)	1:397:A:ILE:HD12	1:418:A:LEU:HD23	6	0.1
(1,212)	1:397:A:ILE:HD13	1:418:A:LEU:HD21	6	0.1
(1,212)	1:397:A:ILE:HD13	1:418:A:LEU:HD22	6	0.1
(1,212)	1:397:A:ILE:HD13	1:418:A:LEU:HD23	6	0.1
(1,212)	1:397:A:ILE:HD11	1:418:A:LEU:HD21	8	0.1
(1,212)	1:397:A:ILE:HD11	1:418:A:LEU:HD22	8	0.1
(1,212)	1:397:A:ILE:HD11	1:418:A:LEU:HD23	8	0.1
(1,212)	1:397:A:ILE:HD12	1:418:A:LEU:HD21	8	0.1
(1,212)	1:397:A:ILE:HD12	1:418:A:LEU:HD22	8	0.1
(1,212)	1:397:A:ILE:HD12	1:418:A:LEU:HD23	8	0.1
(1,212)	1:397:A:ILE:HD13	1:418:A:LEU:HD21	8	0.1
(1,212)	1:397:A:ILE:HD13	1:418:A:LEU:HD22	8	0.1
(1,212)	1:397:A:ILE:HD13	1:418:A:LEU:HD23	8	0.1
(1,212)	1:397:A:ILE:HD11	1:418:A:LEU:HD21	25	0.1
(1,212)	1:397:A:ILE:HD11	1:418:A:LEU:HD22	25	0.1
(1,212)	1:397:A:ILE:HD11	1:418:A:LEU:HD23	25	0.1
(1,212)	1:397:A:ILE:HD12	1:418:A:LEU:HD21	25	0.1
(1,212)	1:397:A:ILE:HD12	1:418:A:LEU:HD22	25	0.1
(1,212)	1:397:A:ILE:HD12	1:418:A:LEU:HD23	25	0.1
(1,212)	1:397:A:ILE:HD13	1:418:A:LEU:HD21	25	0.1
(1,212)	1:397:A:ILE:HD13	1:418:A:LEU:HD22	25	0.1
(1,212)	1:397:A:ILE:HD13	1:418:A:LEU:HD23	25	0.1
(1,178)	1:393:A:ARG:H	1:395:A:ALA:HB1	7	0.1
(1,178)	1:393:A:ARG:H	1:395:A:ALA:HB2	7	0.1
(1,178)	1:393:A:ARG:H	1:395:A:ALA:HB3	7	0.1
(1,178)	1:393:A:ARG:H	1:395:A:ALA:HB1	16	0.1
(1,178)	1:393:A:ARG:H	1:395:A:ALA:HB2	16	0.1
(1,178)	1:393:A:ARG:H	1:395:A:ALA:HB3	16	0.1
(1,154)	1:397:A:ILE:HG12	1:418:A:LEU:HG	5	0.1
(1,154)	1:397:A:ILE:HG13	1:418:A:LEU:HG	5	0.1
(1,130)	1:380:A:ARG:HB2	1:435:A:SER:H	11	0.1
(1,130)	1:380:A:ARG:HB2	1:435:A:SER:H	22	0.1
(1,83)	1:382:A:GLY:HA3	1:392:A:TYR:HB2	8	0.1
(1,83)	1:382:A:GLY:HA3	1:392:A:TYR:HB2	20	0.1
(1,39)	1:366:A:HIS:HA	1:366:A:HIS:HD1	17	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found