



Full wwPDB NMR Structure Validation Report ⓘ

Feb 28, 2026 – 08:59 PM UTC

PDB ID : 6BYV / pdb_00006byv
BMRB ID : 30388
Title : Solution NMR structure of cysteine-rich calcium bound domains of very low density lipoprotein receptor
Authors : Banerjee, K.; Gruschus, J.M.; Tjandra, N.; Yakovlev, S.; Medved, L.
Deposited on : 2017-12-21

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

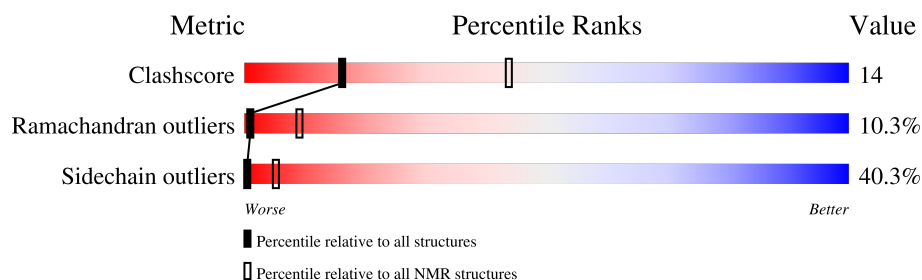
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 84%.

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	121	

2 Ensemble composition and analysis

This entry contains 20 models. Model 16 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:3-A:74 (72)	1.02	16
2	A:75-A:108 (34)	1.43	6

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

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

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

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1659 atoms, of which 753 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Very low-density lipoprotein receptor.

Mol	Chain	Residues	Atoms						Trace
1	A	121	Total	C	H	N	O	S	0
			1656	518	753	160	206	19	

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

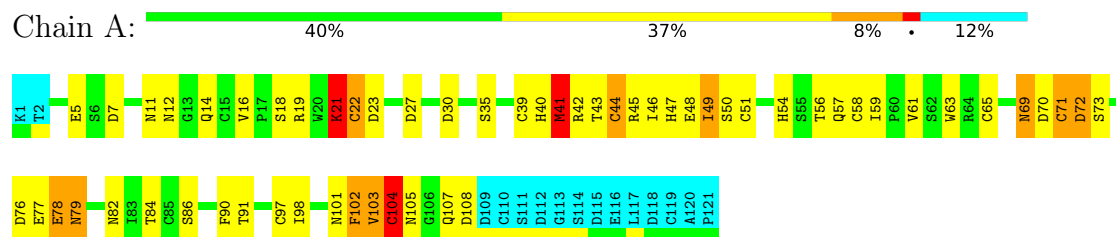
Mol	Chain	Residues	Atoms	
2	A	3	Total	Ca
			3	3

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Very low-density lipoprotein receptor

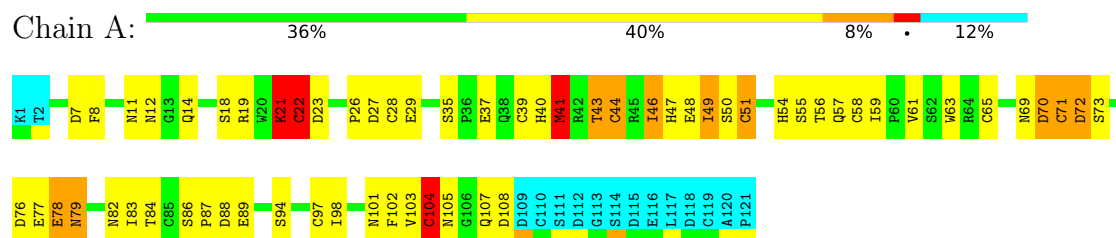


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

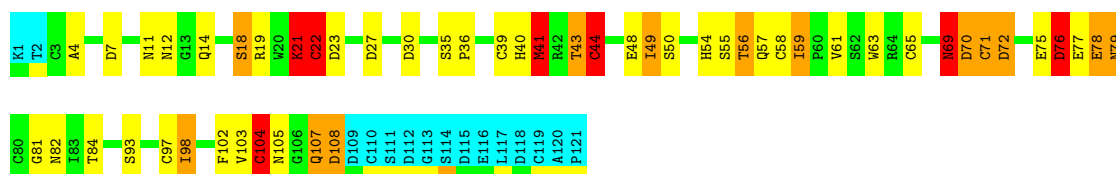
- Molecule 1: Very low-density lipoprotein receptor



4.2.2 Score per residue for model 2

- Molecule 1: Very low-density lipoprotein receptor

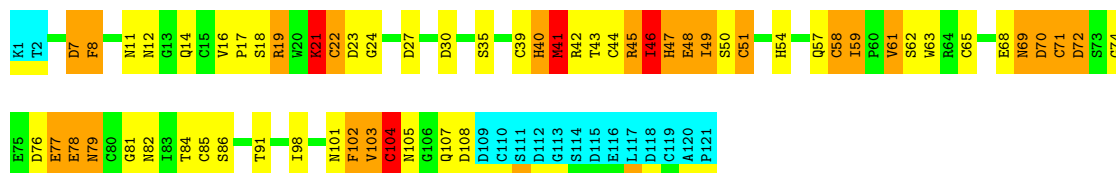




4.2.3 Score per residue for model 3

- Molecule 1: Very low-density lipoprotein receptor

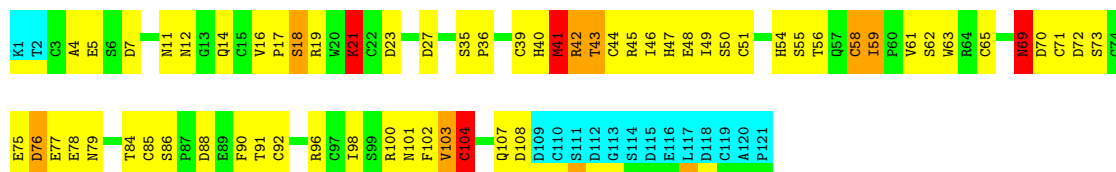
Chain A: 37% 29% 18% 12%



4.2.4 Score per residue for model 4

- Molecule 1: Very low-density lipoprotein receptor

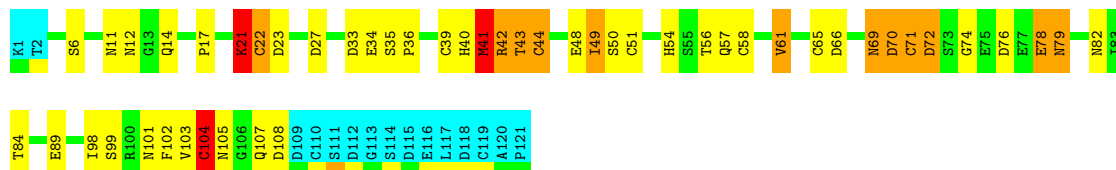
Chain A: 36% 43% 6% 12%



4.2.5 Score per residue for model 5

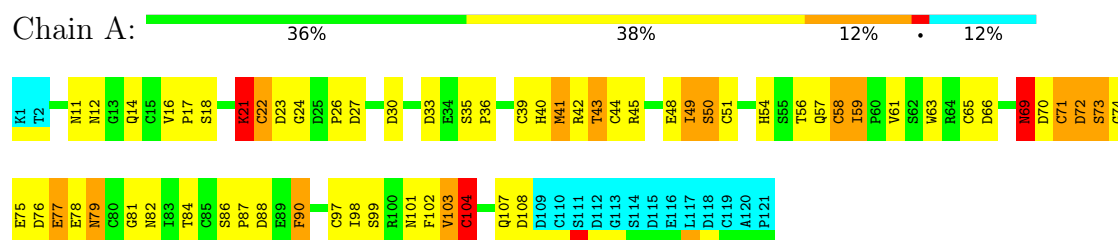
- Molecule 1: Very low-density lipoprotein receptor

Chain A: 46% 29% 10% 12%



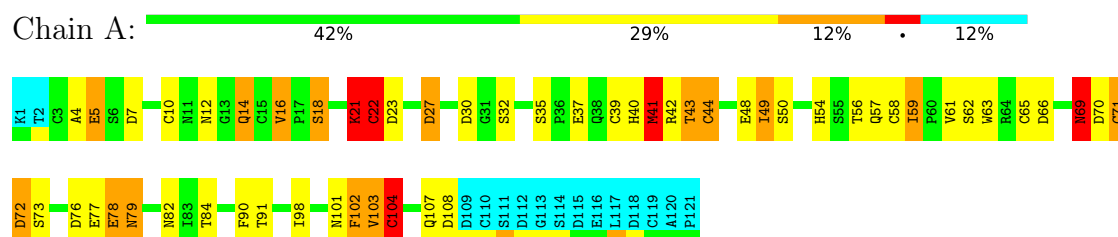
4.2.6 Score per residue for model 6

- Molecule 1: Very low-density lipoprotein receptor



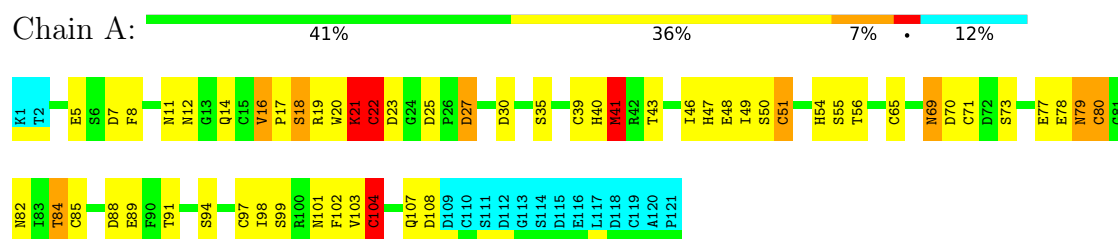
4.2.7 Score per residue for model 7

- Molecule 1: Very low-density lipoprotein receptor



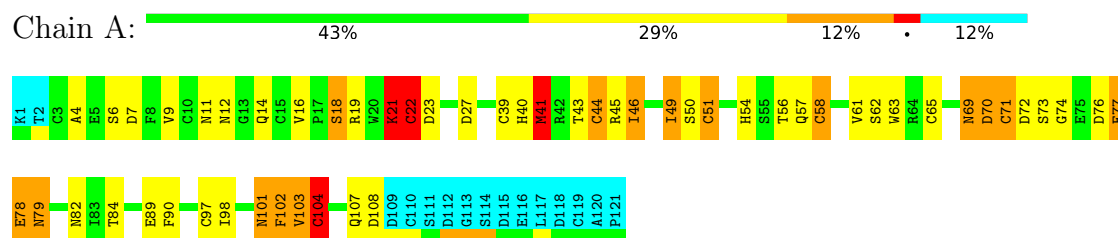
4.2.8 Score per residue for model 8

- Molecule 1: Very low-density lipoprotein receptor



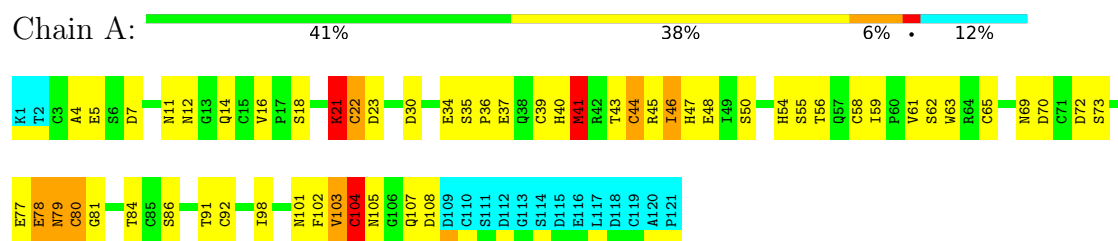
4.2.9 Score per residue for model 9

- Molecule 1: Very low-density lipoprotein receptor



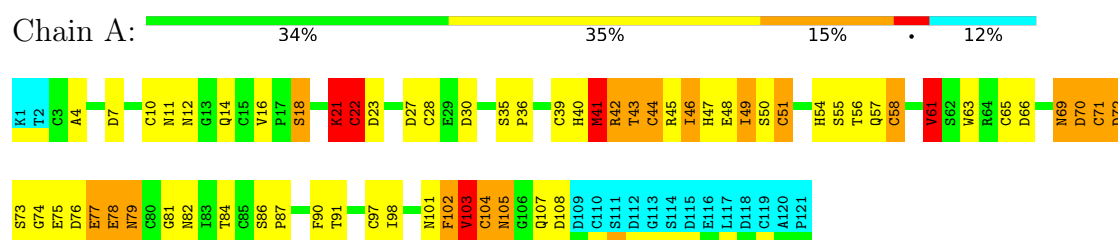
4.2.10 Score per residue for model 10

- Molecule 1: Very low-density lipoprotein receptor



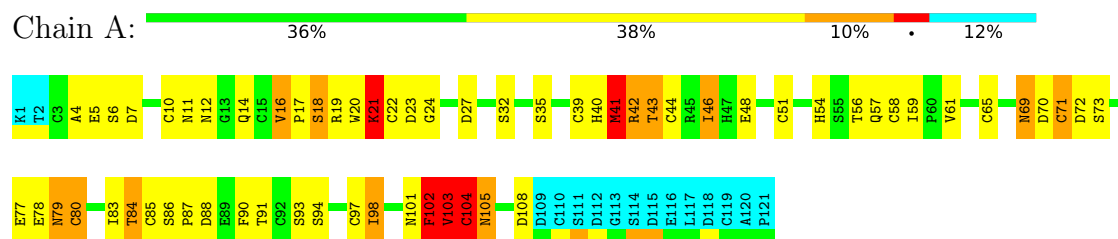
4.2.11 Score per residue for model 11

- Molecule 1: Very low-density lipoprotein receptor



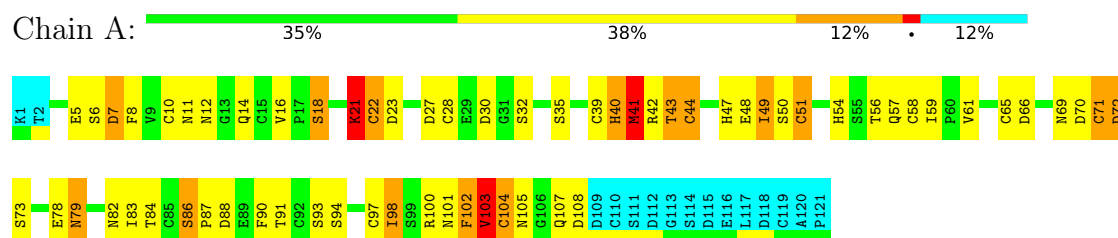
4.2.12 Score per residue for model 12

- Molecule 1: Very low-density lipoprotein receptor



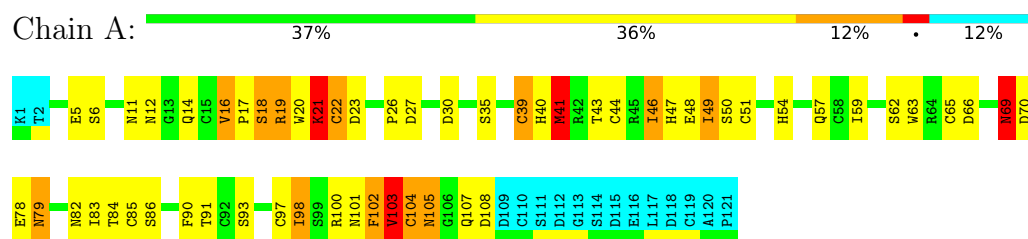
4.2.13 Score per residue for model 13

- Molecule 1: Very low-density lipoprotein receptor



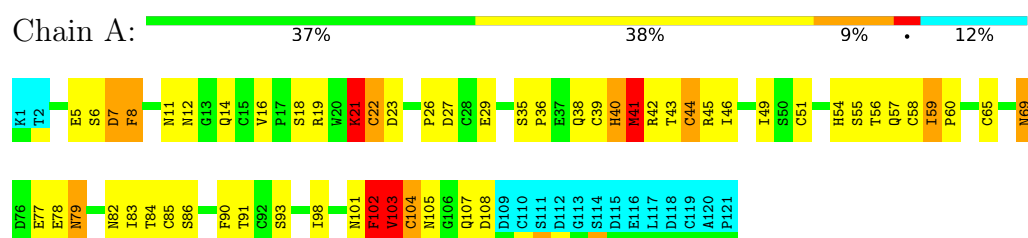
4.2.14 Score per residue for model 14

- Molecule 1: Very low-density lipoprotein receptor



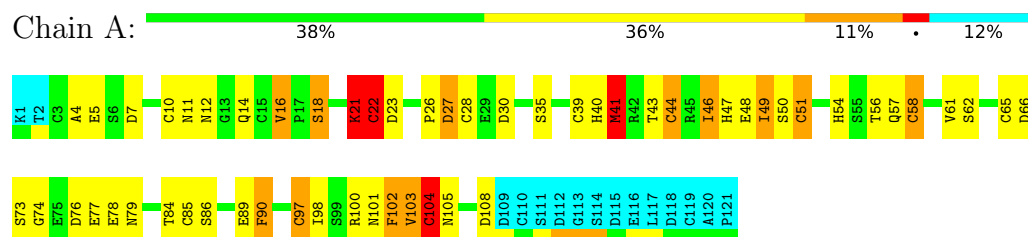
4.2.15 Score per residue for model 15

- Molecule 1: Very low-density lipoprotein receptor



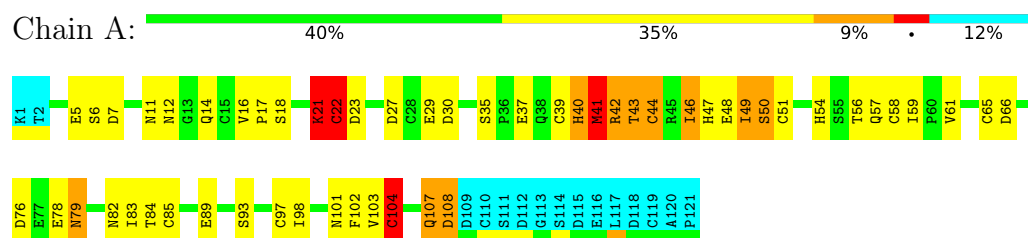
4.2.16 Score per residue for model 16 (medoid)

- Molecule 1: Very low-density lipoprotein receptor



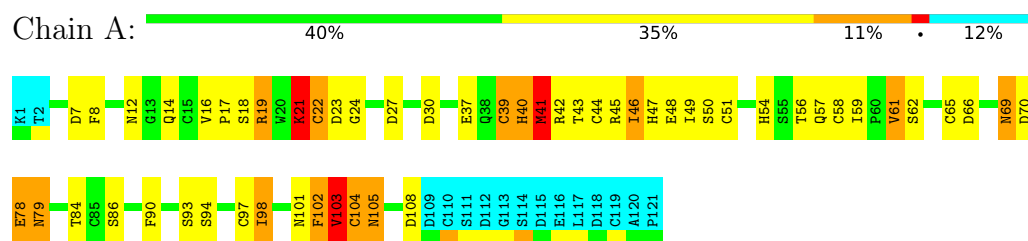
4.2.17 Score per residue for model 17

- Molecule 1: Very low-density lipoprotein receptor



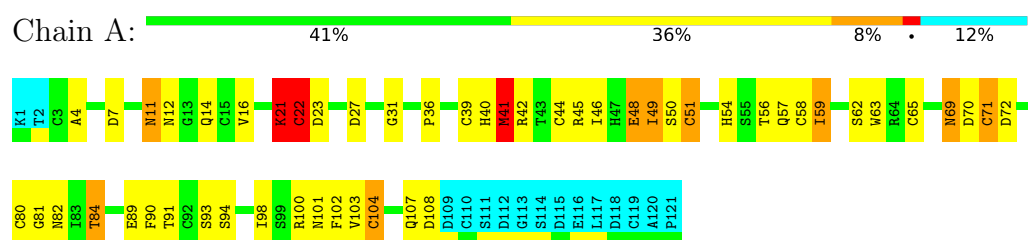
4.2.18 Score per residue for model 18

- Molecule 1: Very low-density lipoprotein receptor



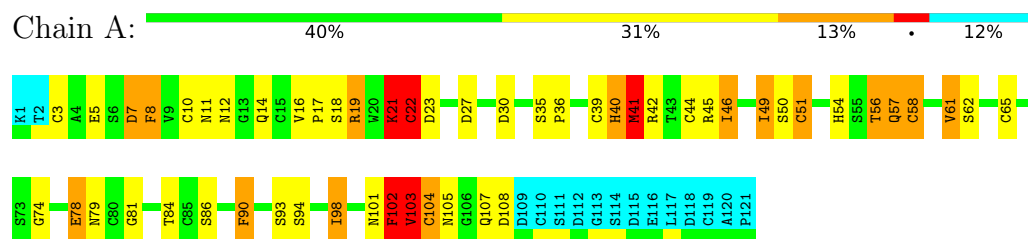
4.2.19 Score per residue for model 19

- Molecule 1: Very low-density lipoprotein receptor



4.2.20 Score per residue for model 20

- Molecule 1: Very low-density lipoprotein receptor



5 Refinement protocol and experimental data overview

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

Of the 500 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	refinement	
TALOS	geometry optimization	

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	1174
Number of shifts mapped to atoms	1174
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.95±0.02	0±0/812 (0.0± 0.0%)	1.31±0.01	2±1/1099 (0.2± 0.1%)
All	All	0.95	0/16240 (0.0%)	1.31	35/21980 (0.2%)

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	69	ASN	CA-CB-CG	-6.62	105.98	112.60	4	7
1	A	102	PHE	CA-CB-CG	-6.36	107.44	113.80	18	5
1	A	8	PHE	CA-CB-CG	-6.27	107.53	113.80	15	6
1	A	51	CYS	N-CA-C	-5.79	106.06	113.23	6	2
1	A	25	ASP	CA-C-N	5.43	126.63	119.84	8	1
1	A	25	ASP	C-N-CA	5.43	126.63	119.84	8	1
1	A	90	PHE	CA-CB-CG	-5.43	108.37	113.80	18	3
1	A	105	ASN	N-CA-C	-5.39	105.40	112.41	16	7
1	A	76	ASP	CA-CB-CG	-5.13	107.47	112.60	2	1
1	A	47	HIS	CA-CB-CG	-5.13	108.67	113.80	11	1
1	A	76	ASP	N-CA-C	5.05	116.87	111.36	16	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	797	665	665	21±4
All	All	16000	13300	13300	418

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 14.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:ILE:HD12	1:A:61:VAL:HG12	0.79	1.53	11	5
1:A:49:ILE:HD12	1:A:61:VAL:HG22	0.76	1.57	2	1
1:A:42:ARG:O	1:A:56:THR:HG23	0.76	1.81	5	7
1:A:57:GLN:NE2	1:A:71:CYS:O	0.73	2.22	13	17
1:A:71:CYS:SG	1:A:71:CYS:O	0.69	2.50	17	2
1:A:98:ILE:HD12	1:A:102:PHE:CB	0.67	2.20	6	15
1:A:69:ASN:ND2	1:A:71:CYS:SG	0.65	2.70	2	12
1:A:59:ILE:HD12	1:A:63:TRP:CE3	0.64	2.26	7	3
1:A:39:CYS:O	1:A:41:MET:N	0.64	2.30	20	20
1:A:71:CYS:O	1:A:72:ASP:C	0.64	2.41	20	17
1:A:4:ALA:HB3	1:A:7:ASP:OD1	0.64	1.92	19	9
1:A:71:CYS:O	1:A:71:CYS:SG	0.62	2.58	20	12
1:A:80:CYS:SG	1:A:84:THR:HG23	0.61	2.35	12	2
1:A:78:GLU:O	1:A:79:ASN:ND2	0.61	2.33	9	13
1:A:69:ASN:ND2	1:A:71:CYS:H	0.60	1.94	12	3
1:A:43:THR:HG23	1:A:44:CYS:O	0.59	1.97	13	6
1:A:59:ILE:HD13	1:A:71:CYS:SG	0.59	2.37	19	1
1:A:49:ILE:HD12	1:A:61:VAL:CG1	0.57	2.25	11	1
1:A:36:PRO:HA	1:A:56:THR:HG21	0.56	1.75	5	7
1:A:49:ILE:HB	1:A:61:VAL:HG22	0.55	1.77	4	1
1:A:51:CYS:SG	1:A:71:CYS:C	0.55	2.90	12	14
1:A:103:VAL:O	1:A:104:CYS:C	0.54	2.49	6	13
1:A:59:ILE:HD12	1:A:63:TRP:HE3	0.54	1.62	7	1
1:A:74:GLY:C	1:A:76:ASP:H	0.54	2.11	6	1
1:A:74:GLY:O	1:A:76:ASP:N	0.54	2.41	6	1
1:A:77:GLU:N	1:A:77:GLU:CD	0.54	2.66	8	6
1:A:98:ILE:HD13	1:A:102:PHE:HB3	0.54	1.79	2	1
1:A:71:CYS:HB2	1:A:74:GLY:HA2	0.53	1.80	11	6
1:A:78:GLU:O	1:A:79:ASN:C	0.53	2.51	12	5
1:A:21:LYS:O	1:A:23:ASP:N	0.53	2.42	5	20
1:A:78:GLU:O	1:A:80:CYS:N	0.52	2.42	8	2
1:A:76:ASP:CG	1:A:76:ASP:O	0.52	2.52	17	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:ILE:HG23	1:A:50:SER:N	0.52	2.20	3	14
1:A:71:CYS:C	1:A:73:SER:H	0.52	2.13	6	1
1:A:70:ASP:O	1:A:74:GLY:N	0.51	2.43	6	1
1:A:59:ILE:HD11	1:A:69:ASN:HD21	0.51	1.66	7	2
1:A:63:TRP:O	1:A:77:GLU:HG3	0.49	2.07	1	3
1:A:49:ILE:HB	1:A:61:VAL:HG12	0.48	1.83	18	1
1:A:59:ILE:HD13	1:A:77:GLU:HB3	0.48	1.83	6	1
1:A:80:CYS:HA	1:A:84:THR:HG23	0.48	1.85	19	1
1:A:63:TRP:O	1:A:77:GLU:HG2	0.47	2.09	7	5
1:A:16:VAL:HG12	1:A:20:TRP:CD1	0.47	2.44	14	3
1:A:12:ASN:ND2	1:A:12:ASN:O	0.47	2.48	17	6
1:A:43:THR:HG21	1:A:50:SER:CB	0.47	2.39	8	1
1:A:98:ILE:HD12	1:A:102:PHE:CG	0.47	2.44	12	3
1:A:34:GLU:HB3	1:A:44:CYS:HA	0.47	1.84	5	1
1:A:39:CYS:O	1:A:39:CYS:SG	0.47	2.72	12	4
1:A:46:ILE:HG23	1:A:47:HIS:H	0.47	1.69	14	2
1:A:12:ASN:O	1:A:12:ASN:ND2	0.47	2.47	7	14
1:A:78:GLU:N	1:A:78:GLU:CD	0.47	2.72	19	3
1:A:69:ASN:C	1:A:69:ASN:ND2	0.47	2.72	6	1
1:A:70:ASP:OD1	1:A:76:ASP:CB	0.47	2.62	7	1
1:A:77:GLU:O	1:A:78:GLU:C	0.47	2.56	12	1
1:A:59:ILE:HD11	1:A:63:TRP:CG	0.46	2.45	10	1
1:A:24:GLY:C	1:A:46:ILE:HD11	0.46	2.35	12	1
1:A:11:ASN:ND2	1:A:31:GLY:O	0.46	2.47	19	1
1:A:62:SER:HG	1:A:63:TRP:CD1	0.46	2.28	10	1
1:A:49:ILE:HG22	1:A:50:SER:N	0.46	2.26	8	1
1:A:98:ILE:HD12	1:A:102:PHE:HB3	0.46	1.86	16	2
1:A:44:CYS:SG	1:A:48:GLU:CB	0.46	3.04	3	1
1:A:44:CYS:H	1:A:58:CYS:CB	0.45	2.25	9	4
1:A:59:ILE:HG21	1:A:71:CYS:SG	0.45	2.51	15	2
1:A:24:GLY:HA2	1:A:45:ARG:O	0.45	2.11	3	1
1:A:44:CYS:H	1:A:58:CYS:HB3	0.45	1.72	11	3
1:A:7:ASP:CG	1:A:8:PHE:N	0.45	2.73	20	4
1:A:77:GLU:CD	1:A:77:GLU:N	0.45	2.74	3	2
1:A:21:LYS:O	1:A:22:CYS:C	0.45	2.60	19	11
1:A:49:ILE:HG21	1:A:69:ASN:HB2	0.45	1.88	14	1
1:A:79:ASN:HB2	1:A:91:THR:HG23	0.45	1.88	8	1
1:A:34:GLU:HB2	1:A:44:CYS:SG	0.45	2.52	10	1
1:A:22:CYS:N	1:A:39:CYS:SG	0.44	2.90	14	1
1:A:44:CYS:SG	1:A:48:GLU:HB2	0.44	2.53	19	1
1:A:17:PRO:O	1:A:19:ARG:N	0.44	2.51	3	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:ASN:O	1:A:101:ASN:CG	0.44	2.60	9	1
1:A:103:VAL:O	1:A:105:ASN:N	0.44	2.51	18	7
1:A:98:ILE:HD12	1:A:102:PHE:HB2	0.44	1.90	6	3
1:A:79:ASN:O	1:A:79:ASN:OD1	0.43	2.36	16	2
1:A:86:SER:O	1:A:88:ASP:N	0.43	2.51	1	4
1:A:43:THR:HG21	1:A:50:SER:HA	0.43	1.91	13	2
1:A:76:ASP:O	1:A:76:ASP:CG	0.43	2.61	14	3
1:A:69:ASN:ND2	1:A:71:CYS:HB3	0.43	2.28	18	1
1:A:45:ARG:C	1:A:46:ILE:HG22	0.43	2.39	3	1
1:A:16:VAL:HG11	1:A:27:ASP:CB	0.43	2.43	7	3
1:A:59:ILE:HD13	1:A:60:PRO:O	0.43	2.13	15	1
1:A:79:ASN:CG	1:A:79:ASN:O	0.43	2.62	19	1
1:A:90:PHE:CE1	1:A:103:VAL:HG23	0.43	2.49	6	1
1:A:57:GLN:NE2	1:A:71:CYS:SG	0.43	2.92	19	2
1:A:107:GLN:HG3	1:A:108:ASP:N	0.42	2.29	2	2
1:A:70:ASP:O	1:A:72:ASP:N	0.42	2.52	6	1
1:A:70:ASP:HB2	1:A:74:GLY:O	0.42	2.14	6	1
1:A:18:SER:O	1:A:21:LYS:CD	0.42	2.67	9	3
1:A:78:GLU:C	1:A:79:ASN:CG	0.42	2.87	7	1
1:A:74:GLY:C	1:A:76:ASP:N	0.42	2.77	6	1
1:A:70:ASP:HB2	1:A:76:ASP:OD1	0.42	2.13	2	1
1:A:78:GLU:O	1:A:78:GLU:OE1	0.42	2.38	3	1
1:A:105:ASN:OD1	1:A:105:ASN:N	0.42	2.53	3	2
1:A:78:GLU:O	1:A:78:GLU:OE2	0.42	2.38	19	1
1:A:43:THR:OG1	1:A:58:CYS:CB	0.42	2.68	4	3
1:A:49:ILE:HD12	1:A:61:VAL:HB	0.42	1.92	13	1
1:A:59:ILE:HD11	1:A:77:GLU:OE1	0.42	2.15	2	1
1:A:39:CYS:O	1:A:56:THR:HG23	0.41	2.14	2	1
1:A:39:CYS:SG	1:A:42:ARG:C	0.41	3.03	17	1
1:A:24:GLY:CA	1:A:45:ARG:O	0.41	2.68	6	2
1:A:46:ILE:HG23	1:A:47:HIS:N	0.41	2.30	14	1
1:A:59:ILE:HD11	1:A:69:ASN:OD1	0.41	2.16	4	1
1:A:66:ASP:OD1	1:A:66:ASP:N	0.41	2.53	6	1
1:A:70:ASP:OD2	1:A:76:ASP:OD2	0.41	2.39	11	5
1:A:70:ASP:O	1:A:74:GLY:CA	0.41	2.69	6	1
1:A:46:ILE:HG22	1:A:47:HIS:N	0.41	2.30	10	1
1:A:78:GLU:O	1:A:78:GLU:CD	0.41	2.64	2	1
1:A:58:CYS:O	1:A:58:CYS:SG	0.40	2.78	12	2
1:A:45:ARG:O	1:A:46:ILE:CB	0.40	2.69	11	2
1:A:78:GLU:C	1:A:80:CYS:N	0.40	2.78	10	1
1:A:17:PRO:C	1:A:19:ARG:H	0.40	2.24	14	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:TRP:O	1:A:77:GLU:CG	0.40	2.69	7	3
1:A:43:THR:OG1	1:A:57:GLN:C	0.40	2.65	11	1
1:A:59:ILE:HD11	1:A:69:ASN:ND2	0.40	2.31	7	1
1:A:90:PHE:O	1:A:97:CYS:HB2	0.40	2.16	16	1
1:A:78:GLU:N	1:A:78:GLU:OE1	0.40	2.55	19	1
1:A:14:GLN:NE2	1:A:27:ASP:O	0.40	2.54	7	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	106/121 (88%)	79±2 (75±2%)	16±2 (15±2%)	11±2 (10±2%)	1	9
All	All	2120/2420 (88%)	1585 (75%)	316 (15%)	219 (10%)	1	9

All 24 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	21	LYS	20
1	A	40	HIS	20
1	A	41	MET	20
1	A	104	CYS	20
1	A	18	SER	18
1	A	22	CYS	16
1	A	46	ILE	15
1	A	71	CYS	15
1	A	82	ASN	13
1	A	5	GLU	8
1	A	61	VAL	7
1	A	81	GLY	7
1	A	103	VAL	7
1	A	44	CYS	6
1	A	26	PRO	5
1	A	87	PRO	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	17	PRO	5
1	A	7	ASP	4
1	A	36	PRO	2
1	A	79	ASN	2
1	A	72	ASP	1
1	A	73	SER	1
1	A	75	GLU	1
1	A	3	CYS	1

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	95/108 (88%)	57±5 (60±5%)	38±5 (40±5%)	0 5
All	All	1900/2160 (88%)	1134 (60%)	766 (40%)	0 5

All 80 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	14	GLN	20
1	A	21	LYS	20
1	A	54	HIS	20
1	A	65	CYS	20
1	A	84	THR	20
1	A	108	ASP	20
1	A	22	CYS	19
1	A	27	ASP	19
1	A	41	MET	19
1	A	101	ASN	19
1	A	104	CYS	19
1	A	11	ASN	18
1	A	70	ASP	18
1	A	35	SER	17
1	A	43	THR	17
1	A	48	GLU	17
1	A	107	GLN	17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	16	VAL	17
1	A	79	ASN	16
1	A	69	ASN	16
1	A	49	ILE	15
1	A	58	CYS	15
1	A	103	VAL	14
1	A	59	ILE	13
1	A	30	ASP	13
1	A	78	GLU	12
1	A	97	CYS	12
1	A	56	THR	11
1	A	72	ASP	11
1	A	44	CYS	11
1	A	90	PHE	11
1	A	19	ARG	10
1	A	51	CYS	10
1	A	73	SER	10
1	A	42	ARG	10
1	A	86	SER	10
1	A	91	THR	10
1	A	102	PHE	10
1	A	93	SER	9
1	A	62	SER	9
1	A	47	HIS	8
1	A	85	CYS	8
1	A	66	ASP	8
1	A	46	ILE	7
1	A	55	SER	7
1	A	89	GLU	7
1	A	94	SER	7
1	A	18	SER	7
1	A	98	ILE	7
1	A	6	SER	7
1	A	83	ILE	6
1	A	40	HIS	6
1	A	45	ARG	6
1	A	61	VAL	6
1	A	10	CYS	6
1	A	37	GLU	5
1	A	75	GLU	5
1	A	77	GLU	5
1	A	50	SER	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	100	ARG	5
1	A	28	CYS	4
1	A	5	GLU	4
1	A	7	ASP	4
1	A	29	GLU	3
1	A	76	ASP	3
1	A	99	SER	3
1	A	32	SER	3
1	A	80	CYS	3
1	A	68	GLU	2
1	A	88	ASP	2
1	A	92	CYS	2
1	A	33	ASP	2
1	A	39	CYS	2
1	A	96	ARG	1
1	A	82	ASN	1
1	A	9	VAL	1
1	A	105	ASN	1
1	A	38	GLN	1
1	A	71	CYS	1
1	A	57	GLN	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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 84% for the well-defined parts and 84% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *Final_CS_2*

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	1174
Number of shifts mapped to atoms	1174
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	120	0.36 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	109	0.45 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	103	0.34 ± 0.18	None needed (< 0.5 ppm)
^{15}N	112	0.32 ± 0.50	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 84%, i.e. 1032 atoms were assigned a chemical shift out of a possible 1232. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	510/529 (96%)	213/216 (99%)	197/212 (93%)	100/101 (99%)
Sidechain	518/628 (82%)	351/394 (89%)	156/204 (76%)	11/30 (37%)

Continued on next page...

Continued from previous page...

	Total	¹H	¹³C	¹⁵N
Aromatic	4/75 (5%)	2/39 (5%)	0/31 (0%)	2/5 (40%)
Overall	1032/1232 (84%)	566/649 (87%)	353/447 (79%)	113/136 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 1163 atoms were assigned a chemical shift out of a possible 1386. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	575/603 (95%)	240/246 (98%)	223/242 (92%)	112/115 (97%)
Sidechain	584/708 (82%)	393/444 (89%)	180/233 (77%)	11/31 (35%)
Aromatic	4/75 (5%)	2/39 (5%)	0/31 (0%)	2/5 (40%)
Overall	1163/1386 (84%)	635/729 (87%)	403/506 (80%)	125/151 (83%)

7.1.4 Statistically unusual chemical shifts [i](#)

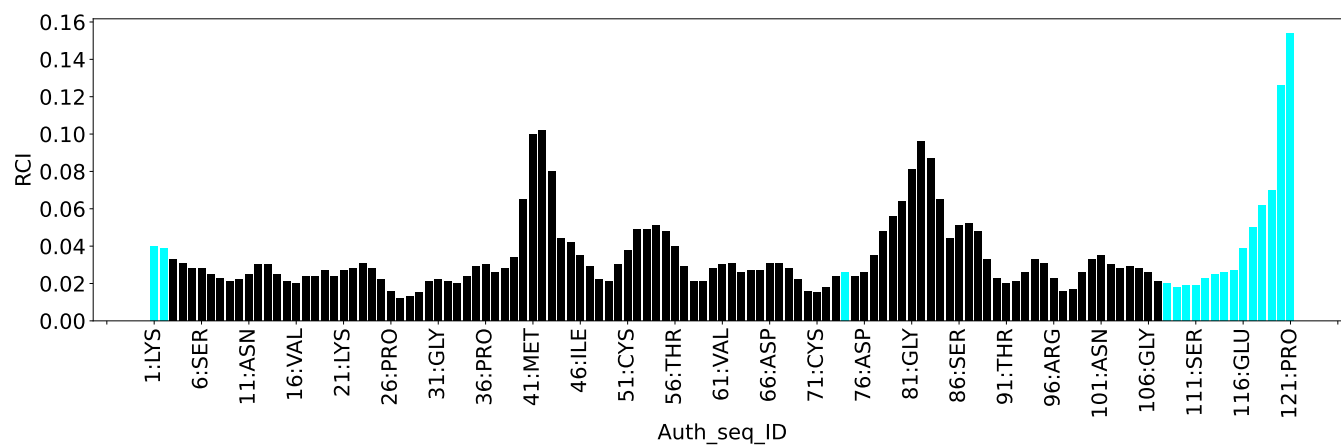
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	60	PRO	HD3	1.61	1.76 – 5.48	-5.4

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1352
Intra-residue ($ i-j =0$)	322
Sequential ($ i-j =1$)	429
Medium range ($ i-j >1$ and $ i-j <5$)	316
Long range ($ i-j \geq 5$)	258
Inter-chain	0
Hydrogen bond restraints	9
Disulfide bond restraints	0
Total dihedral-angle restraints	182
Number of unmapped restraints	0
Number of restraints per residue	12.4
Number of long range restraints per residue ¹	2.1

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)	103.3	0.2
0.2-0.5 (Medium)	148.8	0.5
>0.5 (Large)	67.0	1.95

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	38.2	9.98
10.0-20.0 (Medium)	11.6	19.89
>20.0 (Large)	0.5	29.08

9 Distance violation analysis ⓘ

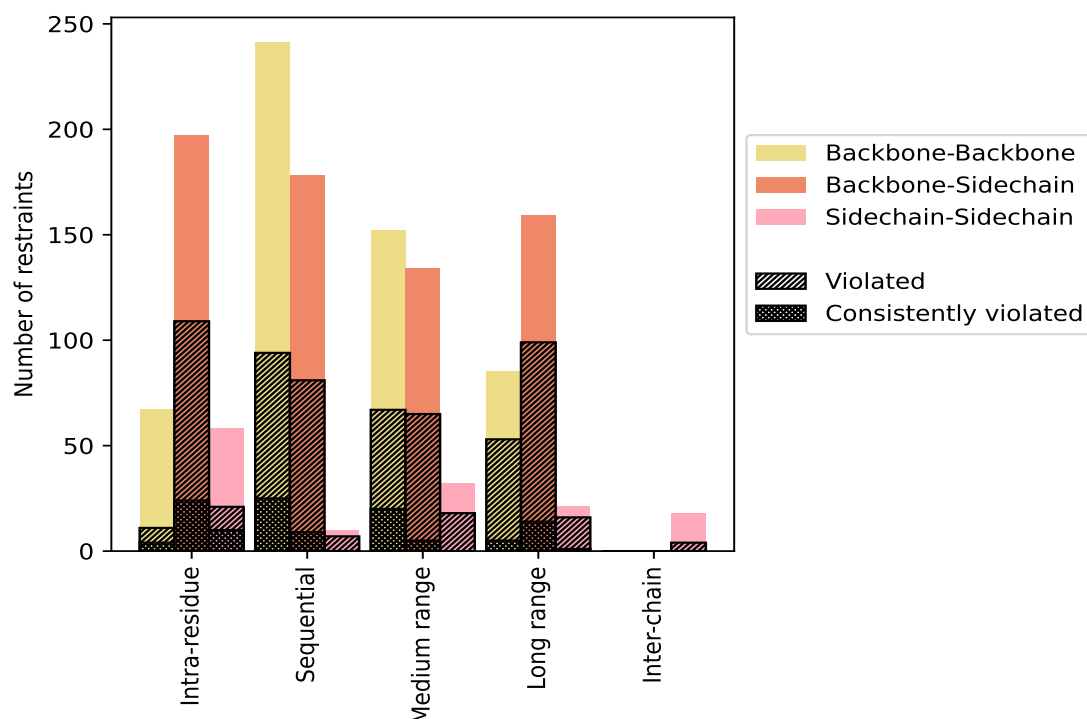
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	322	23.8	141	43.8	10.4	38	11.8	2.8
Backbone-Backbone	67	5.0	11	16.4	0.8	4	6.0	0.3
Backbone-Sidechain	197	14.6	109	55.3	8.1	24	12.2	1.8
Sidechain-Sidechain	58	4.3	21	36.2	1.6	10	17.2	0.7
Sequential (i-j =1)	429	31.7	182	42.4	13.5	34	7.9	2.5
Backbone-Backbone	241	17.8	94	39.0	7.0	25	10.4	1.8
Backbone-Sidechain	178	13.2	81	45.5	6.0	9	5.1	0.7
Sidechain-Sidechain	10	0.7	7	70.0	0.5	0	0.0	0.0
Medium range (i-j >1 & i-j <5)	316	23.4	149	47.2	11.0	25	7.9	1.8
Backbone-Backbone	152	11.2	67	44.1	5.0	20	13.2	1.5
Backbone-Sidechain	132	9.8	64	48.5	4.7	5	3.8	0.4
Sidechain-Sidechain	32	2.4	18	56.2	1.3	0	0.0	0.0
Long range (i-j ≥5)	258	19.1	163	63.2	12.1	19	7.4	1.4
Backbone-Backbone	85	6.3	53	62.4	3.9	5	5.9	0.4
Backbone-Sidechain	152	11.2	94	61.8	7.0	13	8.6	1.0
Sidechain-Sidechain	21	1.6	16	76.2	1.2	1	4.8	0.1
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	9	0.7	6	66.7	0.4	1	11.1	0.1
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1352	100.0	645	47.7	47.7	117	8.7	8.7
Backbone-Backbone	545	40.3	225	41.3	16.6	54	9.9	4.0
Backbone-Sidechain	668	49.4	354	53.0	26.2	52	7.8	3.8
Sidechain-Sidechain	139	10.3	66	47.5	4.9	11	7.9	0.8

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	85	96	75	75	2	333	0.35	1.94	0.25	0.28
2	76	94	70	76	1	317	0.36	1.94	0.24	0.29
3	89	88	82	62	1	322	0.35	1.94	0.25	0.27
4	79	97	87	73	1	337	0.35	1.94	0.24	0.28
5	83	100	72	58	1	314	0.36	1.94	0.26	0.29
6	83	85	71	79	2	320	0.36	1.94	0.25	0.27
7	80	97	70	64	2	313	0.36	1.94	0.26	0.27
8	89	96	76	68	0	329	0.36	1.94	0.26	0.3
9	74	95	76	69	2	316	0.36	1.94	0.26	0.28
10	85	88	81	63	0	317	0.37	1.94	0.26	0.31

Continued on next page...

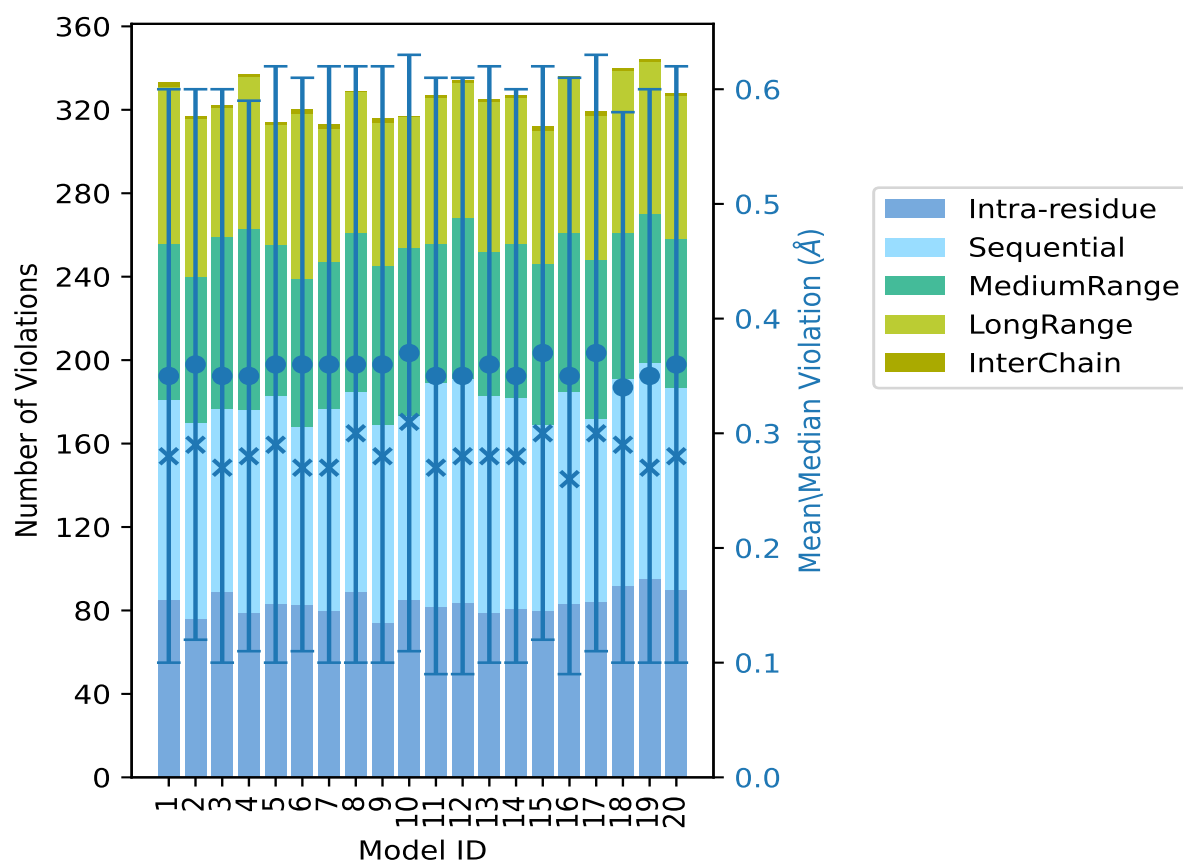
Continued from previous page...

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	82	107	67	70	1	327	0.35	1.94	0.26	0.27
12	84	107	77	65	1	334	0.35	1.94	0.26	0.28
13	79	104	69	72	1	325	0.36	1.95	0.26	0.28
14	81	101	74	70	1	327	0.35	1.94	0.25	0.28
15	80	89	77	64	2	312	0.37	1.94	0.25	0.3
16	83	102	76	74	1	336	0.35	1.94	0.26	0.26
17	84	88	76	69	2	319	0.37	1.94	0.26	0.3
18	92	99	70	78	1	340	0.34	1.94	0.24	0.29
19	95	104	71	73	1	344	0.35	1.94	0.25	0.27
20	90	97	71	69	1	328	0.36	1.94	0.26	0.28

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

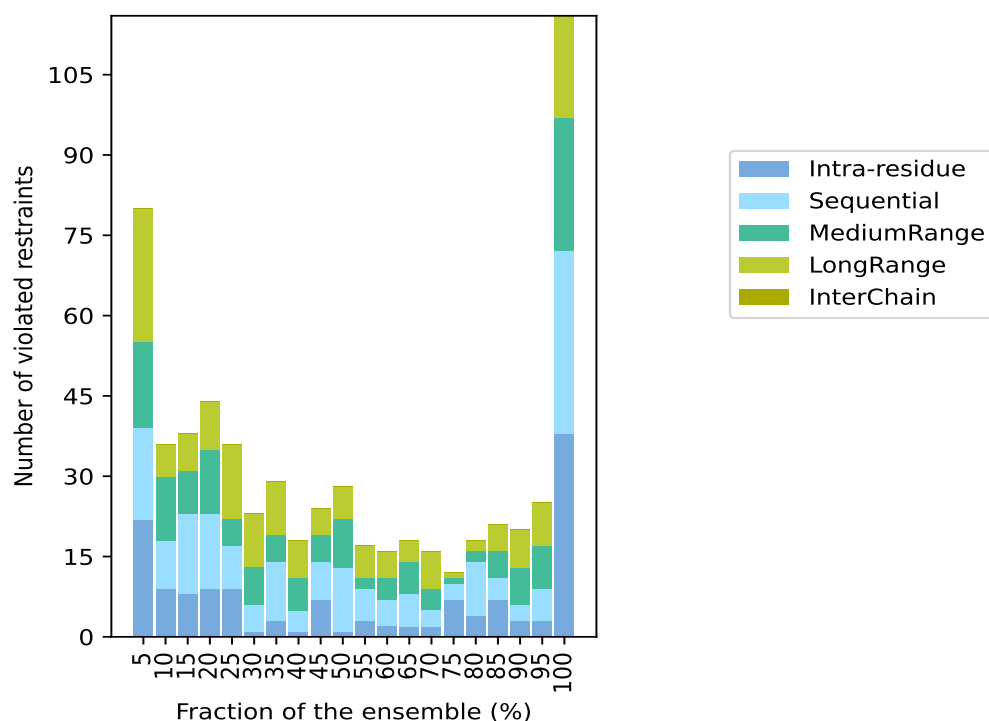
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 690(IR:181, SQ:247, MR:167, LR:95, IC:0) restraints are not 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	%
22	17	16	25	0	80	1	5.0
9	9	12	6	0	36	2	10.0
8	15	8	7	0	38	3	15.0
9	14	12	9	0	44	4	20.0
9	8	5	14	0	36	5	25.0
1	5	7	10	0	23	6	30.0
3	11	5	10	0	29	7	35.0
1	4	6	7	0	18	8	40.0
7	7	5	5	0	24	9	45.0
1	12	9	6	0	28	10	50.0
3	6	2	6	0	17	11	55.0
2	5	4	5	0	16	12	60.0
2	6	6	4	0	18	13	65.0
2	3	4	7	0	16	14	70.0
7	3	1	1	0	12	15	75.0
4	10	2	2	0	18	16	80.0
7	4	5	5	0	21	17	85.0
3	3	7	7	0	20	18	90.0
3	6	8	8	0	25	19	95.0
38	34	25	19	0	116	20	100.0

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

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

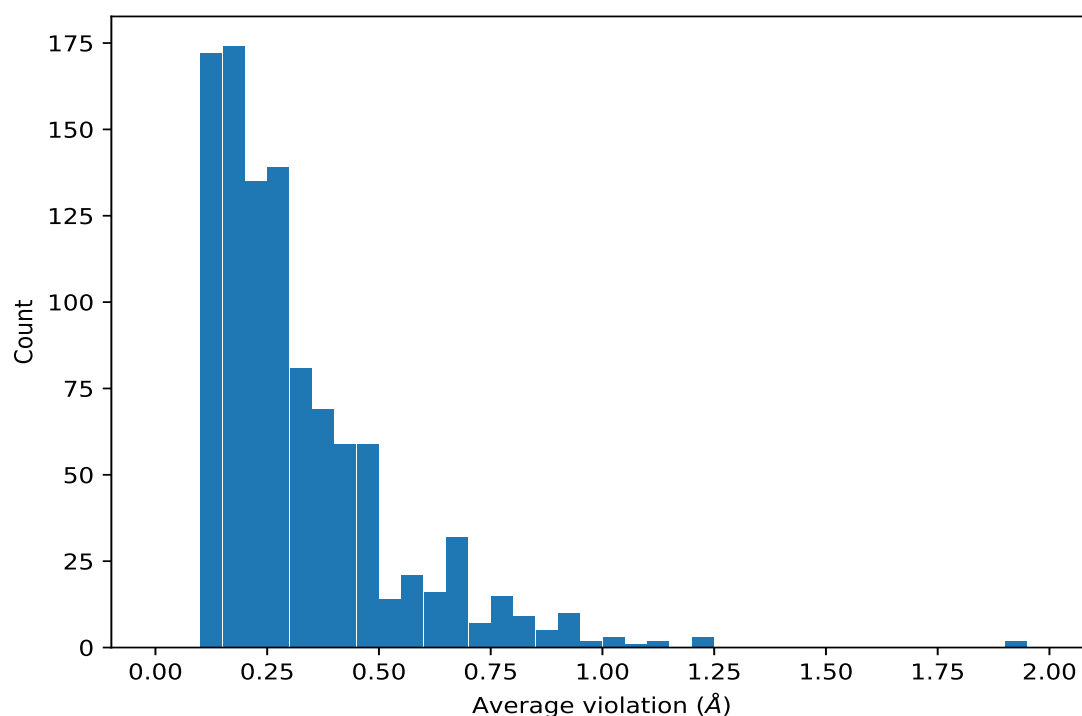
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,384)	1:5:A:GLU:HB2	1:5:A:GLU:HB3	20	1.94	0.0	1.94
(2,384)	1:5:A:GLU:HB3	1:5:A:GLU:HB2	20	1.94	0.0	1.94
(1,740)	1:35:A:SER:H	1:56:A:THR:HG22	20	1.23	0.22	1.22
(1,740)	1:35:A:SER:H	1:56:A:THR:HG23	20	1.23	0.22	1.22
(1,740)	1:35:A:SER:H	1:56:A:THR:HG21	20	1.23	0.22	1.22
(2,145)	1:43:A:THR:HA	1:58:A:CYS:H	20	1.13	0.11	1.12
(2,145)	1:56:A:THR:HB	1:58:A:CYS:H	20	1.13	0.11	1.12
(2,63)	1:82:A:ASN:HA	1:83:A:ILE:H	20	1.02	0.03	1.02
(2,375)	1:60:A:PRO:HD3	1:61:A:VAL:H	20	0.99	0.12	1.02
(2,375)	1:48:A:GLU:HB3	1:61:A:VAL:H	20	0.99	0.12	1.02
(1,713)	1:14:A:GLN:HA	1:12:A:ASN:H	20	0.94	0.08	0.94
(1,4)	1:55:A:SER:H	1:54:A:HIS:H	20	0.93	0.05	0.93
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	20	0.89	0.07	0.9
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	20	0.89	0.07	0.9
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	20	0.89	0.07	0.9
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	20	0.89	0.07	0.9

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,191)	1:100:A:ARG:HA	1:101:A:ASN:H	20	0.86	0.03	0.85
(1,429)	1:69:A:ASN:HA	1:69:A:ASN:H	20	0.8	0.01	0.8
(1,584)	1:27:A:ASP:HB2	1:27:A:ASP:H	20	0.78	0.07	0.79
(1,584)	1:27:A:ASP:HB3	1:27:A:ASP:H	20	0.78	0.07	0.79
(2,337)	1:53:A:ALA:HB3	1:55:A:SER:H	20	0.77	0.15	0.83
(2,337)	1:53:A:ALA:HB2	1:55:A:SER:H	20	0.77	0.15	0.83
(2,337)	1:53:A:ALA:HB1	1:55:A:SER:H	20	0.77	0.15	0.83
(1,909)	1:43:A:THR:HG22	1:46:A:ILE:H	20	0.77	0.15	0.8
(1,909)	1:43:A:THR:HG21	1:46:A:ILE:H	20	0.77	0.15	0.8
(1,909)	1:43:A:THR:HG23	1:46:A:ILE:H	20	0.77	0.15	0.8
(1,688)	1:69:A:ASN:H	1:69:A:ASN:HD22	20	0.76	0.26	0.92
(1,150)	1:104:A:CYS:H	1:106:A:GLY:H	20	0.76	0.05	0.76
(1,459)	1:70:A:ASP:HA	1:76:A:ASP:H	20	0.75	0.25	0.84
(2,281)	1:10:A:CYS:HA	1:11:A:ASN:HD22	20	0.75	0.16	0.8
(2,281)	1:11:A:ASN:HA	1:11:A:ASN:HD22	20	0.75	0.16	0.8
(1,692)	1:8:A:PHE:HB2	1:8:A:PHE:H	20	0.71	0.04	0.71
(1,692)	1:8:A:PHE:HB3	1:8:A:PHE:H	20	0.71	0.04	0.71
(1,824)	1:118:A:ASP:H	1:116:A:GLU:H	20	0.7	0.1	0.73
(1,923)	1:8:A:PHE:HB2	1:16:A:VAL:HA	20	0.69	0.14	0.7
(1,700)	1:69:A:ASN:HB2	1:69:A:ASN:H	20	0.68	0.04	0.68
(1,700)	1:69:A:ASN:HB3	1:69:A:ASN:H	20	0.68	0.04	0.68
(2,39)	1:117:A:LEU:HD22	1:115:A:ASP:H	20	0.67	0.34	0.7
(2,39)	1:117:A:LEU:HD23	1:115:A:ASP:H	20	0.67	0.34	0.7
(2,39)	1:117:A:LEU:HD13	1:115:A:ASP:H	20	0.67	0.34	0.7
(2,39)	1:117:A:LEU:HD12	1:115:A:ASP:H	20	0.67	0.34	0.7
(2,39)	1:117:A:LEU:HD11	1:115:A:ASP:H	20	0.67	0.34	0.7
(2,39)	1:117:A:LEU:HD21	1:115:A:ASP:H	20	0.67	0.34	0.7
(2,327)	1:68:A:GLU:HG2	1:71:A:CYS:H	20	0.67	0.2	0.65
(2,327)	1:64:A:ARG:HG2	1:71:A:CYS:H	20	0.67	0.2	0.65
(2,327)	1:68:A:GLU:HG3	1:71:A:CYS:H	20	0.67	0.2	0.65
(1,502)	1:34:A:GLU:HG2	1:34:A:GLU:H	20	0.66	0.06	0.66
(1,502)	1:34:A:GLU:HG3	1:34:A:GLU:H	20	0.66	0.06	0.66
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	20	0.66	0.09	0.68
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	20	0.66	0.09	0.68
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	20	0.66	0.09	0.68
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	20	0.66	0.09	0.68
(1,491)	1:22:A:CYS:H	1:24:A:GLY:H	20	0.65	0.04	0.65
(1,492)	1:22:A:CYS:H	1:24:A:GLY:H	20	0.65	0.04	0.65
(2,264)	1:49:A:ILE:HB	1:50:A:SER:H	20	0.65	0.2	0.57
(1,391)	1:54:A:HIS:HA	1:53:A:ALA:H	20	0.64	0.04	0.64
(1,898)	1:57:A:GLN:HE22	1:71:A:CYS:H	20	0.62	0.23	0.68
(1,622)	1:12:A:ASN:HB2	1:12:A:ASN:HD21	20	0.62	0.0	0.62

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,622)	1:12:A:ASN:HB3	1:12:A:ASN:HD21	20	0.62	0.0	0.62
(1,687)	1:69:A:ASN:HD21	1:74:A:GLY:H	20	0.62	0.16	0.6
(1,97)	1:98:A:ILE:HD11	1:99:A:SER:H	20	0.61	0.24	0.47
(1,97)	1:98:A:ILE:HD12	1:99:A:SER:H	20	0.61	0.24	0.47
(1,97)	1:98:A:ILE:HD13	1:99:A:SER:H	20	0.61	0.24	0.47
(2,374)	1:25:A:ASP:HA	1:23:A:ASP:H	20	0.61	0.03	0.62
(2,374)	1:20:A:TRP:HA	1:23:A:ASP:H	20	0.61	0.03	0.62
(2,207)	1:79:A:ASN:HB2	1:79:A:ASN:HD22	20	0.6	0.18	0.51
(2,66)	1:5:A:GLU:H	1:7:A:ASP:H	20	0.59	0.13	0.6
(2,66)	1:4:A:ALA:H	1:7:A:ASP:H	20	0.59	0.13	0.6
(1,430)	1:69:A:ASN:HB2	1:69:A:ASN:H	20	0.58	0.04	0.58
(1,430)	1:69:A:ASN:HB3	1:69:A:ASN:H	20	0.58	0.04	0.58
(1,723)	1:23:A:ASP:H	1:21:A:LYS:HA	20	0.58	0.04	0.57
(2,241)	1:12:A:ASN:HD22	1:12:A:ASN:HD21	20	0.56	0.0	0.56
(1,212)	1:96:A:ARG:H	1:92:A:CYS:HA	20	0.55	0.09	0.56
(1,721)	1:21:A:LYS:HG2	1:22:A:CYS:H	20	0.54	0.08	0.53
(1,721)	1:21:A:LYS:HG3	1:22:A:CYS:H	20	0.54	0.08	0.53
(1,27)	1:118:A:ASP:H	1:117:A:LEU:H	20	0.54	0.07	0.55
(1,634)	1:79:A:ASN:HD22	1:79:A:ASN:HA	20	0.53	0.07	0.53
(1,58)	1:66:A:ASP:H	1:65:A:CYS:H	20	0.53	0.04	0.55
(1,583)	1:40:A:HIS:HA	1:38:A:GLN:H	20	0.51	0.07	0.51
(2,212)	1:88:A:ASP:H	1:86:A:SER:H	20	0.51	0.08	0.51
(1,587)	1:14:A:GLN:H	1:12:A:ASN:H	20	0.49	0.05	0.49
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	20	0.47	0.13	0.45
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	20	0.47	0.13	0.45
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	20	0.47	0.13	0.45
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	20	0.47	0.13	0.45
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	20	0.47	0.13	0.45
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	20	0.47	0.13	0.45
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	20	0.47	0.13	0.45
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	20	0.47	0.13	0.45
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	20	0.47	0.13	0.45
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	20	0.47	0.13	0.45
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	20	0.47	0.13	0.45
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	20	0.47	0.13	0.45
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	20	0.47	0.13	0.45
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	20	0.47	0.13	0.45
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	20	0.47	0.13	0.45
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	20	0.47	0.13	0.45
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	20	0.47	0.13	0.45
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	20	0.47	0.13	0.45
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	20	0.47	0.13	0.45
(1,289)	1:8:A:PHE:HA	1:8:A:PHE:H	20	0.47	0.06	0.48

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,619)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	20	0.46	0.0	0.46
(1,608)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	20	0.46	0.05	0.46
(1,608)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	20	0.46	0.05	0.46
(1,555)	1:103:A:VAL:HG11	1:104:A:CYS:H	20	0.45	0.11	0.42
(1,555)	1:103:A:VAL:HG12	1:104:A:CYS:H	20	0.45	0.11	0.42
(1,555)	1:103:A:VAL:HG13	1:104:A:CYS:H	20	0.45	0.11	0.42
(1,555)	1:103:A:VAL:HG21	1:104:A:CYS:H	20	0.45	0.11	0.42
(1,555)	1:103:A:VAL:HG22	1:104:A:CYS:H	20	0.45	0.11	0.42
(1,555)	1:103:A:VAL:HG23	1:104:A:CYS:H	20	0.45	0.11	0.42
(1,657)	1:105:A:ASN:HA	1:105:A:ASN:HD22	20	0.44	0.03	0.44
(1,480)	1:10:A:CYS:HB2	1:10:A:CYS:H	20	0.44	0.13	0.5
(1,480)	1:10:A:CYS:HB3	1:10:A:CYS:H	20	0.44	0.13	0.5
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB2	20	0.43	0.05	0.44
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB3	20	0.43	0.05	0.44
(4,8)	1:8:A:PHE:O	1:16:A:VAL:H	20	0.43	0.11	0.42
(1,73)	1:65:A:CYS:HB2	1:65:A:CYS:H	20	0.42	0.05	0.4
(1,73)	1:65:A:CYS:HB3	1:65:A:CYS:H	20	0.42	0.05	0.4
(1,436)	1:73:A:SER:H	1:72:A:ASP:H	20	0.42	0.12	0.4
(2,278)	1:42:A:ARG:HA	1:42:A:ARG:H	20	0.41	0.01	0.41
(1,706)	1:45:A:ARG:HB2	1:45:A:ARG:H	20	0.41	0.06	0.4
(1,706)	1:45:A:ARG:HB3	1:45:A:ARG:H	20	0.41	0.06	0.4
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD2	20	0.41	0.11	0.4
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD3	20	0.41	0.11	0.4
(1,732)	1:31:A:GLY:HA2	1:32:A:SER:H	20	0.41	0.02	0.4
(1,732)	1:31:A:GLY:HA3	1:32:A:SER:H	20	0.41	0.02	0.4
(1,888)	1:49:A:ILE:HA	1:61:A:VAL:H	20	0.41	0.15	0.38
(1,772)	1:68:A:GLU:H	1:64:A:ARG:H	20	0.4	0.12	0.39
(1,642)	1:82:A:ASN:HA	1:82:A:ASN:HD22	20	0.4	0.08	0.38
(1,327)	1:22:A:CYS:HB2	1:22:A:CYS:H	20	0.4	0.06	0.42
(1,327)	1:22:A:CYS:HB3	1:22:A:CYS:H	20	0.4	0.06	0.42
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	20	0.39	0.03	0.4
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	20	0.39	0.03	0.4
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	20	0.39	0.03	0.4
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	20	0.39	0.03	0.4
(1,398)	1:54:A:HIS:HB2	1:54:A:HIS:H	20	0.38	0.01	0.39
(1,398)	1:54:A:HIS:HB3	1:54:A:HIS:H	20	0.38	0.01	0.39
(1,298)	1:14:A:GLN:H	1:11:A:ASN:H	20	0.38	0.1	0.38
(1,376)	1:49:A:ILE:HA	1:49:A:ILE:H	20	0.37	0.02	0.37
(1,693)	1:21:A:LYS:HD2	1:21:A:LYS:H	20	0.37	0.11	0.34
(1,693)	1:21:A:LYS:HD3	1:21:A:LYS:H	20	0.37	0.11	0.34
(1,158)	1:104:A:CYS:HA	1:105:A:ASN:H	20	0.36	0.05	0.36
(2,114)	1:16:A:VAL:HG11	1:16:A:VAL:H	20	0.36	0.08	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,114)	1:16:A:VAL:HG12	1:16:A:VAL:H	20	0.36	0.08	0.35
(2,114)	1:16:A:VAL:HG13	1:16:A:VAL:H	20	0.36	0.08	0.35
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	20	0.36	0.08	0.35
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	20	0.36	0.08	0.35
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	20	0.36	0.08	0.35
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	20	0.36	0.08	0.35
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	20	0.36	0.08	0.35
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	20	0.36	0.08	0.35
(1,93)	1:8:A:PHE:H	1:7:A:ASP:HA	20	0.36	0.07	0.37
(1,224)	1:92:A:CYS:HA	1:94:A:SER:H	20	0.36	0.05	0.36
(1,486)	1:7:A:ASP:HA	1:19:A:ARG:H	20	0.36	0.09	0.36
(1,735)	1:28:A:CYS:HB2	1:33:A:ASP:H	20	0.35	0.08	0.38
(1,735)	1:28:A:CYS:HB3	1:33:A:ASP:H	20	0.35	0.08	0.38
(1,803)	1:101:A:ASN:HD21	1:99:A:SER:H	20	0.35	0.16	0.3
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD2	20	0.35	0.1	0.36
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD3	20	0.35	0.1	0.36
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB2	20	0.35	0.12	0.37
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB3	20	0.35	0.12	0.37
(1,526)	1:64:A:ARG:H	1:67:A:GLY:H	20	0.35	0.07	0.34
(1,896)	1:64:A:ARG:H	1:66:A:ASP:H	20	0.35	0.08	0.32
(1,85)	1:21:A:LYS:HG2	1:22:A:CYS:H	20	0.34	0.08	0.33
(1,85)	1:21:A:LYS:HG3	1:22:A:CYS:H	20	0.34	0.08	0.33
(1,66)	1:23:A:ASP:H	1:24:A:GLY:H	20	0.32	0.05	0.3
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB2	20	0.31	0.18	0.31
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB3	20	0.31	0.18	0.31
(1,789)	1:85:A:CYS:H	1:84:A:THR:HB	20	0.31	0.07	0.33
(1,365)	1:43:A:THR:HB	1:43:A:THR:H	20	0.31	0.06	0.31
(1,907)	1:39:A:CYS:H	1:41:A:MET:H	20	0.3	0.05	0.31
(1,745)	1:48:A:GLU:HB2	1:49:A:ILE:H	20	0.3	0.12	0.32
(1,745)	1:48:A:GLU:HB3	1:49:A:ILE:H	20	0.3	0.12	0.32
(1,320)	1:7:A:ASP:HA	1:18:A:SER:H	20	0.29	0.09	0.3
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB2	20	0.28	0.01	0.29
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB3	20	0.28	0.01	0.29
(1,666)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	20	0.28	0.01	0.28
(1,666)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	20	0.28	0.01	0.28
(1,904)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	20	0.28	0.01	0.28
(1,904)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	20	0.28	0.01	0.28
(1,504)	1:39:A:CYS:HB2	1:39:A:CYS:H	20	0.27	0.08	0.24
(1,504)	1:39:A:CYS:HB3	1:39:A:CYS:H	20	0.27	0.08	0.24
(1,860)	1:16:A:VAL:HB	1:19:A:ARG:H	20	0.27	0.06	0.26
(1,23)	1:104:A:CYS:H	1:105:A:ASN:H	20	0.27	0.07	0.26
(1,24)	1:104:A:CYS:H	1:105:A:ASN:H	20	0.27	0.07	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,499)	1:33:A:ASP:HB2	1:33:A:ASP:H	20	0.26	0.13	0.22
(1,499)	1:33:A:ASP:HB3	1:33:A:ASP:H	20	0.26	0.13	0.22
(1,768)	1:58:A:CYS:HA	1:59:A:ILE:H	20	0.26	0.04	0.26
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB2	20	0.26	0.07	0.25
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB3	20	0.26	0.07	0.25
(2,29)	1:28:A:CYS:HA	1:29:A:GLU:H	20	0.25	0.03	0.26
(1,569)	1:85:A:CYS:H	1:84:A:THR:H	20	0.25	0.05	0.24
(1,545)	1:103:A:VAL:HA	1:105:A:ASN:H	20	0.25	0.03	0.25
(1,28)	1:118:A:ASP:H	1:117:A:LEU:H	20	0.24	0.07	0.25
(1,744)	1:48:A:GLU:H	1:47:A:HIS:H	20	0.23	0.09	0.2
(2,164)	1:14:A:GLN:HB2	1:14:A:GLN:H	20	0.23	0.09	0.2
(2,164)	1:14:A:GLN:HB3	1:14:A:GLN:H	20	0.23	0.09	0.2
(1,349)	1:32:A:SER:H	1:33:A:ASP:H	20	0.23	0.07	0.22
(1,351)	1:32:A:SER:H	1:33:A:ASP:H	20	0.23	0.07	0.22
(1,283)	1:8:A:PHE:H	1:7:A:ASP:H	20	0.23	0.02	0.22
(2,188)	1:16:A:VAL:HG11	1:19:A:ARG:H	20	0.22	0.09	0.2
(2,188)	1:16:A:VAL:HG12	1:19:A:ARG:H	20	0.22	0.09	0.2
(2,188)	1:16:A:VAL:HG13	1:19:A:ARG:H	20	0.22	0.09	0.2
(2,188)	1:16:A:VAL:HG21	1:19:A:ARG:H	20	0.22	0.09	0.2
(2,188)	1:16:A:VAL:HG22	1:19:A:ARG:H	20	0.22	0.09	0.2
(2,188)	1:16:A:VAL:HG23	1:19:A:ARG:H	20	0.22	0.09	0.2
(1,6)	1:23:A:ASP:H	1:24:A:GLY:H	20	0.22	0.05	0.2
(1,869)	1:14:A:GLN:HE22	1:28:A:CYS:H	20	0.2	0.08	0.2
(1,415)	1:64:A:ARG:HA	1:65:A:CYS:H	20	0.19	0.03	0.2
(1,128)	1:114:A:SER:HA	1:114:A:SER:H	20	0.19	0.04	0.19
(1,664)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	20	0.18	0.01	0.18
(1,664)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	20	0.18	0.01	0.18
(1,290)	1:8:A:PHE:HA	1:9:A:VAL:H	20	0.17	0.03	0.17
(1,473)	1:85:A:CYS:H	1:86:A:SER:H	20	0.15	0.02	0.14
(2,193)	1:98:A:ILE:HD11	1:109:A:ASP:H	19	0.93	0.19	0.9
(2,193)	1:98:A:ILE:HD13	1:109:A:ASP:H	19	0.93	0.19	0.9
(2,193)	1:98:A:ILE:HD12	1:109:A:ASP:H	19	0.93	0.19	0.9
(2,193)	1:117:A:LEU:HD12	1:109:A:ASP:H	19	0.93	0.19	0.9
(2,193)	1:117:A:LEU:HD13	1:109:A:ASP:H	19	0.93	0.19	0.9
(2,193)	1:117:A:LEU:HD11	1:109:A:ASP:H	19	0.93	0.19	0.9
(1,877)	1:22:A:CYS:HA	1:44:A:CYS:H	19	0.78	0.13	0.79
(2,359)	1:98:A:ILE:HD11	1:98:A:ILE:H	19	0.71	0.36	0.84
(2,359)	1:98:A:ILE:HD12	1:98:A:ILE:H	19	0.71	0.36	0.84
(2,359)	1:98:A:ILE:HD13	1:98:A:ILE:H	19	0.71	0.36	0.84
(1,447)	1:71:A:CYS:HA	1:74:A:GLY:H	19	0.64	0.22	0.66
(2,363)	1:49:A:ILE:HB	1:49:A:ILE:H	19	0.6	0.17	0.66
(1,686)	1:74:A:GLY:H	1:69:A:ASN:HD22	19	0.59	0.15	0.64

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,25)	1:79:A:ASN:HD22	1:80:A:CYS:HA	19	0.46	0.12	0.44
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	19	0.45	0.08	0.47
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	19	0.45	0.08	0.47
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	19	0.45	0.08	0.47
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	19	0.45	0.08	0.47
(1,799)	1:85:A:CYS:HA	1:97:A:CYS:H	19	0.41	0.22	0.36
(1,81)	1:28:A:CYS:HA	1:33:A:ASP:H	19	0.4	0.05	0.4
(1,60)	1:56:A:THR:H	1:57:A:GLN:H	19	0.39	0.07	0.42
(1,856)	1:14:A:GLN:H	1:12:A:ASN:HD22	19	0.37	0.09	0.37
(2,190)	1:56:A:THR:HA	1:57:A:GLN:H	19	0.37	0.04	0.36
(1,831)	1:73:A:SER:H	1:75:A:GLU:H	19	0.35	0.08	0.35
(1,849)	1:33:A:ASP:H	1:11:A:ASN:H	19	0.35	0.14	0.29
(1,783)	1:71:A:CYS:HB2	1:74:A:GLY:H	19	0.34	0.08	0.35
(1,783)	1:71:A:CYS:HB3	1:74:A:GLY:H	19	0.34	0.08	0.35
(2,298)	1:28:A:CYS:HB2	1:14:A:GLN:HE22	19	0.32	0.12	0.3
(2,298)	1:28:A:CYS:HB3	1:14:A:GLN:HE22	19	0.32	0.12	0.3
(1,794)	1:82:A:ASN:HD22	1:94:A:SER:H	19	0.3	0.1	0.26
(1,801)	1:102:A:PHE:HB2	1:98:A:ILE:H	19	0.29	0.07	0.28
(1,801)	1:102:A:PHE:HB3	1:98:A:ILE:H	19	0.29	0.07	0.28
(1,375)	1:48:A:GLU:HA	1:49:A:ILE:H	19	0.29	0.07	0.28
(1,585)	1:28:A:CYS:H	1:27:A:ASP:H	19	0.25	0.08	0.24
(1,863)	1:17:A:PRO:HD2	1:20:A:TRP:HE1	19	0.25	0.06	0.25
(1,863)	1:17:A:PRO:HD3	1:20:A:TRP:HE1	19	0.25	0.06	0.25
(1,386)	1:51:A:CYS:HB2	1:51:A:CYS:H	19	0.25	0.06	0.26
(1,386)	1:51:A:CYS:HB3	1:51:A:CYS:H	19	0.25	0.06	0.26
(1,462)	1:79:A:ASN:H	1:78:A:GLU:H	19	0.15	0.03	0.14
(2,233)	1:14:A:GLN:HB2	1:14:A:GLN:HE22	19	0.12	0.01	0.12
(2,233)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	19	0.12	0.01	0.12
(1,819)	1:112:A:ASP:HB2	1:115:A:ASP:H	18	1.02	0.5	1.01
(1,819)	1:112:A:ASP:HB3	1:115:A:ASP:H	18	1.02	0.5	1.01
(2,361)	1:61:A:VAL:HG11	1:64:A:ARG:H	18	0.82	0.34	0.84
(2,361)	1:61:A:VAL:HG13	1:64:A:ARG:H	18	0.82	0.34	0.84
(2,361)	1:61:A:VAL:HG22	1:64:A:ARG:H	18	0.82	0.34	0.84
(2,361)	1:61:A:VAL:HG21	1:64:A:ARG:H	18	0.82	0.34	0.84
(2,361)	1:59:A:ILE:HD11	1:64:A:ARG:H	18	0.82	0.34	0.84
(2,361)	1:61:A:VAL:HG23	1:64:A:ARG:H	18	0.82	0.34	0.84
(2,361)	1:61:A:VAL:HG12	1:64:A:ARG:H	18	0.82	0.34	0.84
(2,354)	1:68:A:GLU:HA	1:69:A:ASN:H	18	0.79	0.03	0.8
(2,296)	1:114:A:SER:HB3	1:117:A:LEU:H	18	0.66	0.19	0.62
(2,296)	1:114:A:SER:HB2	1:117:A:LEU:H	18	0.66	0.19	0.62
(2,296)	1:113:A:GLY:HA2	1:117:A:LEU:H	18	0.66	0.19	0.62
(2,200)	1:77:A:GLU:HG3	1:76:A:ASP:H	18	0.66	0.21	0.73

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,200)	1:77:A:GLU:HG2	1:76:A:ASP:H	18	0.66	0.21	0.73
(2,200)	1:87:A:PRO:HG3	1:76:A:ASP:H	18	0.66	0.21	0.73
(1,543)	1:112:A:ASP:HB2	1:114:A:SER:H	18	0.55	0.22	0.5
(1,543)	1:112:A:ASP:HB3	1:114:A:SER:H	18	0.55	0.22	0.5
(2,323)	1:64:A:ARG:HG2	1:68:A:GLU:H	18	0.46	0.13	0.5
(2,323)	1:68:A:GLU:HG3	1:68:A:GLU:H	18	0.46	0.13	0.5
(1,509)	1:46:A:ILE:HA	1:46:A:ILE:H	18	0.46	0.14	0.53
(2,276)	1:43:A:THR:HA	1:57:A:GLN:H	18	0.35	0.22	0.27
(2,276)	1:56:A:THR:HB	1:57:A:GLN:H	18	0.35	0.22	0.27
(1,859)	1:3:A:CYS:HB2	1:18:A:SER:H	18	0.34	0.1	0.36
(1,859)	1:3:A:CYS:HB3	1:18:A:SER:H	18	0.34	0.1	0.36
(1,596)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	18	0.31	0.12	0.33
(1,596)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	18	0.31	0.12	0.33
(1,454)	1:78:A:GLU:HG2	1:76:A:ASP:H	18	0.28	0.13	0.26
(1,454)	1:78:A:GLU:HG3	1:76:A:ASP:H	18	0.28	0.13	0.26
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB2	18	0.27	0.09	0.29
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB3	18	0.27	0.09	0.29
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB1	18	0.27	0.11	0.27
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB2	18	0.27	0.11	0.27
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB3	18	0.27	0.11	0.27
(1,205)	1:98:A:ILE:HG12	1:98:A:ILE:H	18	0.27	0.05	0.26
(1,205)	1:98:A:ILE:HG13	1:98:A:ILE:H	18	0.27	0.05	0.26
(1,483)	1:10:A:CYS:HB2	1:14:A:GLN:H	18	0.25	0.08	0.25
(1,483)	1:10:A:CYS:HB3	1:14:A:GLN:H	18	0.25	0.08	0.25
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG2	18	0.22	0.1	0.21
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG3	18	0.22	0.1	0.21
(1,418)	1:64:A:ARG:HA	1:66:A:ASP:H	18	0.2	0.05	0.22
(2,218)	1:36:A:PRO:HD2	1:37:A:GLU:H	18	0.19	0.05	0.18
(3,7)	2:202:A:CA:CA	1:63:A:TRP:O	18	0.17	0.04	0.16
(1,383)	1:51:A:CYS:H	1:50:A:SER:HA	18	0.14	0.04	0.12
(1,820)	1:110:A:CYS:H	1:115:A:ASP:H	17	1.09	0.79	1.73
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG12	17	0.74	0.16	0.79
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG13	17	0.74	0.16	0.79
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	17	0.48	0.15	0.46
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	17	0.48	0.15	0.46
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	17	0.48	0.15	0.46
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	17	0.48	0.15	0.46
(1,766)	1:48:A:GLU:HB2	1:58:A:CYS:H	17	0.34	0.16	0.36
(1,766)	1:48:A:GLU:HB3	1:58:A:CYS:H	17	0.34	0.16	0.36
(2,8)	1:45:A:ARG:HA	1:46:A:ILE:H	17	0.32	0.09	0.35
(1,466)	1:80:A:CYS:HA	1:79:A:ASN:H	17	0.31	0.13	0.31
(1,109)	1:119:A:CYS:H	1:117:A:LEU:HG	17	0.29	0.09	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,17)	1:81:A:GLY:H	1:80:A:CYS:H	17	0.26	0.06	0.27
(1,791)	1:85:A:CYS:HB2	1:89:A:GLU:H	17	0.26	0.08	0.24
(1,791)	1:85:A:CYS:HB3	1:89:A:GLU:H	17	0.26	0.08	0.24
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG21	17	0.25	0.1	0.23
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG22	17	0.25	0.1	0.23
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG23	17	0.25	0.1	0.23
(1,886)	1:51:A:CYS:H	1:58:A:CYS:H	17	0.22	0.04	0.23
(1,328)	1:22:A:CYS:HB2	1:22:A:CYS:H	17	0.21	0.04	0.22
(1,328)	1:22:A:CYS:HB3	1:22:A:CYS:H	17	0.21	0.04	0.22
(1,312)	1:14:A:GLN:HG2	1:14:A:GLN:H	17	0.21	0.05	0.21
(1,312)	1:14:A:GLN:HG3	1:14:A:GLN:H	17	0.21	0.05	0.21
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB2	17	0.21	0.06	0.21
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB3	17	0.21	0.06	0.21
(1,842)	1:80:A:CYS:HA	1:84:A:THR:H	17	0.2	0.05	0.21
(1,501)	1:34:A:GLU:HB2	1:34:A:GLU:H	17	0.19	0.05	0.2
(1,501)	1:34:A:GLU:HB3	1:34:A:GLU:H	17	0.19	0.05	0.2
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB2	17	0.19	0.06	0.19
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB3	17	0.19	0.06	0.19
(1,809)	1:106:A:GLY:H	1:104:A:CYS:H	17	0.17	0.05	0.18
(1,550)	1:104:A:CYS:HB2	1:104:A:CYS:H	17	0.17	0.1	0.13
(1,550)	1:104:A:CYS:HB3	1:104:A:CYS:H	17	0.17	0.1	0.13
(1,551)	1:104:A:CYS:HB2	1:104:A:CYS:H	17	0.17	0.1	0.13
(1,551)	1:104:A:CYS:HB3	1:104:A:CYS:H	17	0.17	0.1	0.13
(1,7)	1:22:A:CYS:H	1:23:A:ASP:H	17	0.12	0.02	0.12
(1,2)	1:112:A:ASP:H	1:113:A:GLY:H	16	0.55	0.06	0.54
(2,46)	1:114:A:SER:HG	1:115:A:ASP:H	16	0.46	0.23	0.38
(2,46)	1:116:A:GLU:HA	1:115:A:ASP:H	16	0.46	0.23	0.38
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	16	0.45	0.11	0.44
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	16	0.45	0.11	0.44
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	16	0.45	0.11	0.44
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	16	0.45	0.11	0.44
(1,862)	1:21:A:LYS:HE2	1:19:A:ARG:H	16	0.35	0.11	0.4
(1,862)	1:21:A:LYS:HE3	1:19:A:ARG:H	16	0.35	0.11	0.4
(1,534)	1:77:A:GLU:HB2	1:77:A:GLU:H	16	0.35	0.12	0.38
(1,534)	1:77:A:GLU:HB3	1:77:A:GLU:H	16	0.35	0.12	0.38
(1,806)	1:101:A:ASN:HD21	1:102:A:PHE:H	16	0.27	0.11	0.24
(1,49)	1:94:A:SER:H	1:93:A:SER:H	16	0.24	0.08	0.22
(1,518)	1:49:A:ILE:H	1:61:A:VAL:H	16	0.22	0.06	0.22
(1,658)	1:102:A:PHE:HA	1:105:A:ASN:HD22	16	0.22	0.08	0.24
(1,390)	1:51:A:CYS:HB2	1:52:A:GLY:H	16	0.21	0.09	0.18
(1,390)	1:51:A:CYS:HB3	1:52:A:GLY:H	16	0.21	0.09	0.18
(4,5)	1:49:A:ILE:O	1:59:A:ILE:H	16	0.21	0.06	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,591)	1:69:A:ASN:HB2	1:69:A:ASN:HD21	16	0.18	0.05	0.17
(1,591)	1:69:A:ASN:HB3	1:69:A:ASN:HD21	16	0.18	0.05	0.17
(1,204)	1:98:A:ILE:HG12	1:98:A:ILE:H	16	0.18	0.05	0.17
(1,204)	1:98:A:ILE:HG13	1:98:A:ILE:H	16	0.18	0.05	0.17
(1,308)	1:13:A:GLY:H	1:14:A:GLN:H	16	0.16	0.04	0.16
(1,451)	1:75:A:GLU:H	1:76:A:ASP:H	16	0.16	0.03	0.16
(1,475)	1:75:A:GLU:H	1:76:A:ASP:H	16	0.16	0.03	0.16
(1,409)	1:60:A:PRO:HA	1:61:A:VAL:H	16	0.15	0.02	0.15
(1,59)	1:65:A:CYS:H	1:66:A:ASP:H	16	0.15	0.02	0.15
(2,370)	1:38:A:GLN:HG3	1:38:A:GLN:HE22	16	0.15	0.03	0.14
(2,370)	1:38:A:GLN:HG2	1:38:A:GLN:HE22	16	0.15	0.03	0.14
(2,330)	1:114:A:SER:HG	1:93:A:SER:H	15	0.59	0.15	0.59
(2,330)	1:92:A:CYS:HA	1:93:A:SER:H	15	0.59	0.15	0.59
(2,330)	1:111:A:SER:HG	1:93:A:SER:H	15	0.59	0.15	0.59
(1,531)	1:71:A:CYS:HB2	1:71:A:CYS:H	15	0.5	0.08	0.5
(1,531)	1:71:A:CYS:HB3	1:71:A:CYS:H	15	0.5	0.08	0.5
(1,696)	1:44:A:CYS:HB2	1:34:A:GLU:H	15	0.35	0.14	0.35
(1,696)	1:44:A:CYS:HB3	1:34:A:GLU:H	15	0.35	0.14	0.35
(2,38)	1:96:A:ARG:HB3	1:97:A:CYS:H	15	0.31	0.06	0.32
(1,248)	1:83:A:ILE:HB	1:84:A:THR:H	15	0.21	0.08	0.21
(1,123)	1:115:A:ASP:HB2	1:115:A:ASP:H	15	0.19	0.03	0.18
(1,123)	1:115:A:ASP:HB3	1:115:A:ASP:H	15	0.19	0.03	0.18
(1,372)	1:48:A:GLU:H	1:48:A:GLU:HA	15	0.17	0.04	0.19
(1,277)	1:6:A:SER:HB2	1:6:A:SER:H	15	0.16	0.05	0.13
(1,277)	1:6:A:SER:HB3	1:6:A:SER:H	15	0.16	0.05	0.13
(1,279)	1:6:A:SER:HB2	1:6:A:SER:H	15	0.16	0.05	0.13
(1,279)	1:6:A:SER:HB3	1:6:A:SER:H	15	0.16	0.05	0.13
(1,876)	1:39:A:CYS:HB2	1:43:A:THR:H	15	0.16	0.05	0.15
(1,876)	1:39:A:CYS:HB3	1:43:A:THR:H	15	0.16	0.05	0.15
(1,435)	1:72:A:ASP:HA	1:72:A:ASP:H	15	0.14	0.02	0.15
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	15	0.14	0.03	0.15
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	15	0.14	0.03	0.15
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	15	0.14	0.03	0.15
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	15	0.14	0.03	0.15
(1,371)	1:44:A:CYS:HA	1:45:A:ARG:H	14	0.5	0.06	0.52
(1,118)	1:115:A:ASP:H	1:113:A:GLY:H	14	0.46	0.08	0.45
(1,729)	1:32:A:SER:H	1:28:A:CYS:H	14	0.36	0.05	0.36
(1,733)	1:32:A:SER:H	1:28:A:CYS:H	14	0.36	0.05	0.36
(1,911)	1:57:A:GLN:HE21	1:71:A:CYS:H	14	0.33	0.16	0.37
(1,296)	1:10:A:CYS:HB2	1:10:A:CYS:H	14	0.31	0.07	0.31
(1,296)	1:10:A:CYS:HB3	1:10:A:CYS:H	14	0.31	0.07	0.31
(2,376)	1:87:A:PRO:HB2	1:88:A:ASP:H	14	0.3	0.05	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,916)	1:77:A:GLU:HB2	1:77:A:GLU:H	14	0.28	0.1	0.3
(1,916)	1:77:A:GLU:HB3	1:77:A:GLU:H	14	0.28	0.1	0.3
(4,2)	1:90:A:PHE:O	1:98:A:ILE:H	14	0.25	0.08	0.25
(1,55)	1:71:A:CYS:H	1:70:A:ASP:H	14	0.25	0.07	0.25
(1,724)	1:34:A:GLU:HB2	1:25:A:ASP:H	14	0.22	0.08	0.22
(1,724)	1:34:A:GLU:HB3	1:25:A:ASP:H	14	0.22	0.08	0.22
(1,884)	1:50:A:SER:H	1:59:A:ILE:H	14	0.19	0.05	0.18
(1,516)	1:49:A:ILE:H	1:59:A:ILE:H	14	0.19	0.04	0.18
(2,226)	1:98:A:ILE:H	1:97:A:CYS:H	14	0.17	0.05	0.17
(2,226)	1:92:A:CYS:H	1:97:A:CYS:H	14	0.17	0.05	0.17
(1,560)	1:90:A:PHE:H	1:99:A:SER:H	14	0.16	0.04	0.15
(2,236)	1:21:A:LYS:HB2	1:21:A:LYS:H	14	0.12	0.02	0.12
(1,357)	1:40:A:HIS:H	1:39:A:CYS:HA	14	0.12	0.01	0.12
(1,437)	1:72:A:ASP:H	1:71:A:CYS:H	13	0.45	0.35	0.24
(1,667)	1:107:A:GLN:HG2	1:105:A:ASN:HD22	13	0.38	0.08	0.41
(1,667)	1:107:A:GLN:HG2	1:105:A:ASN:HD22	13	0.38	0.08	0.41
(1,667)	1:107:A:GLN:HG3	1:105:A:ASN:HD22	13	0.38	0.08	0.41
(1,667)	1:107:A:GLN:HG3	1:105:A:ASN:HD22	13	0.38	0.08	0.41
(1,174)	1:103:A:VAL:H	1:101:A:ASN:HB2	13	0.36	0.1	0.39
(1,174)	1:103:A:VAL:H	1:101:A:ASN:HB3	13	0.36	0.1	0.39
(1,711)	1:10:A:CYS:HB2	1:11:A:ASN:H	13	0.35	0.14	0.32
(1,711)	1:10:A:CYS:HB3	1:11:A:ASN:H	13	0.35	0.14	0.32
(2,168)	1:38:A:GLN:HG3	1:38:A:GLN:H	13	0.33	0.15	0.34
(2,168)	1:38:A:GLN:HG2	1:38:A:GLN:H	13	0.33	0.15	0.34
(2,168)	1:37:A:GLU:HG3	1:38:A:GLN:H	13	0.33	0.15	0.34
(2,168)	1:39:A:CYS:HB2	1:38:A:GLN:H	13	0.33	0.15	0.34
(2,168)	1:37:A:GLU:HG2	1:38:A:GLN:H	13	0.33	0.15	0.34
(1,541)	1:115:A:ASP:HB2	1:116:A:GLU:H	13	0.33	0.24	0.2
(1,541)	1:115:A:ASP:HB3	1:116:A:GLU:H	13	0.33	0.24	0.2
(2,83)	1:35:A:SER:HB3	1:38:A:GLN:H	13	0.29	0.18	0.22
(2,83)	1:35:A:SER:HB2	1:38:A:GLN:H	13	0.29	0.18	0.22
(1,592)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	13	0.27	0.07	0.29
(1,592)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	13	0.27	0.07	0.29
(1,800)	1:85:A:CYS:HB2	1:98:A:ILE:H	13	0.26	0.09	0.28
(1,800)	1:85:A:CYS:HB3	1:98:A:ILE:H	13	0.26	0.09	0.28
(1,92)	1:7:A:ASP:HB2	1:8:A:PHE:H	13	0.25	0.08	0.24
(1,92)	1:7:A:ASP:HB3	1:8:A:PHE:H	13	0.25	0.08	0.24
(1,286)	1:7:A:ASP:HB2	1:7:A:ASP:H	13	0.2	0.08	0.16
(1,286)	1:7:A:ASP:HB3	1:7:A:ASP:H	13	0.2	0.08	0.16
(1,810)	1:101:A:ASN:HD21	1:105:A:ASN:HD22	13	0.19	0.03	0.19
(1,718)	1:16:A:VAL:HB	1:20:A:TRP:HE1	13	0.18	0.05	0.17
(1,838)	1:58:A:CYS:HA	1:52:A:GLY:H	13	0.18	0.05	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,726)	1:34:A:GLU:HG2	1:27:A:ASP:H	13	0.17	0.05	0.18
(1,726)	1:34:A:GLU:HG3	1:27:A:ASP:H	13	0.17	0.05	0.18
(2,181)	1:41:A:MET:HG3	1:41:A:MET:H	13	0.17	0.03	0.17
(2,181)	1:41:A:MET:HG2	1:41:A:MET:H	13	0.17	0.03	0.17
(2,181)	1:39:A:CYS:HB3	1:41:A:MET:H	13	0.17	0.03	0.17
(1,369)	1:43:A:THR:HB	1:44:A:CYS:H	13	0.17	0.04	0.16
(1,496)	1:31:A:GLY:HA2	1:31:A:GLY:H	13	0.12	0.01	0.13
(1,496)	1:31:A:GLY:HA3	1:31:A:GLY:H	13	0.12	0.01	0.13
(2,381)	1:100:A:ARG:HD3	1:90:A:PHE:H	12	0.44	0.13	0.44
(2,381)	1:85:A:CYS:HB3	1:90:A:PHE:H	12	0.44	0.13	0.44
(1,879)	1:48:A:GLU:H	1:45:A:ARG:H	12	0.36	0.11	0.36
(1,881)	1:48:A:GLU:H	1:45:A:ARG:H	12	0.36	0.11	0.36
(1,281)	1:5:A:GLU:HB2	1:6:A:SER:H	12	0.3	0.05	0.3
(1,281)	1:5:A:GLU:HB2	1:6:A:SER:H	12	0.3	0.05	0.3
(1,281)	1:5:A:GLU:HB3	1:6:A:SER:H	12	0.3	0.05	0.3
(1,281)	1:5:A:GLU:HB3	1:6:A:SER:H	12	0.3	0.05	0.3
(2,331)	1:101:A:ASN:H	1:99:A:SER:H	12	0.27	0.13	0.23
(1,784)	1:71:A:CYS:HB2	1:76:A:ASP:H	12	0.27	0.17	0.18
(1,784)	1:71:A:CYS:HB3	1:76:A:ASP:H	12	0.27	0.17	0.18
(4,7)	1:8:A:PHE:H	1:16:A:VAL:O	12	0.25	0.07	0.26
(1,837)	1:50:A:SER:H	1:45:A:ARG:HD2	12	0.23	0.08	0.2
(1,837)	1:50:A:SER:H	1:45:A:ARG:HD3	12	0.23	0.08	0.2
(2,89)	1:107:A:GLN:HB2	1:108:A:ASP:H	12	0.23	0.09	0.2
(2,89)	1:107:A:GLN:HB3	1:108:A:ASP:H	12	0.23	0.09	0.2
(2,245)	1:36:A:PRO:HA	1:39:A:CYS:H	12	0.22	0.08	0.23
(1,33)	1:115:A:ASP:H	1:114:A:SER:H	12	0.22	0.09	0.19
(1,731)	1:28:A:CYS:HB2	1:32:A:SER:H	12	0.22	0.06	0.22
(1,731)	1:28:A:CYS:HB3	1:32:A:SER:H	12	0.22	0.06	0.22
(1,187)	1:103:A:VAL:HG11	1:102:A:PHE:H	12	0.21	0.06	0.22
(1,187)	1:103:A:VAL:HG12	1:102:A:PHE:H	12	0.21	0.06	0.22
(1,187)	1:103:A:VAL:HG13	1:102:A:PHE:H	12	0.21	0.06	0.22
(1,187)	1:103:A:VAL:HG21	1:102:A:PHE:H	12	0.21	0.06	0.22
(1,187)	1:103:A:VAL:HG22	1:102:A:PHE:H	12	0.21	0.06	0.22
(1,187)	1:103:A:VAL:HG23	1:102:A:PHE:H	12	0.21	0.06	0.22
(1,9)	1:12:A:ASN:H	1:11:A:ASN:H	12	0.2	0.07	0.2
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG21	12	0.18	0.05	0.18
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG22	12	0.18	0.05	0.18
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG23	12	0.18	0.05	0.18
(1,482)	1:11:A:ASN:HD21	1:11:A:ASN:H	12	0.16	0.04	0.15
(1,74)	1:65:A:CYS:H	1:65:A:CYS:HB2	12	0.15	0.04	0.16
(1,74)	1:65:A:CYS:H	1:65:A:CYS:HB3	12	0.15	0.04	0.16
(1,708)	1:44:A:CYS:HB2	1:45:A:ARG:H	11	0.48	0.2	0.57

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,708)	1:44:A:CYS:HB3	1:45:A:ARG:H	11	0.48	0.2	0.57
(1,833)	1:42:A:ARG:HG2	1:41:A:MET:H	11	0.41	0.06	0.41
(1,833)	1:42:A:ARG:HG2	1:41:A:MET:H	11	0.41	0.06	0.41
(1,833)	1:42:A:ARG:HG3	1:41:A:MET:H	11	0.41	0.06	0.41
(1,833)	1:42:A:ARG:HG3	1:41:A:MET:H	11	0.41	0.06	0.41
(1,685)	1:107:A:GLN:HG2	1:107:A:GLN:HE21	11	0.41	0.07	0.39
(1,685)	1:107:A:GLN:HG2	1:107:A:GLN:HE21	11	0.41	0.07	0.39
(1,685)	1:107:A:GLN:HG3	1:107:A:GLN:HE21	11	0.41	0.07	0.39
(1,685)	1:107:A:GLN:HG3	1:107:A:GLN:HE21	11	0.41	0.07	0.39
(1,807)	1:98:A:ILE:HG12	1:103:A:VAL:H	11	0.39	0.12	0.44
(1,807)	1:98:A:ILE:HG13	1:103:A:VAL:H	11	0.39	0.12	0.44
(1,203)	1:89:A:GLU:HB2	1:98:A:ILE:H	11	0.25	0.06	0.27
(1,203)	1:89:A:GLU:HB3	1:98:A:ILE:H	11	0.25	0.06	0.27
(2,22)	1:75:A:GLU:HA	1:78:A:GLU:H	11	0.25	0.09	0.22
(1,788)	1:80:A:CYS:H	1:78:A:GLU:H	11	0.24	0.1	0.21
(1,228)	1:92:A:CYS:HB2	1:93:A:SER:H	11	0.22	0.07	0.22
(1,228)	1:92:A:CYS:HB3	1:93:A:SER:H	11	0.22	0.07	0.22
(1,679)	1:78:A:GLU:HG2	1:79:A:ASN:HD22	11	0.22	0.09	0.19
(1,679)	1:78:A:GLU:HG3	1:79:A:ASN:HD22	11	0.22	0.09	0.19
(1,510)	1:48:A:GLU:HB2	1:48:A:GLU:H	11	0.18	0.04	0.17
(1,510)	1:48:A:GLU:HB3	1:48:A:GLU:H	11	0.18	0.04	0.17
(1,792)	1:97:A:CYS:HB2	1:91:A:THR:H	11	0.17	0.04	0.17
(1,792)	1:97:A:CYS:HB3	1:91:A:THR:H	11	0.17	0.04	0.17
(1,22)	1:91:A:THR:H	1:92:A:CYS:H	11	0.17	0.03	0.18
(2,280)	1:92:A:CYS:H	1:91:A:THR:H	11	0.17	0.03	0.18
(1,712)	1:32:A:SER:H	1:11:A:ASN:H	11	0.17	0.05	0.15
(1,734)	1:32:A:SER:H	1:11:A:ASN:H	11	0.17	0.05	0.15
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD11	11	0.16	0.04	0.15
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD12	11	0.16	0.04	0.15
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD13	11	0.16	0.04	0.15
(1,607)	1:11:A:ASN:HB2	1:11:A:ASN:HD21	11	0.15	0.02	0.16
(1,607)	1:11:A:ASN:HB3	1:11:A:ASN:HD21	11	0.15	0.02	0.16
(2,244)	1:60:A:PRO:HA	1:47:A:HIS:H	10	0.68	0.21	0.7
(2,244)	1:45:A:ARG:HA	1:47:A:HIS:H	10	0.68	0.21	0.7
(2,257)	1:32:A:SER:HB2	1:38:A:GLN:HE22	10	0.62	0.2	0.64
(2,257)	1:33:A:ASP:HA	1:38:A:GLN:HE22	10	0.62	0.2	0.64
(2,257)	1:32:A:SER:HB3	1:38:A:GLN:HE22	10	0.62	0.2	0.64
(1,654)	1:107:A:GLN:HB2	1:107:A:GLN:HE22	10	0.44	0.04	0.44
(1,654)	1:107:A:GLN:HB2	1:107:A:GLN:HE22	10	0.44	0.04	0.44
(1,654)	1:107:A:GLN:HB3	1:107:A:GLN:HE22	10	0.44	0.04	0.44
(1,654)	1:107:A:GLN:HB3	1:107:A:GLN:HE22	10	0.44	0.04	0.44
(1,80)	1:44:A:CYS:HB2	1:45:A:ARG:H	10	0.41	0.17	0.49

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,80)	1:44:A:CYS:HB3	1:45:A:ARG:H	10	0.41	0.17	0.49
(1,670)	1:107:A:GLN:HB2	1:105:A:ASN:HD22	10	0.4	0.15	0.44
(1,670)	1:107:A:GLN:HB2	1:105:A:ASN:HD22	10	0.4	0.15	0.44
(1,670)	1:107:A:GLN:HB3	1:105:A:ASN:HD22	10	0.4	0.15	0.44
(1,670)	1:107:A:GLN:HB3	1:105:A:ASN:HD22	10	0.4	0.15	0.44
(1,853)	1:10:A:CYS:HB2	1:12:A:ASN:H	10	0.33	0.09	0.37
(1,853)	1:10:A:CYS:HB3	1:12:A:ASN:H	10	0.33	0.09	0.37
(1,99)	1:98:A:ILE:HG12	1:99:A:SER:H	10	0.32	0.1	0.34
(1,99)	1:98:A:ILE:HG13	1:99:A:SER:H	10	0.32	0.1	0.34
(1,628)	1:71:A:CYS:HB2	1:57:A:GLN:HE22	10	0.31	0.13	0.28
(1,628)	1:71:A:CYS:HB3	1:57:A:GLN:HE22	10	0.31	0.13	0.28
(1,759)	1:57:A:GLN:HE21	1:71:A:CYS:HA	10	0.27	0.07	0.28
(2,174)	1:117:A:LEU:HB3	1:116:A:GLU:H	10	0.25	0.09	0.24
(2,174)	1:117:A:LEU:HB2	1:116:A:GLU:H	10	0.25	0.09	0.24
(1,761)	1:72:A:ASP:H	1:57:A:GLN:HE21	10	0.25	0.07	0.24
(2,366)	1:107:A:GLN:HA	1:106:A:GLY:H	10	0.24	0.08	0.24
(2,366)	1:116:A:GLU:HA	1:106:A:GLY:H	10	0.24	0.08	0.24
(2,49)	1:35:A:SER:HB2	1:39:A:CYS:H	10	0.23	0.11	0.2
(2,49)	1:35:A:SER:HB3	1:39:A:CYS:H	10	0.23	0.11	0.2
(2,353)	1:99:A:SER:HG	1:101:A:ASN:HD22	10	0.23	0.05	0.24
(1,900)	1:83:A:ILE:HG12	1:82:A:ASN:H	10	0.2	0.04	0.2
(1,900)	1:83:A:ILE:HG13	1:82:A:ASN:H	10	0.2	0.04	0.2
(1,96)	1:100:A:ARG:H	1:89:A:GLU:HA	10	0.19	0.05	0.2
(1,226)	1:92:A:CYS:HB2	1:94:A:SER:H	10	0.18	0.05	0.18
(1,226)	1:92:A:CYS:HB3	1:94:A:SER:H	10	0.18	0.05	0.18
(1,811)	1:107:A:GLN:H	1:105:A:ASN:HD21	10	0.17	0.04	0.18
(1,378)	1:48:A:GLU:HG2	1:49:A:ILE:H	10	0.16	0.05	0.16
(1,378)	1:48:A:GLU:HG3	1:49:A:ILE:H	10	0.16	0.05	0.16
(1,580)	1:48:A:GLU:HG2	1:49:A:ILE:H	10	0.16	0.05	0.16
(1,580)	1:48:A:GLU:HG3	1:49:A:ILE:H	10	0.16	0.05	0.16
(1,872)	1:32:A:SER:H	1:33:A:ASP:HB2	10	0.16	0.07	0.15
(1,872)	1:32:A:SER:H	1:33:A:ASP:HB3	10	0.16	0.07	0.15
(1,374)	1:61:A:VAL:H	1:49:A:ILE:H	10	0.16	0.04	0.16
(2,382)	1:72:A:ASP:HB2	1:73:A:SER:H	10	0.15	0.03	0.14
(2,382)	1:72:A:ASP:HB3	1:73:A:SER:H	10	0.15	0.03	0.14
(1,444)	1:76:A:ASP:H	1:74:A:GLY:H	10	0.15	0.06	0.12
(1,302)	1:14:A:GLN:H	1:12:A:ASN:H	10	0.13	0.03	0.12
(1,828)	1:85:A:CYS:HA	1:86:A:SER:H	10	0.13	0.02	0.13
(1,392)	1:52:A:GLY:HA2	1:53:A:ALA:H	10	0.12	0.01	0.12
(1,392)	1:52:A:GLY:HA3	1:53:A:ALA:H	10	0.12	0.01	0.12
(1,906)	1:13:A:GLY:HA2	1:12:A:ASN:HD22	10	0.11	0.02	0.11
(1,906)	1:13:A:GLY:HA3	1:12:A:ASN:HD22	10	0.11	0.02	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,770)	1:63:A:TRP:H	1:77:A:GLU:HG2	9	0.7	0.12	0.73
(1,770)	1:63:A:TRP:H	1:77:A:GLU:HG3	9	0.7	0.12	0.73
(2,178)	1:59:A:ILE:HG22	1:57:A:GLN:HE22	9	0.59	0.24	0.7
(2,178)	1:59:A:ILE:HG21	1:57:A:GLN:HE22	9	0.59	0.24	0.7
(2,178)	1:59:A:ILE:HG23	1:57:A:GLN:HE22	9	0.59	0.24	0.7
(1,850)	1:12:A:ASN:H	1:11:A:ASN:HD22	9	0.48	0.05	0.49
(2,304)	1:11:A:ASN:HD21	1:12:A:ASN:H	9	0.48	0.35	0.24
(1,346)	1:32:A:SER:H	1:31:A:GLY:H	9	0.4	0.14	0.42
(1,750)	1:57:A:GLN:HB2	1:52:A:GLY:H	9	0.37	0.13	0.41
(1,750)	1:57:A:GLN:HB2	1:52:A:GLY:H	9	0.37	0.13	0.41
(1,750)	1:57:A:GLN:HB3	1:52:A:GLY:H	9	0.37	0.13	0.41
(1,750)	1:57:A:GLN:HB3	1:52:A:GLY:H	9	0.37	0.13	0.41
(1,704)	1:100:A:ARG:HG2	1:100:A:ARG:H	9	0.36	0.07	0.32
(1,704)	1:100:A:ARG:HG2	1:100:A:ARG:H	9	0.36	0.07	0.32
(1,704)	1:100:A:ARG:HG3	1:100:A:ARG:H	9	0.36	0.07	0.32
(1,704)	1:100:A:ARG:HG3	1:100:A:ARG:H	9	0.36	0.07	0.32
(1,189)	1:101:A:ASN:HB2	1:101:A:ASN:H	9	0.34	0.02	0.34
(1,189)	1:101:A:ASN:HB3	1:101:A:ASN:H	9	0.34	0.02	0.34
(1,14)	1:110:A:CYS:H	1:109:A:ASP:H	9	0.3	0.07	0.34
(2,313)	1:17:A:PRO:HB2	1:20:A:TRP:H	9	0.27	0.13	0.3
(1,553)	1:115:A:ASP:HB2	1:104:A:CYS:H	9	0.25	0.1	0.21
(1,553)	1:115:A:ASP:HB3	1:104:A:CYS:H	9	0.25	0.1	0.21
(1,335)	1:45:A:ARG:HD2	1:24:A:GLY:H	9	0.25	0.1	0.23
(1,335)	1:45:A:ARG:HD3	1:24:A:GLY:H	9	0.25	0.1	0.23
(2,187)	1:118:A:ASP:HA	1:119:A:CYS:H	9	0.2	0.07	0.22
(2,187)	1:116:A:GLU:HA	1:119:A:CYS:H	9	0.2	0.07	0.22
(1,125)	1:114:A:SER:H	1:113:A:GLY:HA2	9	0.2	0.12	0.15
(1,125)	1:114:A:SER:H	1:113:A:GLY:HA3	9	0.2	0.12	0.15
(1,343)	1:28:A:CYS:HB2	1:28:A:CYS:H	9	0.2	0.05	0.19
(1,343)	1:28:A:CYS:HB3	1:28:A:CYS:H	9	0.2	0.05	0.19
(1,184)	1:103:A:VAL:HB	1:102:A:PHE:H	9	0.18	0.04	0.18
(1,180)	1:99:A:SER:HB2	1:102:A:PHE:H	9	0.17	0.05	0.16
(1,180)	1:99:A:SER:HB3	1:102:A:PHE:H	9	0.17	0.05	0.16
(1,864)	1:20:A:TRP:HA	1:20:A:TRP:HE1	9	0.17	0.03	0.17
(1,645)	1:101:A:ASN:HD22	1:101:A:ASN:H	9	0.16	0.04	0.16
(1,623)	1:30:A:ASP:HB2	1:12:A:ASN:HD22	9	0.16	0.04	0.15
(1,623)	1:30:A:ASP:HB3	1:12:A:ASN:HD22	9	0.16	0.04	0.15
(1,781)	1:73:A:SER:H	1:71:A:CYS:HB2	9	0.15	0.04	0.14
(1,781)	1:73:A:SER:H	1:71:A:CYS:HB3	9	0.15	0.04	0.14
(1,313)	1:14:A:GLN:HG2	1:14:A:GLN:H	9	0.15	0.03	0.14
(1,313)	1:14:A:GLN:HG3	1:14:A:GLN:H	9	0.15	0.03	0.14
(1,190)	1:101:A:ASN:HB2	1:101:A:ASN:H	9	0.14	0.02	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,190)	1:101:A:ASN:HB3	1:101:A:ASN:H	9	0.14	0.02	0.14
(2,75)	1:108:A:ASP:HA	1:108:A:ASP:H	9	0.13	0.01	0.13
(1,463)	1:71:A:CYS:HB2	1:78:A:GLU:H	8	0.53	0.25	0.54
(1,463)	1:71:A:CYS:HB3	1:78:A:GLU:H	8	0.53	0.25	0.54
(1,137)	1:109:A:ASP:H	1:113:A:GLY:HA2	8	0.36	0.22	0.37
(1,137)	1:109:A:ASP:H	1:113:A:GLY:HA3	8	0.36	0.22	0.37
(2,44)	1:83:A:ILE:HG22	1:97:A:CYS:H	8	0.34	0.17	0.29
(2,44)	1:83:A:ILE:HG23	1:97:A:CYS:H	8	0.34	0.17	0.29
(2,44)	1:83:A:ILE:HG21	1:97:A:CYS:H	8	0.34	0.17	0.29
(2,12)	1:11:A:ASN:HB2	1:13:A:GLY:H	8	0.3	0.09	0.29
(2,12)	1:10:A:CYS:HB2	1:13:A:GLY:H	8	0.3	0.09	0.29
(2,12)	1:10:A:CYS:HB3	1:13:A:GLY:H	8	0.3	0.09	0.29
(1,98)	1:98:A:ILE:HG12	1:99:A:SER:H	8	0.26	0.06	0.27
(1,98)	1:98:A:ILE:HG13	1:99:A:SER:H	8	0.26	0.06	0.27
(1,808)	1:116:A:GLU:HB2	1:104:A:CYS:H	8	0.25	0.08	0.26
(1,808)	1:116:A:GLU:HB3	1:104:A:CYS:H	8	0.25	0.08	0.26
(2,80)	1:41:A:MET:HA	1:56:A:THR:H	8	0.24	0.1	0.2
(2,80)	1:56:A:THR:HB	1:56:A:THR:H	8	0.24	0.1	0.2
(2,80)	1:42:A:ARG:HA	1:56:A:THR:H	8	0.24	0.1	0.2
(1,897)	1:77:A:GLU:HB2	1:69:A:ASN:HD22	8	0.24	0.11	0.22
(1,897)	1:77:A:GLU:HB3	1:69:A:ASN:HD22	8	0.24	0.11	0.22
(1,56)	1:70:A:ASP:H	1:71:A:CYS:H	8	0.24	0.15	0.15
(1,542)	1:112:A:ASP:H	1:114:A:SER:H	8	0.23	0.06	0.26
(1,840)	1:71:A:CYS:HB2	1:77:A:GLU:H	8	0.22	0.07	0.2
(1,840)	1:71:A:CYS:HB3	1:77:A:GLU:H	8	0.22	0.07	0.2
(1,15)	1:109:A:ASP:H	1:110:A:CYS:H	8	0.22	0.06	0.24
(1,562)	1:102:A:PHE:HB2	1:99:A:SER:H	8	0.21	0.06	0.21
(1,562)	1:102:A:PHE:HB3	1:99:A:SER:H	8	0.21	0.06	0.21
(1,705)	1:100:A:ARG:H	1:100:A:ARG:HD2	8	0.2	0.08	0.18
(1,705)	1:100:A:ARG:H	1:100:A:ARG:HD3	8	0.2	0.08	0.18
(1,627)	1:72:A:ASP:HA	1:57:A:GLN:HE22	8	0.17	0.09	0.12
(1,905)	1:101:A:ASN:HD21	1:105:A:ASN:HD21	8	0.16	0.04	0.18
(1,419)	1:65:A:CYS:HB2	1:66:A:ASP:H	8	0.15	0.03	0.15
(1,419)	1:65:A:CYS:HB3	1:66:A:ASP:H	8	0.15	0.03	0.15
(1,241)	1:86:A:SER:H	1:89:A:GLU:H	8	0.15	0.02	0.15
(2,180)	1:11:A:ASN:HA	1:11:A:ASN:HD21	7	0.52	0.13	0.57
(1,431)	1:72:A:ASP:H	1:70:A:ASP:H	7	0.39	0.21	0.39
(2,210)	1:33:A:ASP:HA	1:38:A:GLN:HE21	7	0.38	0.22	0.3
(1,813)	1:107:A:GLN:HE21	1:108:A:ASP:HA	7	0.37	0.23	0.36
(2,52)	1:60:A:PRO:HD2	1:63:A:TRP:HE1	7	0.36	0.25	0.17
(2,52)	1:80:A:CYS:HB3	1:63:A:TRP:HE1	7	0.36	0.25	0.17
(1,347)	1:31:A:GLY:H	1:28:A:CYS:H	7	0.3	0.15	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,797)	1:91:A:THR:HG21	1:96:A:ARG:H	7	0.29	0.13	0.23
(1,797)	1:91:A:THR:HG23	1:96:A:ARG:H	7	0.29	0.13	0.23
(1,797)	1:91:A:THR:HG22	1:96:A:ARG:H	7	0.29	0.13	0.23
(1,797)	1:91:A:THR:HG1	1:96:A:ARG:H	7	0.29	0.13	0.23
(2,11)	1:110:A:CYS:HA	1:113:A:GLY:H	7	0.28	0.13	0.32
(2,11)	1:109:A:ASP:HA	1:113:A:GLY:H	7	0.28	0.13	0.32
(2,270)	1:113:A:GLY:HA2	1:110:A:CYS:H	7	0.28	0.1	0.29
(2,270)	1:111:A:SER:HA	1:110:A:CYS:H	7	0.28	0.1	0.29
(1,446)	1:73:A:SER:H	1:74:A:GLY:H	7	0.27	0.15	0.19
(1,319)	1:16:A:VAL:H	1:9:A:VAL:HA	7	0.24	0.06	0.24
(1,445)	1:75:A:GLU:H	1:74:A:GLY:H	7	0.24	0.06	0.21
(1,787)	1:73:A:SER:H	1:76:A:ASP:H	7	0.22	0.22	0.11
(1,844)	1:79:A:ASN:HB2	1:92:A:CYS:H	7	0.2	0.04	0.2
(1,844)	1:79:A:ASN:HB3	1:92:A:CYS:H	7	0.2	0.04	0.2
(2,246)	1:90:A:PHE:HB2	1:100:A:ARG:H	7	0.19	0.05	0.16
(2,246)	1:90:A:PHE:HB3	1:100:A:ARG:H	7	0.19	0.05	0.16
(1,612)	1:15:A:CYS:H	1:14:A:GLN:HE22	7	0.16	0.02	0.17
(1,350)	1:31:A:GLY:H	1:32:A:SER:H	7	0.16	0.07	0.13
(1,94)	1:120:A:ALA:H	1:119:A:CYS:HB2	7	0.16	0.05	0.14
(1,94)	1:120:A:ALA:H	1:119:A:CYS:HB3	7	0.16	0.05	0.14
(1,295)	1:15:A:CYS:HA	1:10:A:CYS:H	7	0.16	0.07	0.13
(1,196)	1:98:A:ILE:HA	1:99:A:SER:H	7	0.16	0.03	0.14
(1,603)	1:32:A:SER:HB2	1:11:A:ASN:HD22	7	0.15	0.04	0.14
(1,603)	1:32:A:SER:HB3	1:11:A:ASN:HD22	7	0.15	0.04	0.14
(1,299)	1:11:A:ASN:H	1:12:A:ASN:H	7	0.15	0.04	0.14
(2,74)	1:46:A:ILE:HB	1:46:A:ILE:H	7	0.15	0.02	0.14
(1,882)	1:58:A:CYS:HA	1:50:A:SER:H	7	0.14	0.03	0.13
(1,680)	1:79:A:ASN:HD22	1:79:A:ASN:HB2	7	0.14	0.03	0.14
(1,680)	1:79:A:ASN:HD22	1:79:A:ASN:HB3	7	0.14	0.03	0.14
(1,832)	1:35:A:SER:H	1:38:A:GLN:H	7	0.14	0.02	0.14
(1,116)	1:116:A:GLU:HG2	1:116:A:GLU:H	7	0.14	0.04	0.12
(1,116)	1:116:A:GLU:HG3	1:116:A:GLU:H	7	0.14	0.04	0.12
(1,867)	1:34:A:GLU:HG2	1:24:A:GLY:H	7	0.13	0.02	0.13
(1,867)	1:34:A:GLU:HG3	1:24:A:GLY:H	7	0.13	0.02	0.13
(1,527)	1:67:A:GLY:HA2	1:67:A:GLY:H	7	0.11	0.01	0.11
(1,527)	1:67:A:GLY:HA3	1:67:A:GLY:H	7	0.11	0.01	0.11
(2,154)	1:116:A:GLU:HG3	1:109:A:ASP:H	6	0.38	0.07	0.38
(1,636)	1:78:A:GLU:HB2	1:79:A:ASN:HD22	6	0.36	0.1	0.39
(1,636)	1:78:A:GLU:HB2	1:79:A:ASN:HD22	6	0.36	0.1	0.39
(1,636)	1:78:A:GLU:HB3	1:79:A:ASN:HD22	6	0.36	0.1	0.39
(1,636)	1:78:A:GLU:HB3	1:79:A:ASN:HD22	6	0.36	0.1	0.39
(1,134)	1:110:A:CYS:H	1:109:A:ASP:HB2	6	0.34	0.14	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,134)	1:110:A:CYS:H	1:109:A:ASP:HB2	6	0.34	0.14	0.3
(1,134)	1:110:A:CYS:H	1:109:A:ASP:HB3	6	0.34	0.14	0.3
(1,134)	1:110:A:CYS:H	1:109:A:ASP:HB3	6	0.34	0.14	0.3
(2,329)	1:90:A:PHE:HA	1:98:A:ILE:H	6	0.25	0.07	0.26
(2,329)	1:91:A:THR:HA	1:98:A:ILE:H	6	0.25	0.07	0.26
(1,894)	1:66:A:ASP:H	1:77:A:GLU:HG2	6	0.22	0.11	0.22
(1,894)	1:66:A:ASP:H	1:77:A:GLU:HG3	6	0.22	0.11	0.22
(1,895)	1:77:A:GLU:HG2	1:66:A:ASP:H	6	0.22	0.11	0.22
(1,895)	1:77:A:GLU:HG3	1:66:A:ASP:H	6	0.22	0.11	0.22
(2,307)	1:59:A:ILE:HD12	1:63:A:TRP:H	6	0.22	0.16	0.15
(2,307)	1:60:A:PRO:HB2	1:63:A:TRP:H	6	0.22	0.16	0.15
(2,307)	1:59:A:ILE:HD13	1:63:A:TRP:H	6	0.22	0.16	0.15
(1,597)	1:74:A:GLY:HA2	1:69:A:ASN:HD22	6	0.22	0.1	0.19
(1,597)	1:74:A:GLY:HA3	1:69:A:ASN:HD22	6	0.22	0.1	0.19
(1,598)	1:74:A:GLY:HA2	1:69:A:ASN:HD22	6	0.22	0.1	0.19
(1,598)	1:74:A:GLY:HA3	1:69:A:ASN:HD22	6	0.22	0.1	0.19
(1,822)	1:113:A:GLY:HA2	1:116:A:GLU:H	6	0.21	0.04	0.2
(1,822)	1:113:A:GLY:HA3	1:116:A:GLU:H	6	0.21	0.04	0.2
(1,586)	1:69:A:ASN:HA	1:64:A:ARG:H	6	0.21	0.14	0.16
(1,683)	1:78:A:GLU:HG2	1:79:A:ASN:HD21	6	0.2	0.05	0.2
(1,683)	1:78:A:GLU:HG3	1:79:A:ASN:HD21	6	0.2	0.05	0.2
(1,476)	1:7:A:ASP:H	1:3:A:CYS:HB2	6	0.19	0.04	0.2
(1,476)	1:7:A:ASP:H	1:3:A:CYS:HB3	6	0.19	0.04	0.2
(1,69)	1:78:A:GLU:HG2	1:78:A:GLU:H	6	0.18	0.07	0.16
(1,69)	1:78:A:GLU:HG3	1:78:A:GLU:H	6	0.18	0.07	0.16
(2,56)	1:114:A:SER:HA	1:117:A:LEU:H	6	0.17	0.04	0.18
(1,215)	1:96:A:ARG:H	1:92:A:CYS:HB2	6	0.17	0.04	0.16
(1,215)	1:96:A:ARG:H	1:92:A:CYS:HB3	6	0.17	0.04	0.16
(2,123)	1:16:A:VAL:HG11	1:33:A:ASP:H	6	0.17	0.06	0.16
(2,123)	1:16:A:VAL:HG12	1:33:A:ASP:H	6	0.17	0.06	0.16
(2,123)	1:16:A:VAL:HG13	1:33:A:ASP:H	6	0.17	0.06	0.16
(2,123)	1:16:A:VAL:HG21	1:33:A:ASP:H	6	0.17	0.06	0.16
(2,123)	1:16:A:VAL:HG22	1:33:A:ASP:H	6	0.17	0.06	0.16
(2,123)	1:16:A:VAL:HG23	1:33:A:ASP:H	6	0.17	0.06	0.16
(1,851)	1:32:A:SER:H	1:11:A:ASN:HD22	6	0.16	0.02	0.15
(2,235)	1:80:A:CYS:HA	1:85:A:CYS:H	6	0.16	0.04	0.16
(2,235)	1:86:A:SER:HA	1:85:A:CYS:H	6	0.16	0.04	0.16
(1,41)	1:96:A:ARG:H	1:97:A:CYS:H	6	0.14	0.02	0.15
(1,42)	1:96:A:ARG:H	1:97:A:CYS:H	6	0.14	0.02	0.15
(2,117)	1:14:A:GLN:HB2	1:12:A:ASN:HD21	6	0.12	0.02	0.12
(2,117)	1:14:A:GLN:HB3	1:12:A:ASN:HD21	6	0.12	0.02	0.12
(1,662)	1:102:A:PHE:HB2	1:105:A:ASN:HD21	6	0.12	0.02	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,662)	1:102:A:PHE:HB3	1:105:A:ASN:HD21	6	0.12	0.02	0.12
(1,890)	1:81:A:GLY:HA2	1:63:A:TRP:HE1	5	0.44	0.23	0.5
(1,890)	1:81:A:GLY:HA2	1:63:A:TRP:HE1	5	0.44	0.23	0.5
(1,890)	1:81:A:GLY:HA3	1:63:A:TRP:HE1	5	0.44	0.23	0.5
(1,890)	1:81:A:GLY:HA3	1:63:A:TRP:HE1	5	0.44	0.23	0.5
(2,302)	1:119:A:CYS:HA	1:120:A:ALA:H	5	0.37	0.14	0.41
(2,4)	1:46:A:ILE:HG23	1:46:A:ILE:H	5	0.37	0.06	0.36
(2,4)	1:46:A:ILE:HG22	1:46:A:ILE:H	5	0.37	0.06	0.36
(2,4)	1:46:A:ILE:HG21	1:46:A:ILE:H	5	0.37	0.06	0.36
(2,31)	1:59:A:ILE:HD12	1:71:A:CYS:H	5	0.36	0.12	0.32
(2,31)	1:59:A:ILE:HD11	1:71:A:CYS:H	5	0.36	0.12	0.32
(2,31)	1:59:A:ILE:HD13	1:71:A:CYS:H	5	0.36	0.12	0.32
(1,871)	1:30:A:ASP:HB2	1:32:A:SER:H	5	0.35	0.11	0.37
(1,871)	1:30:A:ASP:HB3	1:32:A:SER:H	5	0.35	0.11	0.37
(2,311)	1:90:A:PHE:HB3	1:91:A:THR:H	5	0.34	0.19	0.26
(2,311)	1:97:A:CYS:HB3	1:91:A:THR:H	5	0.34	0.19	0.26
(2,311)	1:97:A:CYS:HB2	1:91:A:THR:H	5	0.34	0.19	0.26
(2,311)	1:90:A:PHE:HB2	1:91:A:THR:H	5	0.34	0.19	0.26
(1,786)	1:71:A:CYS:H	1:76:A:ASP:H	5	0.3	0.15	0.21
(1,139)	1:109:A:ASP:H	1:109:A:ASP:HB2	5	0.29	0.09	0.3
(1,139)	1:109:A:ASP:H	1:109:A:ASP:HB3	5	0.29	0.09	0.3
(2,322)	1:69:A:ASN:HB3	1:71:A:CYS:H	5	0.28	0.13	0.26
(2,322)	1:70:A:ASP:HB2	1:71:A:CYS:H	5	0.28	0.13	0.26
(2,322)	1:69:A:ASN:HB2	1:71:A:CYS:H	5	0.28	0.13	0.26
(1,293)	1:8:A:PHE:HB2	1:9:A:VAL:H	5	0.25	0.08	0.29
(1,293)	1:8:A:PHE:HB3	1:9:A:VAL:H	5	0.25	0.08	0.29
(1,52)	1:76:A:ASP:H	1:77:A:GLU:H	5	0.23	0.08	0.27
(1,53)	1:77:A:GLU:H	1:76:A:ASP:H	5	0.23	0.08	0.27
(1,165)	1:104:A:CYS:H	1:116:A:GLU:HA	5	0.22	0.1	0.24
(1,379)	1:50:A:SER:H	1:50:A:SER:HA	5	0.22	0.06	0.23
(1,626)	1:71:A:CYS:HA	1:57:A:GLN:HE22	5	0.21	0.09	0.18
(1,639)	1:82:A:ASN:H	1:82:A:ASN:HD21	5	0.2	0.04	0.21
(2,104)	1:80:A:CYS:HB3	1:80:A:CYS:H	5	0.2	0.04	0.22
(1,433)	1:74:A:GLY:HA2	1:71:A:CYS:H	5	0.19	0.04	0.2
(1,433)	1:74:A:GLY:HA3	1:71:A:CYS:H	5	0.19	0.04	0.2
(1,468)	1:78:A:GLU:HG2	1:79:A:ASN:H	5	0.18	0.03	0.18
(1,468)	1:78:A:GLU:HG3	1:79:A:ASN:H	5	0.18	0.03	0.18
(1,816)	1:109:A:ASP:H	1:116:A:GLU:HG2	5	0.17	0.03	0.16
(1,816)	1:109:A:ASP:H	1:116:A:GLU:HG3	5	0.17	0.03	0.16
(1,84)	1:14:A:GLN:HG2	1:29:A:GLU:H	5	0.17	0.05	0.17
(1,84)	1:14:A:GLN:HG3	1:29:A:GLU:H	5	0.17	0.05	0.17
(2,301)	1:11:A:ASN:HD22	1:32:A:SER:H	5	0.16	0.03	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,716)	1:28:A:CYS:HB2	1:14:A:GLN:HE22	5	0.16	0.03	0.16
(1,716)	1:28:A:CYS:HB3	1:14:A:GLN:HE22	5	0.16	0.03	0.16
(1,707)	1:45:A:ARG:HD2	1:45:A:ARG:H	5	0.15	0.04	0.13
(1,707)	1:45:A:ARG:HD3	1:45:A:ARG:H	5	0.15	0.04	0.13
(1,709)	1:45:A:ARG:HD2	1:45:A:ARG:H	5	0.15	0.04	0.13
(1,709)	1:45:A:ARG:HD3	1:45:A:ARG:H	5	0.15	0.04	0.13
(1,439)	1:75:A:GLU:H	1:73:A:SER:H	5	0.15	0.01	0.14
(1,751)	1:52:A:GLY:H	1:57:A:GLN:HG2	5	0.15	0.04	0.12
(1,751)	1:52:A:GLY:H	1:57:A:GLN:HG3	5	0.15	0.04	0.12
(1,432)	1:70:A:ASP:HB2	1:70:A:ASP:H	5	0.15	0.04	0.13
(1,432)	1:70:A:ASP:HB3	1:70:A:ASP:H	5	0.15	0.04	0.13
(1,477)	1:9:A:VAL:HA	1:9:A:VAL:H	5	0.13	0.02	0.12
(1,717)	1:20:A:TRP:HE1	1:20:A:TRP:H	5	0.13	0.02	0.13
(1,512)	1:59:A:ILE:H	1:49:A:ILE:H	5	0.13	0.02	0.14
(1,574)	1:64:A:ARG:H	1:65:A:CYS:H	5	0.13	0.01	0.12
(2,115)	1:80:A:CYS:H	1:81:A:GLY:H	5	0.13	0.02	0.13
(1,329)	1:25:A:ASP:H	1:23:A:ASP:H	5	0.12	0.02	0.13
(1,121)	1:114:A:SER:HA	1:115:A:ASP:H	5	0.12	0.01	0.12
(2,122)	1:16:A:VAL:HA	1:16:A:VAL:H	5	0.11	0.01	0.11
(1,253)	1:83:A:ILE:HB	1:83:A:ILE:H	4	0.84	0.01	0.84
(2,294)	1:61:A:VAL:HG11	1:48:A:GLU:H	4	0.57	0.49	0.36
(2,294)	1:61:A:VAL:HG13	1:48:A:GLU:H	4	0.57	0.49	0.36
(2,166)	1:86:A:SER:HA	1:79:A:ASN:HD21	4	0.5	0.12	0.55
(1,119)	1:112:A:ASP:H	1:115:A:ASP:H	4	0.48	0.03	0.47
(2,72)	1:112:A:ASP:HB2	1:113:A:GLY:H	4	0.4	0.05	0.4
(2,72)	1:112:A:ASP:HB3	1:113:A:GLY:H	4	0.4	0.05	0.4
(2,72)	1:110:A:CYS:HB3	1:113:A:GLY:H	4	0.4	0.05	0.4
(2,90)	1:59:A:ILE:HD12	1:63:A:TRP:HE1	4	0.35	0.12	0.36
(2,90)	1:60:A:PRO:HB2	1:63:A:TRP:HE1	4	0.35	0.12	0.36
(2,90)	1:59:A:ILE:HD11	1:63:A:TRP:HE1	4	0.35	0.12	0.36
(1,582)	1:46:A:ILE:H	1:45:A:ARG:H	4	0.31	0.08	0.35
(2,135)	1:79:A:ASN:HB2	1:79:A:ASN:HD21	4	0.31	0.01	0.31
(1,777)	1:77:A:GLU:HB2	1:70:A:ASP:H	4	0.3	0.1	0.34
(1,777)	1:77:A:GLU:HB3	1:70:A:ASP:H	4	0.3	0.1	0.34
(1,690)	1:61:A:VAL:HG11	1:49:A:ILE:H	4	0.3	0.05	0.29
(1,690)	1:61:A:VAL:HG12	1:49:A:ILE:H	4	0.3	0.05	0.29
(1,690)	1:61:A:VAL:HG13	1:49:A:ILE:H	4	0.3	0.05	0.29
(1,690)	1:61:A:VAL:HG21	1:49:A:ILE:H	4	0.3	0.05	0.29
(1,690)	1:61:A:VAL:HG22	1:49:A:ILE:H	4	0.3	0.05	0.29
(1,690)	1:61:A:VAL:HG23	1:49:A:ILE:H	4	0.3	0.05	0.29
(1,136)	1:112:A:ASP:H	1:110:A:CYS:H	4	0.22	0.02	0.22
(1,549)	1:115:A:ASP:HA	1:104:A:CYS:H	4	0.22	0.06	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,2)	1:35:A:SER:HB2	1:35:A:SER:H	4	0.2	0.08	0.2
(2,2)	1:32:A:SER:HA	1:35:A:SER:H	4	0.2	0.08	0.2
(2,2)	1:32:A:SER:HB2	1:35:A:SER:H	4	0.2	0.08	0.2
(1,18)	1:81:A:GLY:H	1:82:A:ASN:H	4	0.2	0.07	0.18
(2,391)	1:17:A:PRO:HD2	1:16:A:VAL:H	4	0.2	0.05	0.2
(1,873)	1:34:A:GLU:HB2	1:33:A:ASP:H	4	0.19	0.06	0.19
(1,873)	1:34:A:GLU:HB3	1:33:A:ASP:H	4	0.19	0.06	0.19
(1,673)	1:17:A:PRO:HB2	1:20:A:TRP:HE1	4	0.19	0.07	0.2
(1,673)	1:17:A:PRO:HB3	1:20:A:TRP:HE1	4	0.19	0.07	0.2
(1,921)	1:8:A:PHE:HA	1:16:A:VAL:HG21	4	0.19	0.04	0.2
(1,921)	1:8:A:PHE:HA	1:16:A:VAL:HG22	4	0.19	0.04	0.2
(1,921)	1:8:A:PHE:HA	1:16:A:VAL:HG23	4	0.19	0.04	0.2
(1,674)	1:17:A:PRO:HG2	1:20:A:TRP:HE1	4	0.19	0.08	0.14
(1,674)	1:17:A:PRO:HG3	1:20:A:TRP:HE1	4	0.19	0.08	0.14
(1,926)	1:16:A:VAL:HG11	1:20:A:TRP:HZ3	4	0.18	0.06	0.18
(1,926)	1:16:A:VAL:HG12	1:20:A:TRP:HZ3	4	0.18	0.06	0.18
(1,926)	1:16:A:VAL:HG13	1:20:A:TRP:HZ3	4	0.18	0.06	0.18
(1,689)	1:69:A:ASN:HD21	1:69:A:ASN:H	4	0.18	0.04	0.18
(2,173)	1:69:A:ASN:HD21	1:69:A:ASN:H	4	0.18	0.04	0.18
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG11	4	0.16	0.04	0.16
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG12	4	0.16	0.04	0.16
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG13	4	0.16	0.04	0.16
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG21	4	0.16	0.04	0.16
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG22	4	0.16	0.04	0.16
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG23	4	0.16	0.04	0.16
(1,917)	1:28:A:CYS:H	1:14:A:GLN:HG2	4	0.16	0.03	0.16
(1,610)	1:14:A:GLN:HE22	1:29:A:GLU:H	4	0.16	0.02	0.16
(2,263)	1:63:A:TRP:HB2	1:63:A:TRP:H	4	0.16	0.04	0.15
(2,263)	1:62:A:SER:HB2	1:63:A:TRP:H	4	0.16	0.04	0.15
(1,367)	1:42:A:ARG:HG2	1:43:A:THR:H	4	0.16	0.04	0.16
(1,367)	1:42:A:ARG:HG2	1:43:A:THR:H	4	0.16	0.04	0.16
(1,367)	1:42:A:ARG:HG3	1:43:A:THR:H	4	0.16	0.04	0.16
(1,367)	1:42:A:ARG:HG3	1:43:A:THR:H	4	0.16	0.04	0.16
(1,126)	1:117:A:LEU:HD11	1:114:A:SER:H	4	0.15	0.02	0.14
(1,126)	1:117:A:LEU:HD12	1:114:A:SER:H	4	0.15	0.02	0.14
(1,126)	1:117:A:LEU:HD13	1:114:A:SER:H	4	0.15	0.02	0.14
(1,126)	1:117:A:LEU:HD21	1:114:A:SER:H	4	0.15	0.02	0.14
(1,126)	1:117:A:LEU:HD22	1:114:A:SER:H	4	0.15	0.02	0.14
(1,126)	1:117:A:LEU:HD23	1:114:A:SER:H	4	0.15	0.02	0.14
(1,143)	1:106:A:GLY:H	1:107:A:GLN:H	4	0.15	0.02	0.15
(2,362)	1:14:A:GLN:HB2	1:10:A:CYS:H	4	0.15	0.04	0.14
(2,362)	1:14:A:GLN:HB3	1:10:A:CYS:H	4	0.15	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)
(1,127)	1:114:A:SER:H	1:114:A:SER:HB2	4	0.15	0.01	0.15
(1,127)	1:114:A:SER:H	1:114:A:SER:HB3	4	0.15	0.01	0.15
(1,930)	1:102:A:PHE:HE2	1:107:A:GLN:HG2	4	0.15	0.02	0.15
(1,220)	1:92:A:CYS:HB2	1:95:A:GLY:H	4	0.14	0.05	0.12
(1,220)	1:92:A:CYS:HB3	1:95:A:GLY:H	4	0.14	0.05	0.12
(1,57)	1:66:A:ASP:H	1:67:A:GLY:H	4	0.14	0.01	0.14
(2,339)	1:9:A:VAL:HG11	1:13:A:GLY:H	4	0.14	0.01	0.14
(2,339)	1:9:A:VAL:HG12	1:13:A:GLY:H	4	0.14	0.01	0.14
(2,339)	1:9:A:VAL:HG13	1:13:A:GLY:H	4	0.14	0.01	0.14
(2,339)	1:9:A:VAL:HG21	1:13:A:GLY:H	4	0.14	0.01	0.14
(2,339)	1:9:A:VAL:HG22	1:13:A:GLY:H	4	0.14	0.01	0.14
(2,339)	1:9:A:VAL:HG23	1:13:A:GLY:H	4	0.14	0.01	0.14
(1,1)	1:112:A:ASP:H	1:113:A:GLY:H	4	0.14	0.01	0.14
(2,179)	1:9:A:VAL:HG11	1:10:A:CYS:H	4	0.13	0.01	0.14
(2,179)	1:9:A:VAL:HG12	1:10:A:CYS:H	4	0.13	0.01	0.14
(2,179)	1:9:A:VAL:HG13	1:10:A:CYS:H	4	0.13	0.01	0.14
(2,179)	1:9:A:VAL:HG21	1:10:A:CYS:H	4	0.13	0.01	0.14
(2,179)	1:9:A:VAL:HG22	1:10:A:CYS:H	4	0.13	0.01	0.14
(2,179)	1:9:A:VAL:HG23	1:10:A:CYS:H	4	0.13	0.01	0.14
(1,122)	1:115:A:ASP:HB2	1:115:A:ASP:H	4	0.13	0.02	0.12
(1,122)	1:115:A:ASP:HB3	1:115:A:ASP:H	4	0.13	0.02	0.12
(1,478)	1:9:A:VAL:HB	1:9:A:VAL:H	4	0.13	0.01	0.14
(1,547)	1:104:A:CYS:HB2	1:105:A:ASN:H	4	0.12	0.01	0.13
(1,547)	1:104:A:CYS:HB3	1:105:A:ASN:H	4	0.12	0.01	0.13
(1,247)	1:83:A:ILE:HA	1:84:A:THR:H	4	0.12	0.02	0.12
(1,387)	1:51:A:CYS:H	1:51:A:CYS:HB2	4	0.12	0.01	0.12
(1,387)	1:51:A:CYS:H	1:51:A:CYS:HB3	4	0.12	0.01	0.12
(2,61)	1:4:A:ALA:HA	1:5:A:GLU:H	4	0.12	0.01	0.12
(1,315)	1:15:A:CYS:H	1:15:A:CYS:HB2	4	0.11	0.01	0.11
(1,315)	1:15:A:CYS:H	1:15:A:CYS:HB3	4	0.11	0.01	0.11
(2,88)	1:78:A:GLU:HG2	1:79:A:ASN:HD21	3	0.91	0.06	0.89
(2,88)	1:78:A:GLU:HG3	1:79:A:ASN:HD21	3	0.91	0.06	0.89
(2,253)	1:86:A:SER:HB3	1:89:A:GLU:H	3	0.48	0.21	0.46
(2,253)	1:86:A:SER:HB2	1:89:A:GLU:H	3	0.48	0.21	0.46
(1,529)	1:59:A:ILE:HD11	1:70:A:ASP:H	3	0.46	0.06	0.43
(1,529)	1:59:A:ILE:HD12	1:70:A:ASP:H	3	0.46	0.06	0.43
(1,529)	1:59:A:ILE:HD13	1:70:A:ASP:H	3	0.46	0.06	0.43
(2,98)	1:28:A:CYS:HB3	1:11:A:ASN:H	3	0.38	0.17	0.48
(2,98)	1:32:A:SER:HB3	1:11:A:ASN:H	3	0.38	0.17	0.48
(1,878)	1:48:A:GLU:HB2	1:45:A:ARG:H	3	0.37	0.19	0.49
(1,878)	1:48:A:GLU:HB3	1:45:A:ARG:H	3	0.37	0.19	0.49
(2,20)	1:82:A:ASN:H	1:83:A:ILE:H	3	0.33	0.06	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,280)	1:5:A:GLU:HG2	1:6:A:SER:H	3	0.28	0.1	0.35
(1,280)	1:5:A:GLU:HG2	1:6:A:SER:H	3	0.28	0.1	0.35
(1,280)	1:5:A:GLU:HG3	1:6:A:SER:H	3	0.28	0.1	0.35
(1,280)	1:5:A:GLU:HG3	1:6:A:SER:H	3	0.28	0.1	0.35
(1,51)	1:78:A:GLU:H	1:77:A:GLU:H	3	0.27	0.02	0.26
(1,776)	1:77:A:GLU:HG2	1:70:A:ASP:H	3	0.26	0.14	0.21
(1,776)	1:77:A:GLU:HG3	1:70:A:ASP:H	3	0.26	0.14	0.21
(2,82)	1:94:A:SER:HB3	1:94:A:SER:H	3	0.25	0.06	0.27
(2,82)	1:94:A:SER:HB2	1:94:A:SER:H	3	0.25	0.06	0.27
(2,394)	1:86:A:SER:HB2	1:86:A:SER:H	3	0.24	0.05	0.24
(2,394)	1:86:A:SER:HB3	1:86:A:SER:H	3	0.24	0.05	0.24
(1,348)	1:30:A:ASP:HB2	1:31:A:GLY:H	3	0.23	0.1	0.17
(1,348)	1:30:A:ASP:HB3	1:31:A:GLY:H	3	0.23	0.1	0.17
(2,30)	1:14:A:GLN:H	1:10:A:CYS:H	3	0.2	0.07	0.18
(2,30)	1:9:A:VAL:H	1:10:A:CYS:H	3	0.2	0.07	0.18
(1,826)	1:114:A:SER:H	1:117:A:LEU:H	3	0.2	0.04	0.22
(1,479)	1:9:A:VAL:HG11	1:9:A:VAL:H	3	0.19	0.09	0.13
(1,479)	1:9:A:VAL:HG12	1:9:A:VAL:H	3	0.19	0.09	0.13
(1,479)	1:9:A:VAL:HG13	1:9:A:VAL:H	3	0.19	0.09	0.13
(1,479)	1:9:A:VAL:HG21	1:9:A:VAL:H	3	0.19	0.09	0.13
(1,479)	1:9:A:VAL:HG22	1:9:A:VAL:H	3	0.19	0.09	0.13
(1,479)	1:9:A:VAL:HG23	1:9:A:VAL:H	3	0.19	0.09	0.13
(1,694)	1:21:A:LYS:HE2	1:21:A:LYS:H	3	0.18	0.04	0.2
(1,694)	1:21:A:LYS:HE3	1:21:A:LYS:H	3	0.18	0.04	0.2
(4,6)	1:51:A:CYS:H	1:57:A:GLN:O	3	0.18	0.05	0.2
(1,91)	1:14:A:GLN:HG2	1:15:A:CYS:H	3	0.17	0.04	0.19
(1,91)	1:14:A:GLN:HG3	1:15:A:CYS:H	3	0.17	0.04	0.19
(1,915)	1:51:A:CYS:HA	1:71:A:CYS:H	3	0.17	0.05	0.16
(1,273)	1:7:A:ASP:HB2	1:4:A:ALA:H	3	0.16	0.03	0.14
(1,273)	1:7:A:ASP:HB3	1:4:A:ALA:H	3	0.16	0.03	0.14
(2,320)	1:59:A:ILE:HA	1:58:A:CYS:H	3	0.16	0.04	0.14
(1,130)	1:115:A:ASP:HB2	1:113:A:GLY:H	3	0.16	0.01	0.16
(1,130)	1:115:A:ASP:HB3	1:113:A:GLY:H	3	0.16	0.01	0.16
(1,470)	1:79:A:ASN:HB2	1:79:A:ASN:H	3	0.16	0.07	0.12
(1,470)	1:79:A:ASN:HB3	1:79:A:ASN:H	3	0.16	0.07	0.12
(2,112)	1:84:A:THR:HG1	1:84:A:THR:H	3	0.15	0.06	0.13
(1,12)	1:34:A:GLU:H	1:33:A:ASP:H	3	0.15	0.01	0.15
(1,875)	1:38:A:GLN:HE22	1:38:A:GLN:H	3	0.15	0.04	0.13
(1,63)	1:39:A:CYS:H	1:40:A:HIS:H	3	0.14	0.01	0.13
(1,377)	1:60:A:PRO:HA	1:49:A:ILE:H	3	0.14	0.02	0.13
(1,495)	1:31:A:GLY:H	1:29:A:GLU:H	3	0.13	0.02	0.13
(1,536)	1:89:A:GLU:HB2	1:86:A:SER:H	3	0.13	0.02	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,536)	1:89:A:GLU:HB3	1:86:A:SER:H	3	0.13	0.02	0.12
(1,601)	1:11:A:ASN:H	1:11:A:ASN:HD22	3	0.13	0.01	0.13
(1,719)	1:19:A:ARG:HH21	1:20:A:TRP:HE1	3	0.13	0.01	0.14
(3,10)	2:202:A:CA:CA	1:70:A:ASP:OD2	3	0.13	0.02	0.13
(1,67)	1:19:A:ARG:H	1:18:A:SER:H	3	0.12	0.01	0.12
(2,288)	1:75:A:GLU:HB2	1:75:A:GLU:H	3	0.12	0.02	0.11
(2,288)	1:75:A:GLU:HB3	1:75:A:GLU:H	3	0.12	0.02	0.11
(1,129)	1:114:A:SER:H	1:114:A:SER:HG	3	0.12	0.02	0.11
(1,631)	1:79:A:ASN:HD22	1:79:A:ASN:H	3	0.12	0.01	0.11
(2,385)	1:66:A:ASP:HA	1:68:A:GLU:H	3	0.12	0.0	0.12
(1,588)	1:12:A:ASN:HA	1:13:A:GLY:H	3	0.11	0.01	0.11
(2,338)	1:99:A:SER:H	1:98:A:ILE:H	3	0.11	0.0	0.11
(2,338)	1:97:A:CYS:H	1:98:A:ILE:H	3	0.11	0.0	0.11
(2,371)	1:83:A:ILE:HG21	1:83:A:ILE:H	2	0.62	0.14	0.62
(2,371)	1:83:A:ILE:HD13	1:83:A:ILE:H	2	0.62	0.14	0.62
(1,635)	1:78:A:GLU:HB2	1:79:A:ASN:HD21	2	0.43	0.08	0.43
(1,635)	1:78:A:GLU:HB2	1:79:A:ASN:HD21	2	0.43	0.08	0.43
(1,635)	1:78:A:GLU:HB3	1:79:A:ASN:HD21	2	0.43	0.08	0.43
(1,635)	1:78:A:GLU:HB3	1:79:A:ASN:HD21	2	0.43	0.08	0.43
(1,747)	1:57:A:GLN:HB2	1:51:A:CYS:H	2	0.4	0.05	0.4
(1,747)	1:57:A:GLN:HB2	1:51:A:CYS:H	2	0.4	0.05	0.4
(1,747)	1:57:A:GLN:HB3	1:51:A:CYS:H	2	0.4	0.05	0.4
(1,747)	1:57:A:GLN:HB3	1:51:A:CYS:H	2	0.4	0.05	0.4
(2,368)	1:87:A:PRO:HD2	1:88:A:ASP:H	2	0.32	0.1	0.32
(2,159)	1:39:A:CYS:HB3	1:43:A:THR:H	2	0.31	0.17	0.31
(2,159)	1:42:A:ARG:HD2	1:43:A:THR:H	2	0.31	0.17	0.31
(1,544)	1:110:A:CYS:H	1:108:A:ASP:HB2	2	0.3	0.0	0.3
(1,544)	1:110:A:CYS:H	1:108:A:ASP:HB2	2	0.3	0.0	0.3
(1,544)	1:110:A:CYS:H	1:108:A:ASP:HB3	2	0.3	0.0	0.3
(1,544)	1:110:A:CYS:H	1:108:A:ASP:HB3	2	0.3	0.0	0.3
(1,795)	1:91:A:THR:HG23	1:95:A:GLY:H	2	0.3	0.1	0.3
(1,54)	1:73:A:SER:H	1:74:A:GLY:H	2	0.29	0.05	0.29
(2,196)	1:56:A:THR:HA	1:42:A:ARG:H	2	0.28	0.11	0.28
(2,196)	1:40:A:HIS:HA	1:42:A:ARG:H	2	0.28	0.11	0.28
(1,565)	1:91:A:THR:HG1	1:91:A:THR:H	2	0.28	0.13	0.28
(1,565)	1:91:A:THR:HG22	1:91:A:THR:H	2	0.28	0.13	0.28
(2,357)	1:70:A:ASP:HA	1:69:A:ASN:HD21	2	0.24	0.03	0.24
(2,357)	1:69:A:ASN:HA	1:69:A:ASN:HD21	2	0.24	0.03	0.24
(1,737)	1:33:A:ASP:HB2	1:34:A:GLU:H	2	0.22	0.02	0.22
(1,737)	1:33:A:ASP:HB3	1:34:A:GLU:H	2	0.22	0.02	0.22
(1,70)	1:77:A:GLU:HB2	1:78:A:GLU:H	2	0.2	0.02	0.2
(1,70)	1:77:A:GLU:HB3	1:78:A:GLU:H	2	0.2	0.02	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,79)	1:61:A:VAL:HB	1:61:A:VAL:H	2	0.2	0.09	0.2
(1,460)	1:74:A:GLY:HA2	1:77:A:GLU:H	2	0.2	0.02	0.2
(1,460)	1:74:A:GLY:HA3	1:77:A:GLU:H	2	0.2	0.02	0.2
(1,438)	1:72:A:ASP:H	1:73:A:SER:H	2	0.18	0.02	0.18
(1,35)	1:115:A:ASP:H	1:116:A:GLU:H	2	0.18	0.02	0.18
(1,847)	1:13:A:GLY:H	1:10:A:CYS:H	2	0.18	0.08	0.18
(1,578)	1:52:A:GLY:H	1:50:A:SER:HB2	2	0.16	0.02	0.16
(1,578)	1:52:A:GLY:H	1:50:A:SER:HB3	2	0.16	0.02	0.16
(1,902)	1:94:A:SER:HB2	1:82:A:ASN:HD21	2	0.16	0.02	0.16
(1,902)	1:94:A:SER:HB3	1:82:A:ASN:HD21	2	0.16	0.02	0.16
(1,469)	1:78:A:GLU:HB2	1:79:A:ASN:H	2	0.16	0.01	0.16
(1,469)	1:78:A:GLU:HB2	1:79:A:ASN:H	2	0.16	0.01	0.16
(1,469)	1:78:A:GLU:HB3	1:79:A:ASN:H	2	0.16	0.01	0.16
(1,469)	1:78:A:GLU:HB3	1:79:A:ASN:H	2	0.16	0.01	0.16
(1,798)	1:85:A:CYS:HB2	1:97:A:CYS:H	2	0.15	0.02	0.15
(1,798)	1:85:A:CYS:HB3	1:97:A:CYS:H	2	0.15	0.02	0.15
(1,741)	1:9:A:VAL:HG11	1:38:A:GLN:HE21	2	0.14	0.02	0.14
(1,741)	1:9:A:VAL:HG12	1:38:A:GLN:HE21	2	0.14	0.02	0.14
(1,741)	1:9:A:VAL:HG13	1:38:A:GLN:HE21	2	0.14	0.02	0.14
(1,741)	1:9:A:VAL:HG21	1:38:A:GLN:HE21	2	0.14	0.02	0.14
(1,741)	1:9:A:VAL:HG22	1:38:A:GLN:HE21	2	0.14	0.02	0.14
(1,741)	1:9:A:VAL:HG23	1:38:A:GLN:HE21	2	0.14	0.02	0.14
(1,928)	1:102:A:PHE:HA	1:103:A:VAL:HG11	2	0.14	0.01	0.14
(1,928)	1:102:A:PHE:HA	1:103:A:VAL:HG12	2	0.14	0.01	0.14
(1,928)	1:102:A:PHE:HA	1:103:A:VAL:HG13	2	0.14	0.01	0.14
(2,285)	1:112:A:ASP:HB2	1:112:A:ASP:H	2	0.14	0.01	0.14
(1,442)	1:73:A:SER:HB2	1:73:A:SER:H	2	0.12	0.02	0.12
(1,442)	1:73:A:SER:HB3	1:73:A:SER:H	2	0.12	0.02	0.12
(1,682)	1:79:A:ASN:HD22	1:87:A:PRO:HD2	2	0.12	0.02	0.12
(1,682)	1:79:A:ASN:HD22	1:87:A:PRO:HD3	2	0.12	0.02	0.12
(1,931)	1:99:A:SER:HB2	1:102:A:PHE:HD1	2	0.12	0.02	0.12
(1,931)	1:99:A:SER:HB2	1:102:A:PHE:HD2	2	0.12	0.02	0.12
(1,931)	1:99:A:SER:HB3	1:102:A:PHE:HD1	2	0.12	0.02	0.12
(1,931)	1:99:A:SER:HB3	1:102:A:PHE:HD2	2	0.12	0.02	0.12
(1,861)	1:17:A:PRO:HD2	1:19:A:ARG:H	2	0.12	0.02	0.12
(1,861)	1:17:A:PRO:HD3	1:19:A:ARG:H	2	0.12	0.02	0.12
(1,600)	1:11:A:ASN:H	1:11:A:ASN:HD21	2	0.11	0.0	0.11
(1,602)	1:32:A:SER:HB2	1:11:A:ASN:HD21	2	0.11	0.01	0.11
(1,602)	1:32:A:SER:HB3	1:11:A:ASN:HD21	2	0.11	0.01	0.11
(1,652)	1:101:A:ASN:HD21	1:101:A:ASN:HB2	2	0.11	0.0	0.11
(1,652)	1:101:A:ASN:HD21	1:101:A:ASN:HB3	2	0.11	0.0	0.11
(2,111)	1:72:A:ASP:H	1:71:A:CYS:H	2	0.11	0.01	0.11

Continued on next page...

Continued from previous page...

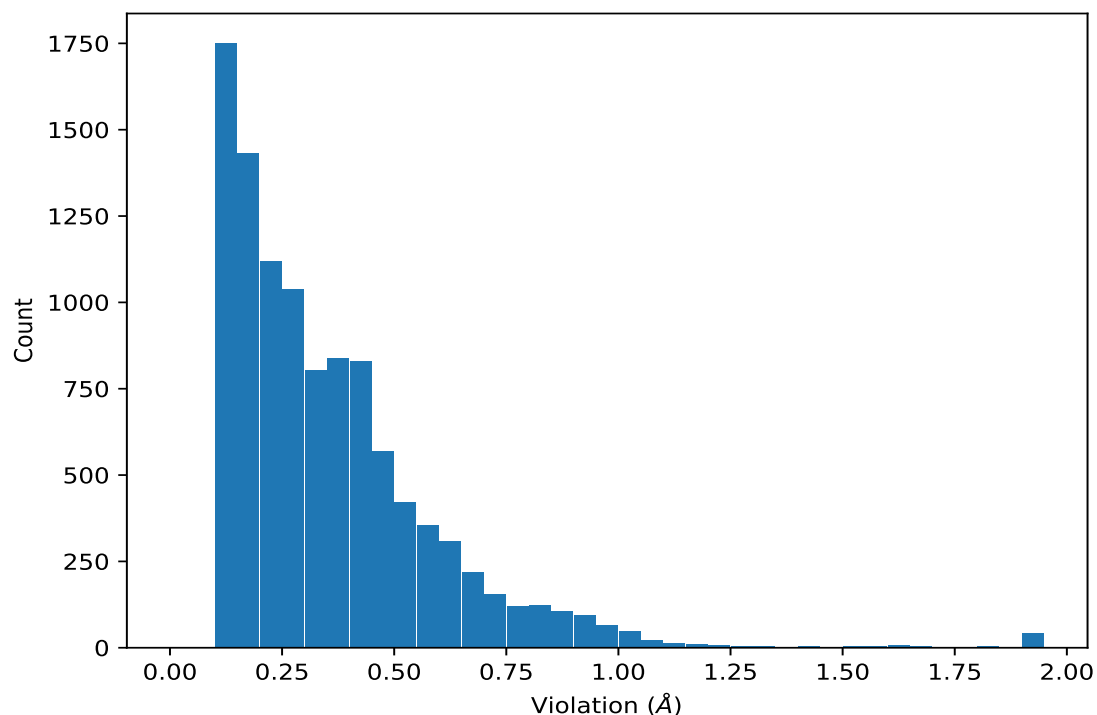
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,191)	1:54:A:HIS:H	1:55:A:SER:H	2	0.11	0.01	0.11
(2,287)	1:5:A:GLU:HB2	1:5:A:GLU:H	2	0.11	0.0	0.11
(2,287)	1:5:A:GLU:HB3	1:5:A:GLU:H	2	0.11	0.0	0.11
(3,11)	2:202:A:CA:CA	1:76:A:ASP:OD2	2	0.11	0.0	0.11
(1,108)	1:119:A:CYS:H	1:119:A:CYS:HB2	2	0.1	0.0	0.1
(1,108)	1:119:A:CYS:H	1:119:A:CYS:HB3	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)
(1,820)	1:110:A:CYS:H	1:115:A:ASP:H	13	1.95
(2,384)	1:5:A:GLU:HB2	1:5:A:GLU:HB3	1	1.94
(2,384)	1:5:A:GLU:HB3	1:5:A:GLU:HB2	1	1.94
(2,384)	1:5:A:GLU:HB2	1:5:A:GLU:HB3	2	1.94
(2,384)	1:5:A:GLU:HB3	1:5:A:GLU:HB2	2	1.94
(2,384)	1:5:A:GLU:HB2	1:5:A:GLU:HB3	3	1.94
(2,384)	1:5:A:GLU:HB3	1:5:A:GLU:HB2	3	1.94
(2,384)	1:5:A:GLU:HB2	1:5:A:GLU:HB3	4	1.94
(2,384)	1:5:A:GLU:HB3	1:5:A:GLU:HB2	4	1.94
(2,384)	1:5:A:GLU:HB2	1:5:A:GLU:HB3	5	1.94
(2,384)	1:5:A:GLU:HB3	1:5:A:GLU:HB2	5	1.94
(2,384)	1:5:A:GLU:HB2	1:5:A:GLU:HB3	6	1.94
(2,384)	1:5:A:GLU:HB3	1:5:A:GLU:HB2	6	1.94
(2,384)	1:5:A:GLU:HB2	1:5:A:GLU:HB3	7	1.94
(2,384)	1:5:A:GLU:HB3	1:5:A:GLU:HB2	7	1.94
(2,384)	1:5:A:GLU:HB2	1:5:A:GLU:HB3	8	1.94
(2,384)	1:5:A:GLU:HB3	1:5:A:GLU:HB2	8	1.94
(2,384)	1:5:A:GLU:HB2	1:5:A:GLU:HB3	9	1.94
(2,384)	1:5:A:GLU:HB3	1:5:A:GLU:HB2	9	1.94
(2,384)	1:5:A:GLU:HB2	1:5:A:GLU:HB3	10	1.94
(2,384)	1:5:A:GLU:HB3	1:5:A:GLU:HB2	10	1.94
(2,384)	1:5:A:GLU:HB2	1:5:A:GLU:HB3	11	1.94
(2,384)	1:5:A:GLU:HB3	1:5:A:GLU:HB2	11	1.94
(2,384)	1:5:A:GLU:HB2	1:5:A:GLU:HB3	12	1.94
(2,384)	1:5:A:GLU:HB3	1:5:A:GLU:HB2	12	1.94
(2,384)	1:5:A:GLU:HB2	1:5:A:GLU:HB3	13	1.94
(2,384)	1:5:A:GLU:HB3	1:5:A:GLU:HB2	13	1.94
(2,384)	1:5:A:GLU:HB2	1:5:A:GLU:HB3	14	1.94
(2,384)	1:5:A:GLU:HB3	1:5:A:GLU:HB2	14	1.94
(2,384)	1:5:A:GLU:HB2	1:5:A:GLU:HB3	15	1.94
(2,384)	1:5:A:GLU:HB3	1:5:A:GLU:HB2	15	1.94
(2,384)	1:5:A:GLU:HB2	1:5:A:GLU:HB3	16	1.94
(2,384)	1:5:A:GLU:HB3	1:5:A:GLU:HB2	16	1.94
(2,384)	1:5:A:GLU:HB2	1:5:A:GLU:HB3	17	1.94
(2,384)	1:5:A:GLU:HB3	1:5:A:GLU:HB2	17	1.94
(2,384)	1:5:A:GLU:HB2	1:5:A:GLU:HB3	18	1.94
(2,384)	1:5:A:GLU:HB3	1:5:A:GLU:HB2	18	1.94
(2,384)	1:5:A:GLU:HB2	1:5:A:GLU:HB3	19	1.94
(2,384)	1:5:A:GLU:HB3	1:5:A:GLU:HB2	19	1.94
(2,384)	1:5:A:GLU:HB2	1:5:A:GLU:HB3	20	1.94
(2,384)	1:5:A:GLU:HB3	1:5:A:GLU:HB2	20	1.94
(1,820)	1:110:A:CYS:H	1:115:A:ASP:H	11	1.91
(1,820)	1:110:A:CYS:H	1:115:A:ASP:H	14	1.88

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,820)	1:110:A:CYS:H	1:115:A:ASP:H	9	1.82
(1,820)	1:110:A:CYS:H	1:115:A:ASP:H	12	1.82
(1,820)	1:110:A:CYS:H	1:115:A:ASP:H	18	1.81
(1,820)	1:110:A:CYS:H	1:115:A:ASP:H	20	1.81
(1,820)	1:110:A:CYS:H	1:115:A:ASP:H	16	1.8
(1,820)	1:110:A:CYS:H	1:115:A:ASP:H	15	1.73
(1,819)	1:112:A:ASP:HB2	1:115:A:ASP:H	17	1.67
(1,819)	1:112:A:ASP:HB3	1:115:A:ASP:H	17	1.67
(1,740)	1:35:A:SER:H	1:56:A:THR:HG22	3	1.65
(1,819)	1:112:A:ASP:HB2	1:115:A:ASP:H	5	1.63
(1,819)	1:112:A:ASP:HB3	1:115:A:ASP:H	5	1.63
(1,819)	1:112:A:ASP:HB2	1:115:A:ASP:H	2	1.61
(1,819)	1:112:A:ASP:HB3	1:115:A:ASP:H	2	1.61
(1,819)	1:112:A:ASP:HB2	1:115:A:ASP:H	19	1.6
(1,819)	1:112:A:ASP:HB3	1:115:A:ASP:H	19	1.6
(1,819)	1:112:A:ASP:HB2	1:115:A:ASP:H	8	1.58
(1,819)	1:112:A:ASP:HB3	1:115:A:ASP:H	8	1.58
(1,819)	1:112:A:ASP:HB2	1:115:A:ASP:H	1	1.55
(1,819)	1:112:A:ASP:HB3	1:115:A:ASP:H	1	1.55
(1,740)	1:35:A:SER:H	1:56:A:THR:HG22	17	1.53
(1,819)	1:112:A:ASP:HB2	1:115:A:ASP:H	10	1.52
(1,819)	1:112:A:ASP:HB3	1:115:A:ASP:H	10	1.52
(1,740)	1:35:A:SER:H	1:56:A:THR:HG22	19	1.49
(1,740)	1:35:A:SER:H	1:56:A:THR:HG21	12	1.47
(1,740)	1:35:A:SER:H	1:56:A:THR:HG23	11	1.44
(2,145)	1:56:A:THR:HB	1:58:A:CYS:H	10	1.43
(2,294)	1:61:A:VAL:HG13	1:48:A:GLU:H	12	1.4
(1,740)	1:35:A:SER:H	1:56:A:THR:HG22	9	1.4
(1,740)	1:35:A:SER:H	1:56:A:THR:HG21	5	1.38
(1,740)	1:35:A:SER:H	1:56:A:THR:HG22	1	1.36
(2,361)	1:61:A:VAL:HG23	1:64:A:ARG:H	7	1.32
(2,39)	1:117:A:LEU:HD11	1:115:A:ASP:H	10	1.31
(2,145)	1:43:A:THR:HA	1:58:A:CYS:H	8	1.3
(2,193)	1:98:A:ILE:HD12	1:109:A:ASP:H	16	1.28
(1,459)	1:70:A:ASP:HA	1:76:A:ASP:H	7	1.27
(1,740)	1:35:A:SER:H	1:56:A:THR:HG22	13	1.25
(1,740)	1:35:A:SER:H	1:56:A:THR:HG23	16	1.25
(2,361)	1:61:A:VAL:HG21	1:64:A:ARG:H	8	1.24
(2,145)	1:43:A:THR:HA	1:58:A:CYS:H	2	1.24
(2,145)	1:43:A:THR:HA	1:58:A:CYS:H	20	1.22
(2,375)	1:60:A:PRO:HD3	1:61:A:VAL:H	5	1.21
(2,193)	1:98:A:ILE:HD11	1:109:A:ASP:H	19	1.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,145)	1:43:A:THR:HA	1:58:A:CYS:H	6	1.21
(2,361)	1:61:A:VAL:HG22	1:64:A:ARG:H	11	1.19
(1,740)	1:35:A:SER:H	1:56:A:THR:HG23	7	1.19
(2,193)	1:98:A:ILE:HD11	1:109:A:ASP:H	9	1.18
(2,145)	1:43:A:THR:HA	1:58:A:CYS:H	7	1.18
(2,145)	1:43:A:THR:HA	1:58:A:CYS:H	1	1.17
(2,375)	1:48:A:GLU:HB3	1:61:A:VAL:H	11	1.16
(2,375)	1:60:A:PRO:HD3	1:61:A:VAL:H	17	1.16
(2,145)	1:43:A:THR:HA	1:58:A:CYS:H	9	1.16
(2,145)	1:43:A:THR:HA	1:58:A:CYS:H	17	1.16
(2,361)	1:61:A:VAL:HG21	1:64:A:ARG:H	9	1.15
(2,361)	1:61:A:VAL:HG21	1:64:A:ARG:H	5	1.14
(2,193)	1:98:A:ILE:HD12	1:109:A:ASP:H	7	1.13
(2,145)	1:43:A:THR:HA	1:58:A:CYS:H	13	1.13
(1,740)	1:35:A:SER:H	1:56:A:THR:HG22	18	1.13
(2,39)	1:117:A:LEU:HD11	1:115:A:ASP:H	6	1.12
(1,740)	1:35:A:SER:H	1:56:A:THR:HG23	2	1.12
(1,459)	1:70:A:ASP:HA	1:76:A:ASP:H	17	1.12
(2,375)	1:60:A:PRO:HD3	1:61:A:VAL:H	1	1.11
(2,145)	1:43:A:THR:HA	1:58:A:CYS:H	4	1.11
(1,740)	1:35:A:SER:H	1:56:A:THR:HG21	4	1.11
(2,359)	1:98:A:ILE:HD11	1:98:A:ILE:H	17	1.1
(2,145)	1:43:A:THR:HA	1:58:A:CYS:H	16	1.1
(1,740)	1:35:A:SER:H	1:56:A:THR:HG21	14	1.1
(2,361)	1:59:A:ILE:HD11	1:64:A:ARG:H	6	1.09
(2,145)	1:43:A:THR:HA	1:58:A:CYS:H	5	1.09
(2,145)	1:43:A:THR:HA	1:58:A:CYS:H	15	1.09
(2,63)	1:82:A:ASN:HA	1:83:A:ILE:H	8	1.09
(2,359)	1:98:A:ILE:HD11	1:98:A:ILE:H	1	1.08
(2,193)	1:117:A:LEU:HD12	1:109:A:ASP:H	15	1.08
(2,145)	1:43:A:THR:HA	1:58:A:CYS:H	19	1.08
(2,359)	1:98:A:ILE:HD11	1:98:A:ILE:H	5	1.07
(2,262)	1:71:A:CYS:HB2	1:74:A:GLY:H	6	1.07
(2,193)	1:98:A:ILE:HD12	1:109:A:ASP:H	5	1.07
(2,63)	1:82:A:ASN:HA	1:83:A:ILE:H	16	1.07
(2,359)	1:98:A:ILE:HD12	1:98:A:ILE:H	6	1.06
(2,145)	1:43:A:THR:HA	1:58:A:CYS:H	3	1.06
(2,63)	1:82:A:ASN:HA	1:83:A:ILE:H	4	1.06
(2,63)	1:82:A:ASN:HA	1:83:A:ILE:H	10	1.06
(2,39)	1:117:A:LEU:HD11	1:115:A:ASP:H	19	1.06
(2,375)	1:60:A:PRO:HD3	1:61:A:VAL:H	14	1.05
(2,375)	1:48:A:GLU:HB3	1:61:A:VAL:H	16	1.05

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,264)	1:49:A:ILE:HB	1:50:A:SER:H	4	1.05
(2,264)	1:49:A:ILE:HB	1:50:A:SER:H	12	1.05
(2,63)	1:82:A:ASN:HA	1:83:A:ILE:H	12	1.05
(2,39)	1:117:A:LEU:HD23	1:115:A:ASP:H	9	1.05
(1,898)	1:57:A:GLN:HE22	1:71:A:CYS:H	17	1.05
(2,375)	1:48:A:GLU:HB3	1:61:A:VAL:H	10	1.04
(2,375)	1:48:A:GLU:HB3	1:61:A:VAL:H	20	1.04
(1,713)	1:14:A:GLN:HA	1:12:A:ASN:H	13	1.04
(2,375)	1:48:A:GLU:HB3	1:61:A:VAL:H	13	1.03
(2,63)	1:82:A:ASN:HA	1:83:A:ILE:H	2	1.03
(2,63)	1:82:A:ASN:HA	1:83:A:ILE:H	6	1.03
(2,63)	1:82:A:ASN:HA	1:83:A:ILE:H	15	1.03
(2,63)	1:82:A:ASN:HA	1:83:A:ILE:H	18	1.03
(2,63)	1:82:A:ASN:HA	1:83:A:ILE:H	20	1.03
(2,39)	1:117:A:LEU:HD22	1:115:A:ASP:H	17	1.03
(1,713)	1:14:A:GLN:HA	1:12:A:ASN:H	11	1.03
(1,713)	1:14:A:GLN:HA	1:12:A:ASN:H	16	1.03
(1,713)	1:14:A:GLN:HA	1:12:A:ASN:H	20	1.03
(2,375)	1:48:A:GLU:HB3	1:61:A:VAL:H	12	1.02
(2,375)	1:48:A:GLU:HB3	1:61:A:VAL:H	18	1.02
(2,359)	1:98:A:ILE:HD11	1:98:A:ILE:H	19	1.02
(2,304)	1:11:A:ASN:HD21	1:12:A:ASN:H	17	1.02
(2,193)	1:98:A:ILE:HD11	1:109:A:ASP:H	4	1.02
(2,193)	1:98:A:ILE:HD11	1:109:A:ASP:H	8	1.02
(2,63)	1:82:A:ASN:HA	1:83:A:ILE:H	3	1.02
(2,63)	1:82:A:ASN:HA	1:83:A:ILE:H	14	1.02
(1,447)	1:71:A:CYS:HA	1:74:A:GLY:H	8	1.02
(1,4)	1:55:A:SER:H	1:54:A:HIS:H	1	1.02
(2,359)	1:98:A:ILE:HD12	1:98:A:ILE:H	4	1.01
(2,359)	1:98:A:ILE:HD11	1:98:A:ILE:H	8	1.01
(2,63)	1:82:A:ASN:HA	1:83:A:ILE:H	11	1.01
(1,819)	1:112:A:ASP:HB2	1:115:A:ASP:H	4	1.01
(1,819)	1:112:A:ASP:HB3	1:115:A:ASP:H	4	1.01
(1,819)	1:112:A:ASP:HB2	1:115:A:ASP:H	6	1.01
(1,819)	1:112:A:ASP:HB3	1:115:A:ASP:H	6	1.01
(1,819)	1:112:A:ASP:HB2	1:115:A:ASP:H	7	1.01
(1,819)	1:112:A:ASP:HB3	1:115:A:ASP:H	7	1.01
(1,740)	1:35:A:SER:H	1:56:A:THR:HG22	6	1.01
(1,688)	1:69:A:ASN:H	1:69:A:ASN:HD22	1	1.01
(2,375)	1:48:A:GLU:HB3	1:61:A:VAL:H	8	1.0
(2,361)	1:61:A:VAL:HG23	1:64:A:ARG:H	20	1.0
(2,337)	1:53:A:ALA:HB2	1:55:A:SER:H	2	1.0

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,327)	1:68:A:GLU:HG2	1:71:A:CYS:H	8	1.0
(2,327)	1:68:A:GLU:HG2	1:71:A:CYS:H	19	1.0
(2,39)	1:117:A:LEU:HD11	1:115:A:ASP:H	8	1.0
(1,740)	1:35:A:SER:H	1:56:A:THR:HG21	10	1.0
(1,713)	1:14:A:GLN:HA	1:12:A:ASN:H	7	1.0
(1,459)	1:70:A:ASP:HA	1:76:A:ASP:H	20	1.0
(1,97)	1:98:A:ILE:HD11	1:99:A:SER:H	9	1.0
(1,97)	1:98:A:ILE:HD12	1:99:A:SER:H	9	1.0
(1,97)	1:98:A:ILE:HD13	1:99:A:SER:H	9	1.0
(1,4)	1:55:A:SER:H	1:54:A:HIS:H	18	1.0
(2,327)	1:64:A:ARG:HG2	1:71:A:CYS:H	6	0.99
(2,264)	1:49:A:ILE:HB	1:50:A:SER:H	18	0.99
(2,244)	1:45:A:ARG:HA	1:47:A:HIS:H	17	0.99
(2,145)	1:43:A:THR:HA	1:58:A:CYS:H	18	0.99
(2,88)	1:78:A:GLU:HG2	1:79:A:ASN:HD21	15	0.99
(2,63)	1:82:A:ASN:HA	1:83:A:ILE:H	1	0.99
(2,63)	1:82:A:ASN:HA	1:83:A:ILE:H	5	0.99
(2,63)	1:82:A:ASN:HA	1:83:A:ILE:H	7	0.99
(2,63)	1:82:A:ASN:HA	1:83:A:ILE:H	9	0.99
(2,63)	1:82:A:ASN:HA	1:83:A:ILE:H	13	0.99
(2,63)	1:82:A:ASN:HA	1:83:A:ILE:H	17	0.99
(2,63)	1:82:A:ASN:HA	1:83:A:ILE:H	19	0.99
(1,713)	1:14:A:GLN:HA	1:12:A:ASN:H	12	0.99
(1,688)	1:69:A:ASN:H	1:69:A:ASN:HD22	10	0.99
(1,97)	1:98:A:ILE:HD11	1:99:A:SER:H	16	0.99
(1,97)	1:98:A:ILE:HD12	1:99:A:SER:H	16	0.99
(1,97)	1:98:A:ILE:HD13	1:99:A:SER:H	16	0.99
(2,375)	1:48:A:GLU:HB3	1:61:A:VAL:H	6	0.98
(2,296)	1:113:A:GLY:HA2	1:117:A:LEU:H	4	0.98
(2,296)	1:113:A:GLY:HA2	1:117:A:LEU:H	7	0.98
(2,145)	1:43:A:THR:HA	1:58:A:CYS:H	12	0.98
(2,145)	1:43:A:THR:HA	1:58:A:CYS:H	14	0.98
(1,909)	1:43:A:THR:HG22	1:46:A:ILE:H	3	0.98
(1,877)	1:22:A:CYS:HA	1:44:A:CYS:H	12	0.98
(1,688)	1:69:A:ASN:H	1:69:A:ASN:HD22	5	0.98
(1,688)	1:69:A:ASN:H	1:69:A:ASN:HD22	9	0.98
(1,688)	1:69:A:ASN:H	1:69:A:ASN:HD22	16	0.98
(1,4)	1:55:A:SER:H	1:54:A:HIS:H	5	0.98
(2,359)	1:98:A:ILE:HD13	1:98:A:ILE:H	7	0.97
(2,178)	1:59:A:ILE:HG23	1:57:A:GLN:HE22	10	0.97
(2,145)	1:43:A:THR:HA	1:58:A:CYS:H	11	0.97
(1,819)	1:112:A:ASP:HB2	1:115:A:ASP:H	3	0.97

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,819)	1:112:A:ASP:HB3	1:115:A:ASP:H	3	0.97
(1,740)	1:35:A:SER:H	1:56:A:THR:HG21	20	0.97
(1,688)	1:69:A:ASN:H	1:69:A:ASN:HD22	3	0.97
(1,688)	1:69:A:ASN:H	1:69:A:ASN:HD22	11	0.97
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	20	0.97
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	20	0.97
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	20	0.97
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	20	0.97
(1,4)	1:55:A:SER:H	1:54:A:HIS:H	14	0.97
(1,4)	1:55:A:SER:H	1:54:A:HIS:H	15	0.97
(2,304)	1:11:A:ASN:HD21	1:12:A:ASN:H	1	0.96
(2,200)	1:87:A:PRO:HG3	1:76:A:ASP:H	17	0.96
(1,909)	1:43:A:THR:HG22	1:46:A:ILE:H	19	0.96
(1,687)	1:69:A:ASN:HD21	1:74:A:GLY:H	19	0.96
(1,463)	1:71:A:CYS:HB2	1:78:A:GLU:H	8	0.96
(1,463)	1:71:A:CYS:HB3	1:78:A:GLU:H	8	0.96
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	14	0.96
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	14	0.96
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	14	0.96
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	14	0.96
(2,281)	1:11:A:ASN:HA	1:11:A:ASN:HD22	12	0.95
(1,923)	1:8:A:PHE:HB2	1:16:A:VAL:HA	5	0.95
(1,877)	1:22:A:CYS:HA	1:44:A:CYS:H	8	0.95
(1,877)	1:22:A:CYS:HA	1:44:A:CYS:H	20	0.95
(1,713)	1:14:A:GLN:HA	1:12:A:ASN:H	8	0.95
(1,713)	1:14:A:GLN:HA	1:12:A:ASN:H	18	0.95
(1,688)	1:69:A:ASN:H	1:69:A:ASN:HD22	7	0.95
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	7	0.95
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	7	0.95
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	7	0.95
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	7	0.95
(1,447)	1:71:A:CYS:HA	1:74:A:GLY:H	10	0.95
(1,4)	1:55:A:SER:H	1:54:A:HIS:H	12	0.95
(1,4)	1:55:A:SER:H	1:54:A:HIS:H	13	0.95
(2,361)	1:61:A:VAL:HG21	1:64:A:ARG:H	12	0.94
(2,304)	1:11:A:ASN:HD21	1:12:A:ASN:H	2	0.94
(2,244)	1:45:A:ARG:HA	1:47:A:HIS:H	16	0.94
(2,207)	1:79:A:ASN:HB2	1:79:A:ASN:HD22	16	0.94
(2,207)	1:79:A:ASN:HB2	1:79:A:ASN:HD22	20	0.94
(2,193)	1:98:A:ILE:HD11	1:109:A:ASP:H	6	0.94
(1,898)	1:57:A:GLN:HE22	1:71:A:CYS:H	13	0.94
(1,740)	1:35:A:SER:H	1:56:A:THR:HG21	15	0.94

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,713)	1:14:A:GLN:HA	1:12:A:ASN:H	3	0.94
(1,713)	1:14:A:GLN:HA	1:12:A:ASN:H	4	0.94
(1,688)	1:69:A:ASN:H	1:69:A:ASN:HD22	13	0.94
(1,688)	1:69:A:ASN:H	1:69:A:ASN:HD22	20	0.94
(1,543)	1:112:A:ASP:HB2	1:114:A:SER:H	3	0.94
(1,543)	1:112:A:ASP:HB3	1:114:A:SER:H	3	0.94
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	4	0.94
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	4	0.94
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	4	0.94
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	4	0.94
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	8	0.94
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	8	0.94
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	8	0.94
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	8	0.94
(1,191)	1:100:A:ARG:HA	1:101:A:ASN:H	16	0.94
(1,4)	1:55:A:SER:H	1:54:A:HIS:H	10	0.94
(1,4)	1:55:A:SER:H	1:54:A:HIS:H	11	0.94
(2,375)	1:48:A:GLU:HB3	1:61:A:VAL:H	9	0.93
(2,337)	1:53:A:ALA:HB3	1:55:A:SER:H	1	0.93
(2,337)	1:53:A:ALA:HB2	1:55:A:SER:H	15	0.93
(2,207)	1:79:A:ASN:HB2	1:79:A:ASN:HD22	8	0.93
(2,207)	1:79:A:ASN:HB2	1:79:A:ASN:HD22	19	0.93
(1,713)	1:14:A:GLN:HA	1:12:A:ASN:H	1	0.93
(1,713)	1:14:A:GLN:HA	1:12:A:ASN:H	9	0.93
(1,543)	1:112:A:ASP:HB2	1:114:A:SER:H	4	0.93
(1,543)	1:112:A:ASP:HB3	1:114:A:SER:H	4	0.93
(1,459)	1:70:A:ASP:HA	1:76:A:ASP:H	2	0.93
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	10	0.93
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	10	0.93
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	10	0.93
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	10	0.93
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	11	0.93
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	11	0.93
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	11	0.93
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	11	0.93
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	17	0.93
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	17	0.93
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	17	0.93
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	17	0.93
(1,4)	1:55:A:SER:H	1:54:A:HIS:H	4	0.93
(1,4)	1:55:A:SER:H	1:54:A:HIS:H	16	0.93
(2,359)	1:98:A:ILE:HD12	1:98:A:ILE:H	10	0.92

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,337)	1:53:A:ALA:HB2	1:55:A:SER:H	18	0.92
(1,898)	1:57:A:GLN:HE22	1:71:A:CYS:H	7	0.92
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG12	1	0.92
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG13	1	0.92
(1,713)	1:14:A:GLN:HA	1:12:A:ASN:H	2	0.92
(1,713)	1:14:A:GLN:HA	1:12:A:ASN:H	19	0.92
(1,459)	1:70:A:ASP:HA	1:76:A:ASP:H	5	0.92
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	3	0.92
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	3	0.92
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	3	0.92
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	3	0.92
(1,437)	1:72:A:ASP:H	1:71:A:CYS:H	18	0.92
(1,4)	1:55:A:SER:H	1:54:A:HIS:H	7	0.92
(2,375)	1:48:A:GLU:HB3	1:61:A:VAL:H	15	0.91
(2,281)	1:11:A:ASN:HA	1:11:A:ASN:HD22	8	0.91
(1,909)	1:43:A:THR:HG21	1:46:A:ILE:H	8	0.91
(1,877)	1:22:A:CYS:HA	1:44:A:CYS:H	9	0.91
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG12	20	0.91
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG13	20	0.91
(1,713)	1:14:A:GLN:HA	1:12:A:ASN:H	6	0.91
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	18	0.91
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	18	0.91
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	18	0.91
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	18	0.91
(1,97)	1:98:A:ILE:HD11	1:99:A:SER:H	20	0.91
(1,97)	1:98:A:ILE:HD12	1:99:A:SER:H	20	0.91
(1,97)	1:98:A:ILE:HD13	1:99:A:SER:H	20	0.91
(1,4)	1:55:A:SER:H	1:54:A:HIS:H	9	0.91
(2,375)	1:60:A:PRO:HD3	1:61:A:VAL:H	4	0.9
(2,375)	1:48:A:GLU:HB3	1:61:A:VAL:H	7	0.9
(2,281)	1:11:A:ASN:HA	1:11:A:ASN:HD22	4	0.9
(2,264)	1:49:A:ILE:HB	1:50:A:SER:H	15	0.9
(2,193)	1:117:A:LEU:HD13	1:109:A:ASP:H	20	0.9
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG12	17	0.9
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG13	17	0.9
(1,543)	1:112:A:ASP:HB2	1:114:A:SER:H	7	0.9
(1,543)	1:112:A:ASP:HB3	1:114:A:SER:H	7	0.9
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	12	0.9
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	12	0.9
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	12	0.9
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	12	0.9
(1,437)	1:72:A:ASP:H	1:71:A:CYS:H	14	0.9

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,191)	1:100:A:ARG:HA	1:101:A:ASN:H	3	0.9
(2,361)	1:61:A:VAL:HG23	1:64:A:ARG:H	13	0.89
(2,337)	1:53:A:ALA:HB3	1:55:A:SER:H	4	0.89
(2,337)	1:53:A:ALA:HB1	1:55:A:SER:H	14	0.89
(2,296)	1:113:A:GLY:HA2	1:117:A:LEU:H	6	0.89
(2,276)	1:43:A:THR:HA	1:57:A:GLN:H	12	0.89
(2,264)	1:49:A:ILE:HB	1:50:A:SER:H	10	0.89
(2,257)	1:33:A:ASP:HA	1:38:A:GLN:HE22	6	0.89
(2,200)	1:77:A:GLU:HG3	1:76:A:ASP:H	10	0.89
(2,193)	1:117:A:LEU:HD11	1:109:A:ASP:H	13	0.89
(2,88)	1:78:A:GLU:HG2	1:79:A:ASN:HD21	17	0.89
(1,909)	1:43:A:THR:HG22	1:46:A:ILE:H	10	0.89
(1,909)	1:43:A:THR:HG21	1:46:A:ILE:H	14	0.89
(1,713)	1:14:A:GLN:HA	1:12:A:ASN:H	14	0.89
(1,688)	1:69:A:ASN:H	1:69:A:ASN:HD22	4	0.89
(1,543)	1:112:A:ASP:HB2	1:114:A:SER:H	6	0.89
(1,543)	1:112:A:ASP:HB3	1:114:A:SER:H	6	0.89
(1,459)	1:70:A:ASP:HA	1:76:A:ASP:H	16	0.89
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	9	0.89
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	9	0.89
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	9	0.89
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	9	0.89
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	19	0.89
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	19	0.89
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	19	0.89
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	19	0.89
(1,4)	1:55:A:SER:H	1:54:A:HIS:H	2	0.89
(1,4)	1:55:A:SER:H	1:54:A:HIS:H	6	0.89
(1,4)	1:55:A:SER:H	1:54:A:HIS:H	17	0.89
(2,337)	1:53:A:ALA:HB2	1:55:A:SER:H	7	0.88
(2,327)	1:68:A:GLU:HG2	1:71:A:CYS:H	12	0.88
(2,200)	1:87:A:PRO:HG3	1:76:A:ASP:H	15	0.88
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG12	3	0.88
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG13	3	0.88
(1,740)	1:35:A:SER:H	1:56:A:THR:HG23	8	0.88
(1,713)	1:14:A:GLN:HA	1:12:A:ASN:H	10	0.88
(1,687)	1:69:A:ASN:HD21	1:74:A:GLY:H	12	0.88
(1,459)	1:70:A:ASP:HA	1:76:A:ASP:H	19	0.88
(1,447)	1:71:A:CYS:HA	1:74:A:GLY:H	15	0.88
(1,437)	1:72:A:ASP:H	1:71:A:CYS:H	10	0.88
(1,191)	1:100:A:ARG:HA	1:101:A:ASN:H	10	0.88
(1,191)	1:100:A:ARG:HA	1:101:A:ASN:H	20	0.88

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:55:A:SER:H	1:54:A:HIS:H	19	0.88
(2,337)	1:53:A:ALA:HB1	1:55:A:SER:H	5	0.87
(2,244)	1:60:A:PRO:HA	1:47:A:HIS:H	1	0.87
(2,193)	1:98:A:ILE:HD11	1:109:A:ASP:H	1	0.87
(2,193)	1:98:A:ILE:HD11	1:109:A:ASP:H	10	0.87
(2,46)	1:116:A:GLU:HA	1:115:A:ASP:H	14	0.87
(1,923)	1:8:A:PHE:HB2	1:16:A:VAL:HA	20	0.87
(1,909)	1:43:A:THR:HG21	1:46:A:ILE:H	9	0.87
(1,713)	1:14:A:GLN:HA	1:12:A:ASN:H	15	0.87
(1,688)	1:69:A:ASN:H	1:69:A:ASN:HD22	14	0.87
(1,688)	1:69:A:ASN:H	1:69:A:ASN:HD22	18	0.87
(1,584)	1:27:A:ASP:HB2	1:27:A:ASP:H	10	0.87
(1,584)	1:27:A:ASP:HB3	1:27:A:ASP:H	10	0.87
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	1	0.87
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	1	0.87
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	1	0.87
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	1	0.87
(1,191)	1:100:A:ARG:HA	1:101:A:ASN:H	7	0.87
(1,191)	1:100:A:ARG:HA	1:101:A:ASN:H	14	0.87
(1,191)	1:100:A:ARG:HA	1:101:A:ASN:H	15	0.87
(1,150)	1:104:A:CYS:H	1:106:A:GLY:H	3	0.87
(1,4)	1:55:A:SER:H	1:54:A:HIS:H	3	0.87
(2,337)	1:53:A:ALA:HB3	1:55:A:SER:H	12	0.86
(2,257)	1:33:A:ASP:HA	1:38:A:GLN:HE22	9	0.86
(2,200)	1:87:A:PRO:HG3	1:76:A:ASP:H	13	0.86
(2,46)	1:116:A:GLU:HA	1:115:A:ASP:H	13	0.86
(1,888)	1:49:A:ILE:HA	1:61:A:VAL:H	10	0.86
(1,877)	1:22:A:CYS:HA	1:44:A:CYS:H	19	0.86
(1,824)	1:118:A:ASP:H	1:116:A:GLU:H	6	0.86
(1,584)	1:27:A:ASP:HB2	1:27:A:ASP:H	19	0.86
(1,584)	1:27:A:ASP:HB3	1:27:A:ASP:H	19	0.86
(1,459)	1:70:A:ASP:HA	1:76:A:ASP:H	11	0.86
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	6	0.86
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	6	0.86
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	6	0.86
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	6	0.86
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	15	0.86
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	15	0.86
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	15	0.86
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	15	0.86
(1,191)	1:100:A:ARG:HA	1:101:A:ASN:H	2	0.86
(1,191)	1:100:A:ARG:HA	1:101:A:ASN:H	9	0.86

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,97)	1:98:A:ILE:HD11	1:99:A:SER:H	15	0.86
(1,97)	1:98:A:ILE:HD12	1:99:A:SER:H	15	0.86
(1,97)	1:98:A:ILE:HD13	1:99:A:SER:H	15	0.86
(2,375)	1:48:A:GLU:HB3	1:61:A:VAL:H	3	0.85
(2,337)	1:53:A:ALA:HB1	1:55:A:SER:H	13	0.85
(2,296)	1:114:A:SER:HB3	1:117:A:LEU:H	13	0.85
(2,39)	1:117:A:LEU:HD11	1:115:A:ASP:H	7	0.85
(1,898)	1:57:A:GLN:HE22	1:71:A:CYS:H	2	0.85
(1,877)	1:22:A:CYS:HA	1:44:A:CYS:H	5	0.85
(1,877)	1:22:A:CYS:HA	1:44:A:CYS:H	14	0.85
(1,877)	1:22:A:CYS:HA	1:44:A:CYS:H	17	0.85
(1,459)	1:70:A:ASP:HA	1:76:A:ASP:H	3	0.85
(1,447)	1:71:A:CYS:HA	1:74:A:GLY:H	4	0.85
(1,447)	1:71:A:CYS:HA	1:74:A:GLY:H	12	0.85
(1,437)	1:72:A:ASP:H	1:71:A:CYS:H	8	0.85
(1,253)	1:83:A:ILE:HB	1:83:A:ILE:H	17	0.85
(1,191)	1:100:A:ARG:HA	1:101:A:ASN:H	4	0.85
(1,191)	1:100:A:ARG:HA	1:101:A:ASN:H	11	0.85
(1,191)	1:100:A:ARG:HA	1:101:A:ASN:H	13	0.85
(1,97)	1:98:A:ILE:HD11	1:99:A:SER:H	13	0.85
(1,97)	1:98:A:ILE:HD12	1:99:A:SER:H	13	0.85
(1,97)	1:98:A:ILE:HD13	1:99:A:SER:H	13	0.85
(2,359)	1:98:A:ILE:HD12	1:98:A:ILE:H	3	0.84
(2,296)	1:113:A:GLY:HA2	1:117:A:LEU:H	3	0.84
(2,281)	1:11:A:ASN:HA	1:11:A:ASN:HD22	6	0.84
(2,88)	1:78:A:GLU:HG3	1:79:A:ASN:HD21	12	0.84
(2,39)	1:117:A:LEU:HD13	1:115:A:ASP:H	3	0.84
(2,39)	1:117:A:LEU:HD12	1:115:A:ASP:H	4	0.84
(1,687)	1:69:A:ASN:HD21	1:74:A:GLY:H	8	0.84
(1,584)	1:27:A:ASP:HB2	1:27:A:ASP:H	2	0.84
(1,584)	1:27:A:ASP:HB3	1:27:A:ASP:H	2	0.84
(1,584)	1:27:A:ASP:HB2	1:27:A:ASP:H	4	0.84
(1,584)	1:27:A:ASP:HB3	1:27:A:ASP:H	4	0.84
(1,459)	1:70:A:ASP:HA	1:76:A:ASP:H	9	0.84
(1,253)	1:83:A:ILE:HB	1:83:A:ILE:H	13	0.84
(1,253)	1:83:A:ILE:HB	1:83:A:ILE:H	15	0.84
(1,191)	1:100:A:ARG:HA	1:101:A:ASN:H	1	0.84
(1,191)	1:100:A:ARG:HA	1:101:A:ASN:H	5	0.84
(1,191)	1:100:A:ARG:HA	1:101:A:ASN:H	6	0.84
(1,191)	1:100:A:ARG:HA	1:101:A:ASN:H	8	0.84
(1,191)	1:100:A:ARG:HA	1:101:A:ASN:H	12	0.84
(1,191)	1:100:A:ARG:HA	1:101:A:ASN:H	17	0.84

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,191)	1:100:A:ARG:HA	1:101:A:ASN:H	18	0.84
(1,150)	1:104:A:CYS:H	1:106:A:GLY:H	7	0.84
(1,4)	1:55:A:SER:H	1:54:A:HIS:H	8	0.84
(1,4)	1:55:A:SER:H	1:54:A:HIS:H	20	0.84
(2,330)	1:92:A:CYS:HA	1:93:A:SER:H	9	0.83
(2,330)	1:111:A:SER:HG	1:93:A:SER:H	16	0.83
(2,281)	1:11:A:ASN:HA	1:11:A:ASN:HD22	11	0.83
(2,281)	1:10:A:CYS:HA	1:11:A:ASN:HD22	16	0.83
(2,200)	1:77:A:GLU:HG3	1:76:A:ASP:H	14	0.83
(2,200)	1:77:A:GLU:HG3	1:76:A:ASP:H	18	0.83
(1,909)	1:43:A:THR:HG22	1:46:A:ILE:H	1	0.83
(1,824)	1:118:A:ASP:H	1:116:A:GLU:H	17	0.83
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG12	2	0.83
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG13	2	0.83
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG12	6	0.83
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG13	6	0.83
(1,713)	1:14:A:GLN:HA	1:12:A:ASN:H	5	0.83
(1,584)	1:27:A:ASP:HB2	1:27:A:ASP:H	3	0.83
(1,584)	1:27:A:ASP:HB3	1:27:A:ASP:H	3	0.83
(1,584)	1:27:A:ASP:HB2	1:27:A:ASP:H	9	0.83
(1,584)	1:27:A:ASP:HB3	1:27:A:ASP:H	9	0.83
(1,459)	1:70:A:ASP:HA	1:76:A:ASP:H	1	0.83
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	13	0.83
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	13	0.83
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	13	0.83
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	13	0.83
(1,437)	1:72:A:ASP:H	1:71:A:CYS:H	4	0.83
(1,150)	1:104:A:CYS:H	1:106:A:GLY:H	4	0.83
(2,354)	1:68:A:GLU:HA	1:69:A:ASN:H	3	0.82
(2,354)	1:68:A:GLU:HA	1:69:A:ASN:H	7	0.82
(2,281)	1:11:A:ASN:HA	1:11:A:ASN:HD22	9	0.82
(1,877)	1:22:A:CYS:HA	1:44:A:CYS:H	16	0.82
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	20	0.82
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	20	0.82
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	20	0.82
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	20	0.82
(1,584)	1:27:A:ASP:HB2	1:27:A:ASP:H	18	0.82
(1,584)	1:27:A:ASP:HB3	1:27:A:ASP:H	18	0.82
(1,253)	1:83:A:ILE:HB	1:83:A:ILE:H	14	0.82
(1,191)	1:100:A:ARG:HA	1:101:A:ASN:H	19	0.82
(1,97)	1:98:A:ILE:HD11	1:99:A:SER:H	14	0.82
(1,97)	1:98:A:ILE:HD12	1:99:A:SER:H	14	0.82

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,97)	1:98:A:ILE:HD13	1:99:A:SER:H	14	0.82
(2,354)	1:68:A:GLU:HA	1:69:A:ASN:H	6	0.81
(2,354)	1:68:A:GLU:HA	1:69:A:ASN:H	18	0.81
(2,354)	1:68:A:GLU:HA	1:69:A:ASN:H	20	0.81
(2,337)	1:53:A:ALA:HB2	1:55:A:SER:H	10	0.81
(2,327)	1:68:A:GLU:HG2	1:71:A:CYS:H	1	0.81
(2,281)	1:11:A:ASN:HA	1:11:A:ASN:HD22	15	0.81
(2,46)	1:114:A:SER:HG	1:115:A:ASP:H	15	0.81
(1,909)	1:43:A:THR:HG22	1:46:A:ILE:H	5	0.81
(1,909)	1:43:A:THR:HG22	1:46:A:ILE:H	7	0.81
(1,909)	1:43:A:THR:HG23	1:46:A:ILE:H	15	0.81
(1,766)	1:48:A:GLU:HB2	1:58:A:CYS:H	10	0.81
(1,766)	1:48:A:GLU:HB3	1:58:A:CYS:H	10	0.81
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG12	9	0.81
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG13	9	0.81
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG12	13	0.81
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG13	13	0.81
(1,584)	1:27:A:ASP:HB2	1:27:A:ASP:H	15	0.81
(1,584)	1:27:A:ASP:HB3	1:27:A:ASP:H	15	0.81
(1,447)	1:71:A:CYS:HA	1:74:A:GLY:H	18	0.81
(1,429)	1:69:A:ASN:HA	1:69:A:ASN:H	3	0.81
(1,429)	1:69:A:ASN:HA	1:69:A:ASN:H	10	0.81
(1,429)	1:69:A:ASN:HA	1:69:A:ASN:H	11	0.81
(1,150)	1:104:A:CYS:H	1:106:A:GLY:H	6	0.81
(1,150)	1:104:A:CYS:H	1:106:A:GLY:H	10	0.81
(1,97)	1:98:A:ILE:HD11	1:99:A:SER:H	11	0.81
(1,97)	1:98:A:ILE:HD12	1:99:A:SER:H	11	0.81
(1,97)	1:98:A:ILE:HD13	1:99:A:SER:H	11	0.81
(2,375)	1:48:A:GLU:HB3	1:61:A:VAL:H	2	0.8
(2,354)	1:68:A:GLU:HA	1:69:A:ASN:H	11	0.8
(2,354)	1:68:A:GLU:HA	1:69:A:ASN:H	12	0.8
(2,354)	1:68:A:GLU:HA	1:69:A:ASN:H	13	0.8
(2,354)	1:68:A:GLU:HA	1:69:A:ASN:H	17	0.8
(2,354)	1:68:A:GLU:HA	1:69:A:ASN:H	19	0.8
(2,327)	1:68:A:GLU:HG2	1:71:A:CYS:H	7	0.8
(2,281)	1:11:A:ASN:HA	1:11:A:ASN:HD22	10	0.8
(2,281)	1:11:A:ASN:HA	1:11:A:ASN:HD22	14	0.8
(2,244)	1:45:A:ARG:HA	1:47:A:HIS:H	20	0.8
(2,200)	1:77:A:GLU:HG3	1:76:A:ASP:H	4	0.8
(1,923)	1:8:A:PHE:HB2	1:16:A:VAL:HA	1	0.8
(1,923)	1:8:A:PHE:HB2	1:16:A:VAL:HA	2	0.8
(1,909)	1:43:A:THR:HG21	1:46:A:ILE:H	2	0.8

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,909)	1:43:A:THR:HG22	1:46:A:ILE:H	17	0.8
(1,799)	1:85:A:CYS:HA	1:97:A:CYS:H	16	0.8
(1,692)	1:8:A:PHE:HB2	1:8:A:PHE:H	19	0.8
(1,692)	1:8:A:PHE:HB3	1:8:A:PHE:H	19	0.8
(1,686)	1:74:A:GLY:H	1:69:A:ASN:HD22	7	0.8
(1,584)	1:27:A:ASP:HB2	1:27:A:ASP:H	7	0.8
(1,584)	1:27:A:ASP:HB3	1:27:A:ASP:H	7	0.8
(1,429)	1:69:A:ASN:HA	1:69:A:ASN:H	1	0.8
(1,429)	1:69:A:ASN:HA	1:69:A:ASN:H	4	0.8
(1,429)	1:69:A:ASN:HA	1:69:A:ASN:H	7	0.8
(1,429)	1:69:A:ASN:HA	1:69:A:ASN:H	8	0.8
(1,429)	1:69:A:ASN:HA	1:69:A:ASN:H	9	0.8
(1,429)	1:69:A:ASN:HA	1:69:A:ASN:H	12	0.8
(1,429)	1:69:A:ASN:HA	1:69:A:ASN:H	13	0.8
(1,429)	1:69:A:ASN:HA	1:69:A:ASN:H	14	0.8
(1,429)	1:69:A:ASN:HA	1:69:A:ASN:H	16	0.8
(1,429)	1:69:A:ASN:HA	1:69:A:ASN:H	18	0.8
(1,429)	1:69:A:ASN:HA	1:69:A:ASN:H	19	0.8
(1,429)	1:69:A:ASN:HA	1:69:A:ASN:H	20	0.8
(2,361)	1:61:A:VAL:HG12	1:64:A:ARG:H	14	0.79
(2,354)	1:68:A:GLU:HA	1:69:A:ASN:H	5	0.79
(2,354)	1:68:A:GLU:HA	1:69:A:ASN:H	16	0.79
(2,281)	1:11:A:ASN:HA	1:11:A:ASN:HD22	5	0.79
(2,257)	1:33:A:ASP:HA	1:38:A:GLN:HE22	15	0.79
(1,923)	1:8:A:PHE:HB2	1:16:A:VAL:HA	13	0.79
(1,877)	1:22:A:CYS:HA	1:44:A:CYS:H	15	0.79
(1,824)	1:118:A:ASP:H	1:116:A:GLU:H	4	0.79
(1,770)	1:63:A:TRP:H	1:77:A:GLU:HG2	3	0.79
(1,770)	1:63:A:TRP:H	1:77:A:GLU:HG3	3	0.79
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG12	7	0.79
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG13	7	0.79
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG12	19	0.79
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG13	19	0.79
(1,687)	1:69:A:ASN:HD21	1:74:A:GLY:H	15	0.79
(1,584)	1:27:A:ASP:HB2	1:27:A:ASP:H	1	0.79
(1,584)	1:27:A:ASP:HB3	1:27:A:ASP:H	1	0.79
(1,584)	1:27:A:ASP:HB2	1:27:A:ASP:H	11	0.79
(1,584)	1:27:A:ASP:HB3	1:27:A:ASP:H	11	0.79
(1,584)	1:27:A:ASP:HB2	1:27:A:ASP:H	12	0.79
(1,584)	1:27:A:ASP:HB3	1:27:A:ASP:H	12	0.79
(1,584)	1:27:A:ASP:HB2	1:27:A:ASP:H	14	0.79
(1,584)	1:27:A:ASP:HB3	1:27:A:ASP:H	14	0.79

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,584)	1:27:A:ASP:HB2	1:27:A:ASP:H	20	0.79
(1,584)	1:27:A:ASP:HB3	1:27:A:ASP:H	20	0.79
(1,502)	1:34:A:GLU:HG2	1:34:A:GLU:H	7	0.79
(1,502)	1:34:A:GLU:HG3	1:34:A:GLU:H	7	0.79
(1,502)	1:34:A:GLU:HG2	1:34:A:GLU:H	16	0.79
(1,502)	1:34:A:GLU:HG3	1:34:A:GLU:H	16	0.79
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	5	0.79
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	5	0.79
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	5	0.79
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	5	0.79
(1,429)	1:69:A:ASN:HA	1:69:A:ASN:H	5	0.79
(1,429)	1:69:A:ASN:HA	1:69:A:ASN:H	6	0.79
(1,429)	1:69:A:ASN:HA	1:69:A:ASN:H	15	0.79
(1,150)	1:104:A:CYS:H	1:106:A:GLY:H	9	0.79
(1,97)	1:98:A:ILE:HD11	1:99:A:SER:H	12	0.79
(1,97)	1:98:A:ILE:HD12	1:99:A:SER:H	12	0.79
(1,97)	1:98:A:ILE:HD13	1:99:A:SER:H	12	0.79
(2,354)	1:68:A:GLU:HA	1:69:A:ASN:H	1	0.78
(2,354)	1:68:A:GLU:HA	1:69:A:ASN:H	9	0.78
(2,296)	1:114:A:SER:HB2	1:117:A:LEU:H	2	0.78
(2,281)	1:10:A:CYS:HA	1:11:A:ASN:HD22	20	0.78
(2,178)	1:59:A:ILE:HG21	1:57:A:GLN:HE22	6	0.78
(2,178)	1:59:A:ILE:HG21	1:57:A:GLN:HE22	8	0.78
(1,923)	1:8:A:PHE:HB2	1:16:A:VAL:HA	19	0.78
(1,824)	1:118:A:ASP:H	1:116:A:GLU:H	5	0.78
(1,824)	1:118:A:ASP:H	1:116:A:GLU:H	7	0.78
(1,824)	1:118:A:ASP:H	1:116:A:GLU:H	13	0.78
(1,770)	1:63:A:TRP:H	1:77:A:GLU:HG2	11	0.78
(1,770)	1:63:A:TRP:H	1:77:A:GLU:HG3	11	0.78
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG12	5	0.78
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG13	5	0.78
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG12	11	0.78
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG13	11	0.78
(1,686)	1:74:A:GLY:H	1:69:A:ASN:HD22	3	0.78
(1,584)	1:27:A:ASP:HB2	1:27:A:ASP:H	5	0.78
(1,584)	1:27:A:ASP:HB3	1:27:A:ASP:H	5	0.78
(1,584)	1:27:A:ASP:HB2	1:27:A:ASP:H	6	0.78
(1,584)	1:27:A:ASP:HB3	1:27:A:ASP:H	6	0.78
(1,429)	1:69:A:ASN:HA	1:69:A:ASN:H	2	0.78
(1,150)	1:104:A:CYS:H	1:106:A:GLY:H	1	0.78
(1,150)	1:104:A:CYS:H	1:106:A:GLY:H	8	0.78
(1,150)	1:104:A:CYS:H	1:106:A:GLY:H	20	0.78

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,97)	1:98:A:ILE:HD11	1:99:A:SER:H	18	0.78
(1,97)	1:98:A:ILE:HD12	1:99:A:SER:H	18	0.78
(1,97)	1:98:A:ILE:HD13	1:99:A:SER:H	18	0.78
(2,361)	1:61:A:VAL:HG22	1:64:A:ARG:H	3	0.77
(2,337)	1:53:A:ALA:HB2	1:55:A:SER:H	6	0.77
(2,330)	1:114:A:SER:HG	1:93:A:SER:H	19	0.77
(2,276)	1:43:A:THR:HA	1:57:A:GLN:H	4	0.77
(2,210)	1:33:A:ASP:HA	1:38:A:GLN:HE21	14	0.77
(2,66)	1:4:A:ALA:H	1:7:A:ASP:H	20	0.77
(1,923)	1:8:A:PHE:HB2	1:16:A:VAL:HA	3	0.77
(1,877)	1:22:A:CYS:HA	1:44:A:CYS:H	1	0.77
(1,877)	1:22:A:CYS:HA	1:44:A:CYS:H	3	0.77
(1,799)	1:85:A:CYS:HA	1:97:A:CYS:H	20	0.77
(1,770)	1:63:A:TRP:H	1:77:A:GLU:HG2	20	0.77
(1,770)	1:63:A:TRP:H	1:77:A:GLU:HG3	20	0.77
(1,584)	1:27:A:ASP:HB2	1:27:A:ASP:H	13	0.77
(1,584)	1:27:A:ASP:HB3	1:27:A:ASP:H	13	0.77
(1,447)	1:71:A:CYS:HA	1:74:A:GLY:H	14	0.77
(1,429)	1:69:A:ASN:HA	1:69:A:ASN:H	17	0.77
(1,150)	1:104:A:CYS:H	1:106:A:GLY:H	11	0.77
(2,354)	1:68:A:GLU:HA	1:69:A:ASN:H	2	0.76
(2,354)	1:68:A:GLU:HA	1:69:A:ASN:H	8	0.76
(2,281)	1:11:A:ASN:HA	1:11:A:ASN:HD22	13	0.76
(2,200)	1:77:A:GLU:HG3	1:76:A:ASP:H	8	0.76
(2,83)	1:35:A:SER:HB3	1:38:A:GLN:H	13	0.76
(1,923)	1:8:A:PHE:HB2	1:16:A:VAL:HA	18	0.76
(1,909)	1:43:A:THR:HG21	1:46:A:ILE:H	6	0.76
(1,787)	1:73:A:SER:H	1:76:A:ASP:H	6	0.76
(1,770)	1:63:A:TRP:H	1:77:A:GLU:HG2	16	0.76
(1,770)	1:63:A:TRP:H	1:77:A:GLU:HG3	16	0.76
(1,692)	1:8:A:PHE:HB2	1:8:A:PHE:H	2	0.76
(1,692)	1:8:A:PHE:HB3	1:8:A:PHE:H	2	0.76
(1,692)	1:8:A:PHE:HB2	1:8:A:PHE:H	8	0.76
(1,692)	1:8:A:PHE:HB3	1:8:A:PHE:H	8	0.76
(1,692)	1:8:A:PHE:HB2	1:8:A:PHE:H	11	0.76
(1,692)	1:8:A:PHE:HB3	1:8:A:PHE:H	11	0.76
(1,463)	1:71:A:CYS:HB2	1:78:A:GLU:H	10	0.76
(1,463)	1:71:A:CYS:HB3	1:78:A:GLU:H	10	0.76
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	2	0.76
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	2	0.76
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	2	0.76
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	2	0.76

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,150)	1:104:A:CYS:H	1:106:A:GLY:H	15	0.76
(2,371)	1:83:A:ILE:HG21	1:83:A:ILE:H	18	0.75
(2,363)	1:49:A:ILE:HB	1:49:A:ILE:H	14	0.75
(2,281)	1:11:A:ASN:HA	1:11:A:ASN:HD22	18	0.75
(2,66)	1:5:A:GLU:H	1:7:A:ASP:H	6	0.75
(1,700)	1:69:A:ASN:HB2	1:69:A:ASN:H	14	0.75
(1,700)	1:69:A:ASN:HB3	1:69:A:ASN:H	14	0.75
(1,692)	1:8:A:PHE:HB2	1:8:A:PHE:H	13	0.75
(1,692)	1:8:A:PHE:HB3	1:8:A:PHE:H	13	0.75
(1,692)	1:8:A:PHE:HB2	1:8:A:PHE:H	17	0.75
(1,692)	1:8:A:PHE:HB3	1:8:A:PHE:H	17	0.75
(1,686)	1:74:A:GLY:H	1:69:A:ASN:HD22	1	0.75
(1,447)	1:71:A:CYS:HA	1:74:A:GLY:H	2	0.75
(1,150)	1:104:A:CYS:H	1:106:A:GLY:H	14	0.75
(2,363)	1:49:A:ILE:HB	1:49:A:ILE:H	20	0.74
(2,354)	1:68:A:GLU:HA	1:69:A:ASN:H	10	0.74
(2,337)	1:53:A:ALA:HB2	1:55:A:SER:H	11	0.74
(2,327)	1:64:A:ARG:HG2	1:71:A:CYS:H	11	0.74
(2,296)	1:114:A:SER:HB3	1:117:A:LEU:H	19	0.74
(2,281)	1:11:A:ASN:HA	1:11:A:ASN:HD22	3	0.74
(2,257)	1:32:A:SER:HB2	1:38:A:GLN:HE22	4	0.74
(2,253)	1:86:A:SER:HB3	1:89:A:GLU:H	11	0.74
(2,244)	1:45:A:ARG:HA	1:47:A:HIS:H	9	0.74
(2,200)	1:77:A:GLU:HG3	1:76:A:ASP:H	12	0.74
(2,193)	1:98:A:ILE:HD13	1:109:A:ASP:H	2	0.74
(2,52)	1:60:A:PRO:HD2	1:63:A:TRP:HE1	15	0.74
(1,909)	1:43:A:THR:HG23	1:46:A:ILE:H	18	0.74
(1,898)	1:57:A:GLN:HE22	1:71:A:CYS:H	1	0.74
(1,849)	1:33:A:ASP:H	1:11:A:ASN:H	8	0.74
(1,824)	1:118:A:ASP:H	1:116:A:GLU:H	3	0.74
(1,824)	1:118:A:ASP:H	1:116:A:GLU:H	18	0.74
(1,824)	1:118:A:ASP:H	1:116:A:GLU:H	20	0.74
(1,799)	1:85:A:CYS:HA	1:97:A:CYS:H	8	0.74
(1,799)	1:85:A:CYS:HA	1:97:A:CYS:H	10	0.74
(1,447)	1:71:A:CYS:HA	1:74:A:GLY:H	13	0.74
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	1	0.74
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	1	0.74
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	1	0.74
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	1	0.74
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	12	0.74
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	12	0.74
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	12	0.74

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	12	0.74
(1,150)	1:104:A:CYS:H	1:106:A:GLY:H	13	0.74
(2,363)	1:49:A:ILE:HB	1:49:A:ILE:H	3	0.73
(2,363)	1:49:A:ILE:HB	1:49:A:ILE:H	16	0.73
(2,193)	1:117:A:LEU:HD12	1:109:A:ASP:H	11	0.73
(2,193)	1:98:A:ILE:HD12	1:109:A:ASP:H	17	0.73
(2,66)	1:5:A:GLU:H	1:7:A:ASP:H	19	0.73
(1,923)	1:8:A:PHE:HB2	1:16:A:VAL:HA	8	0.73
(1,909)	1:43:A:THR:HG21	1:46:A:ILE:H	20	0.73
(1,898)	1:57:A:GLN:HE22	1:71:A:CYS:H	9	0.73
(1,824)	1:118:A:ASP:H	1:116:A:GLU:H	11	0.73
(1,824)	1:118:A:ASP:H	1:116:A:GLU:H	14	0.73
(1,824)	1:118:A:ASP:H	1:116:A:GLU:H	16	0.73
(1,770)	1:63:A:TRP:H	1:77:A:GLU:HG2	5	0.73
(1,770)	1:63:A:TRP:H	1:77:A:GLU:HG3	5	0.73
(1,770)	1:63:A:TRP:H	1:77:A:GLU:HG2	9	0.73
(1,770)	1:63:A:TRP:H	1:77:A:GLU:HG3	9	0.73
(1,700)	1:69:A:ASN:HB2	1:69:A:ASN:H	18	0.73
(1,700)	1:69:A:ASN:HB3	1:69:A:ASN:H	18	0.73
(1,150)	1:104:A:CYS:H	1:106:A:GLY:H	19	0.73
(2,363)	1:49:A:ILE:HB	1:49:A:ILE:H	19	0.72
(2,359)	1:98:A:ILE:HD11	1:98:A:ILE:H	9	0.72
(2,354)	1:68:A:GLU:HA	1:69:A:ASN:H	15	0.72
(2,281)	1:11:A:ASN:HA	1:11:A:ASN:HD22	19	0.72
(2,200)	1:77:A:GLU:HG2	1:76:A:ASP:H	20	0.72
(2,193)	1:98:A:ILE:HD11	1:109:A:ASP:H	3	0.72
(2,178)	1:59:A:ILE:HG21	1:57:A:GLN:HE22	17	0.72
(2,66)	1:4:A:ALA:H	1:7:A:ASP:H	9	0.72
(2,46)	1:114:A:SER:HG	1:115:A:ASP:H	12	0.72
(2,39)	1:117:A:LEU:HD21	1:115:A:ASP:H	16	0.72
(1,713)	1:14:A:GLN:HA	1:12:A:ASN:H	17	0.72
(1,696)	1:44:A:CYS:HB2	1:34:A:GLU:H	10	0.72
(1,696)	1:44:A:CYS:HB3	1:34:A:GLU:H	10	0.72
(1,692)	1:8:A:PHE:HB2	1:8:A:PHE:H	7	0.72
(1,692)	1:8:A:PHE:HB3	1:8:A:PHE:H	7	0.72
(1,692)	1:8:A:PHE:HB2	1:8:A:PHE:H	10	0.72
(1,692)	1:8:A:PHE:HB3	1:8:A:PHE:H	10	0.72
(1,541)	1:115:A:ASP:HB2	1:116:A:GLU:H	15	0.72
(1,541)	1:115:A:ASP:HB3	1:116:A:GLU:H	15	0.72
(1,502)	1:34:A:GLU:HG2	1:34:A:GLU:H	1	0.72
(1,502)	1:34:A:GLU:HG3	1:34:A:GLU:H	1	0.72
(1,502)	1:34:A:GLU:HG2	1:34:A:GLU:H	11	0.72

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,502)	1:34:A:GLU:HG3	1:34:A:GLU:H	11	0.72
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	16	0.72
(1,455)	1:76:A:ASP:HB2	1:76:A:ASP:H	16	0.72
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	16	0.72
(1,455)	1:76:A:ASP:HB3	1:76:A:ASP:H	16	0.72
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	9	0.72
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	9	0.72
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	9	0.72
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	9	0.72
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	17	0.72
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	17	0.72
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	17	0.72
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	17	0.72
(1,150)	1:104:A:CYS:H	1:106:A:GLY:H	17	0.72
(2,363)	1:49:A:ILE:HB	1:49:A:ILE:H	13	0.71
(2,193)	1:117:A:LEU:HD13	1:109:A:ASP:H	14	0.71
(1,923)	1:8:A:PHE:HB2	1:16:A:VAL:HA	17	0.71
(1,898)	1:57:A:GLN:HE22	1:71:A:CYS:H	6	0.71
(1,898)	1:57:A:GLN:HE22	1:71:A:CYS:H	16	0.71
(1,890)	1:81:A:GLY:HA2	1:63:A:TRP:HE1	8	0.71
(1,890)	1:81:A:GLY:HA2	1:63:A:TRP:HE1	8	0.71
(1,890)	1:81:A:GLY:HA3	1:63:A:TRP:HE1	8	0.71
(1,890)	1:81:A:GLY:HA3	1:63:A:TRP:HE1	8	0.71
(1,877)	1:22:A:CYS:HA	1:44:A:CYS:H	13	0.71
(1,784)	1:71:A:CYS:HB2	1:76:A:ASP:H	6	0.71
(1,784)	1:71:A:CYS:HB3	1:76:A:ASP:H	6	0.71
(1,708)	1:44:A:CYS:HB2	1:45:A:ARG:H	5	0.71
(1,708)	1:44:A:CYS:HB3	1:45:A:ARG:H	5	0.71
(1,700)	1:69:A:ASN:HB2	1:69:A:ASN:H	4	0.71
(1,700)	1:69:A:ASN:HB3	1:69:A:ASN:H	4	0.71
(1,700)	1:69:A:ASN:HB2	1:69:A:ASN:H	6	0.71
(1,700)	1:69:A:ASN:HB3	1:69:A:ASN:H	6	0.71
(1,692)	1:8:A:PHE:HB2	1:8:A:PHE:H	3	0.71
(1,692)	1:8:A:PHE:HB3	1:8:A:PHE:H	3	0.71
(1,692)	1:8:A:PHE:HB2	1:8:A:PHE:H	6	0.71
(1,692)	1:8:A:PHE:HB3	1:8:A:PHE:H	6	0.71
(1,692)	1:8:A:PHE:HB2	1:8:A:PHE:H	16	0.71
(1,692)	1:8:A:PHE:HB3	1:8:A:PHE:H	16	0.71
(1,502)	1:34:A:GLU:HG2	1:34:A:GLU:H	2	0.71
(1,502)	1:34:A:GLU:HG3	1:34:A:GLU:H	2	0.71
(1,492)	1:22:A:CYS:H	1:24:A:GLY:H	19	0.71
(1,491)	1:22:A:CYS:H	1:24:A:GLY:H	19	0.71

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,459)	1:70:A:ASP:HA	1:76:A:ASP:H	6	0.71
(1,391)	1:54:A:HIS:HA	1:53:A:ALA:H	12	0.71
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	5	0.71
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	5	0.71
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	5	0.71
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	5	0.71
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	7	0.71
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	7	0.71
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	7	0.71
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	7	0.71
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	19	0.71
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	19	0.71
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	19	0.71
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	19	0.71
(1,150)	1:104:A:CYS:H	1:106:A:GLY:H	12	0.71
(2,375)	1:48:A:GLU:HB3	1:61:A:VAL:H	19	0.7
(2,363)	1:49:A:ILE:HB	1:49:A:ILE:H	7	0.7
(2,330)	1:92:A:CYS:HA	1:93:A:SER:H	4	0.7
(2,178)	1:59:A:ILE:HG21	1:57:A:GLN:HE22	15	0.7
(1,877)	1:22:A:CYS:HA	1:44:A:CYS:H	7	0.7
(1,824)	1:118:A:ASP:H	1:116:A:GLU:H	12	0.7
(1,721)	1:21:A:LYS:HG2	1:22:A:CYS:H	10	0.7
(1,721)	1:21:A:LYS:HG3	1:22:A:CYS:H	10	0.7
(1,721)	1:21:A:LYS:HG2	1:22:A:CYS:H	11	0.7
(1,721)	1:21:A:LYS:HG3	1:22:A:CYS:H	11	0.7
(1,700)	1:69:A:ASN:HB2	1:69:A:ASN:H	10	0.7
(1,700)	1:69:A:ASN:HB3	1:69:A:ASN:H	10	0.7
(1,700)	1:69:A:ASN:HB2	1:69:A:ASN:H	13	0.7
(1,700)	1:69:A:ASN:HB3	1:69:A:ASN:H	13	0.7
(1,700)	1:69:A:ASN:HB2	1:69:A:ASN:H	20	0.7
(1,700)	1:69:A:ASN:HB3	1:69:A:ASN:H	20	0.7
(1,686)	1:74:A:GLY:H	1:69:A:ASN:HD22	4	0.7
(1,541)	1:115:A:ASP:HB2	1:116:A:GLU:H	14	0.7
(1,541)	1:115:A:ASP:HB3	1:116:A:GLU:H	14	0.7
(1,492)	1:22:A:CYS:H	1:24:A:GLY:H	9	0.7
(1,491)	1:22:A:CYS:H	1:24:A:GLY:H	9	0.7
(1,436)	1:73:A:SER:H	1:72:A:ASP:H	8	0.7
(1,391)	1:54:A:HIS:HA	1:53:A:ALA:H	14	0.7
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	13	0.7
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	13	0.7
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	13	0.7
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	13	0.7

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,150)	1:104:A:CYS:H	1:106:A:GLY:H	2	0.7
(1,150)	1:104:A:CYS:H	1:106:A:GLY:H	16	0.7
(4,8)	1:8:A:PHE:O	1:16:A:VAL:H	16	0.69
(2,363)	1:49:A:ILE:HB	1:49:A:ILE:H	9	0.69
(2,337)	1:53:A:ALA:HB1	1:55:A:SER:H	17	0.69
(2,257)	1:33:A:ASP:HA	1:38:A:GLN:HE22	12	0.69
(2,66)	1:4:A:ALA:H	1:7:A:ASP:H	10	0.69
(2,66)	1:4:A:ALA:H	1:7:A:ASP:H	11	0.69
(2,39)	1:117:A:LEU:HD23	1:115:A:ASP:H	2	0.69
(1,923)	1:8:A:PHE:HB2	1:16:A:VAL:HA	10	0.69
(1,909)	1:43:A:THR:HG23	1:46:A:ILE:H	13	0.69
(1,877)	1:22:A:CYS:HA	1:44:A:CYS:H	4	0.69
(1,770)	1:63:A:TRP:H	1:77:A:GLU:HG2	19	0.69
(1,770)	1:63:A:TRP:H	1:77:A:GLU:HG3	19	0.69
(1,700)	1:69:A:ASN:HB2	1:69:A:ASN:H	3	0.69
(1,700)	1:69:A:ASN:HB3	1:69:A:ASN:H	3	0.69
(1,700)	1:69:A:ASN:HB2	1:69:A:ASN:H	12	0.69
(1,700)	1:69:A:ASN:HB3	1:69:A:ASN:H	12	0.69
(1,692)	1:8:A:PHE:HB2	1:8:A:PHE:H	18	0.69
(1,692)	1:8:A:PHE:HB3	1:8:A:PHE:H	18	0.69
(1,692)	1:8:A:PHE:HB2	1:8:A:PHE:H	20	0.69
(1,692)	1:8:A:PHE:HB3	1:8:A:PHE:H	20	0.69
(1,686)	1:74:A:GLY:H	1:69:A:ASN:HD22	16	0.69
(1,541)	1:115:A:ASP:HB2	1:116:A:GLU:H	13	0.69
(1,541)	1:115:A:ASP:HB3	1:116:A:GLU:H	13	0.69
(1,502)	1:34:A:GLU:HG2	1:34:A:GLU:H	13	0.69
(1,502)	1:34:A:GLU:HG3	1:34:A:GLU:H	13	0.69
(1,502)	1:34:A:GLU:HG2	1:34:A:GLU:H	19	0.69
(1,502)	1:34:A:GLU:HG3	1:34:A:GLU:H	19	0.69
(1,492)	1:22:A:CYS:H	1:24:A:GLY:H	7	0.69
(1,491)	1:22:A:CYS:H	1:24:A:GLY:H	7	0.69
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	14	0.69
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	14	0.69
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	14	0.69
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	14	0.69
(1,212)	1:96:A:ARG:H	1:92:A:CYS:HA	1	0.69
(1,150)	1:104:A:CYS:H	1:106:A:GLY:H	18	0.69
(2,359)	1:98:A:ILE:HD11	1:98:A:ILE:H	2	0.68
(2,327)	1:64:A:ARG:HG2	1:71:A:CYS:H	16	0.68
(2,66)	1:4:A:ALA:H	1:7:A:ASP:H	17	0.68
(1,911)	1:57:A:GLN:HE21	1:71:A:CYS:H	20	0.68
(1,898)	1:57:A:GLN:HE22	1:71:A:CYS:H	5	0.68

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,898)	1:57:A:GLN:HE22	1:71:A:CYS:H	19	0.68
(1,877)	1:22:A:CYS:HA	1:44:A:CYS:H	2	0.68
(1,824)	1:118:A:ASP:H	1:116:A:GLU:H	15	0.68
(1,770)	1:63:A:TRP:H	1:77:A:GLU:HG2	7	0.68
(1,770)	1:63:A:TRP:H	1:77:A:GLU:HG3	7	0.68
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	17	0.68
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	17	0.68
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	17	0.68
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	17	0.68
(1,721)	1:21:A:LYS:HG2	1:22:A:CYS:H	13	0.68
(1,721)	1:21:A:LYS:HG3	1:22:A:CYS:H	13	0.68
(1,708)	1:44:A:CYS:HB2	1:45:A:ARG:H	1	0.68
(1,708)	1:44:A:CYS:HB3	1:45:A:ARG:H	1	0.68
(1,700)	1:69:A:ASN:HB2	1:69:A:ASN:H	8	0.68
(1,700)	1:69:A:ASN:HB3	1:69:A:ASN:H	8	0.68
(1,700)	1:69:A:ASN:HB2	1:69:A:ASN:H	11	0.68
(1,700)	1:69:A:ASN:HB3	1:69:A:ASN:H	11	0.68
(1,700)	1:69:A:ASN:HB2	1:69:A:ASN:H	16	0.68
(1,700)	1:69:A:ASN:HB3	1:69:A:ASN:H	16	0.68
(1,692)	1:8:A:PHE:HB2	1:8:A:PHE:H	1	0.68
(1,692)	1:8:A:PHE:HB3	1:8:A:PHE:H	1	0.68
(1,692)	1:8:A:PHE:HB2	1:8:A:PHE:H	9	0.68
(1,692)	1:8:A:PHE:HB3	1:8:A:PHE:H	9	0.68
(1,686)	1:74:A:GLY:H	1:69:A:ASN:HD22	11	0.68
(1,492)	1:22:A:CYS:H	1:24:A:GLY:H	2	0.68
(1,492)	1:22:A:CYS:H	1:24:A:GLY:H	17	0.68
(1,491)	1:22:A:CYS:H	1:24:A:GLY:H	2	0.68
(1,491)	1:22:A:CYS:H	1:24:A:GLY:H	17	0.68
(1,459)	1:70:A:ASP:HA	1:76:A:ASP:H	12	0.68
(1,391)	1:54:A:HIS:HA	1:53:A:ALA:H	4	0.68
(1,391)	1:54:A:HIS:HA	1:53:A:ALA:H	15	0.68
(1,391)	1:54:A:HIS:HA	1:53:A:ALA:H	19	0.68
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	6	0.68
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	6	0.68
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	6	0.68
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	6	0.68
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	11	0.68
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	11	0.68
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	11	0.68
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	11	0.68
(1,212)	1:96:A:ARG:H	1:92:A:CYS:HA	6	0.68
(2,381)	1:85:A:CYS:HB3	1:90:A:PHE:H	2	0.67

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,374)	1:25:A:ASP:HA	1:23:A:ASP:H	17	0.67
(2,363)	1:49:A:ILE:HB	1:49:A:ILE:H	5	0.67
(2,361)	1:61:A:VAL:HG13	1:64:A:ARG:H	2	0.67
(2,337)	1:53:A:ALA:HB1	1:55:A:SER:H	16	0.67
(2,327)	1:64:A:ARG:HG2	1:71:A:CYS:H	2	0.67
(2,323)	1:68:A:GLU:HG3	1:68:A:GLU:H	15	0.67
(2,281)	1:11:A:ASN:HA	1:11:A:ASN:HD22	7	0.67
(2,210)	1:33:A:ASP:HA	1:38:A:GLN:HE21	18	0.67
(1,909)	1:43:A:THR:HG23	1:46:A:ILE:H	11	0.67
(1,898)	1:57:A:GLN:HE22	1:71:A:CYS:H	11	0.67
(1,803)	1:101:A:ASN:HD21	1:99:A:SER:H	2	0.67
(1,700)	1:69:A:ASN:HB2	1:69:A:ASN:H	5	0.67
(1,700)	1:69:A:ASN:HB3	1:69:A:ASN:H	5	0.67
(1,700)	1:69:A:ASN:HB2	1:69:A:ASN:H	15	0.67
(1,700)	1:69:A:ASN:HB3	1:69:A:ASN:H	15	0.67
(1,692)	1:8:A:PHE:HB2	1:8:A:PHE:H	5	0.67
(1,692)	1:8:A:PHE:HB3	1:8:A:PHE:H	5	0.67
(1,692)	1:8:A:PHE:HB2	1:8:A:PHE:H	12	0.67
(1,692)	1:8:A:PHE:HB3	1:8:A:PHE:H	12	0.67
(1,692)	1:8:A:PHE:HB2	1:8:A:PHE:H	14	0.67
(1,692)	1:8:A:PHE:HB3	1:8:A:PHE:H	14	0.67
(1,687)	1:69:A:ASN:HD21	1:74:A:GLY:H	2	0.67
(1,686)	1:74:A:GLY:H	1:69:A:ASN:HD22	10	0.67
(1,686)	1:74:A:GLY:H	1:69:A:ASN:HD22	18	0.67
(1,502)	1:34:A:GLU:HG2	1:34:A:GLU:H	6	0.67
(1,502)	1:34:A:GLU:HG3	1:34:A:GLU:H	6	0.67
(1,492)	1:22:A:CYS:H	1:24:A:GLY:H	6	0.67
(1,492)	1:22:A:CYS:H	1:24:A:GLY:H	16	0.67
(1,491)	1:22:A:CYS:H	1:24:A:GLY:H	6	0.67
(1,491)	1:22:A:CYS:H	1:24:A:GLY:H	16	0.67
(1,436)	1:73:A:SER:H	1:72:A:ASP:H	10	0.67
(1,391)	1:54:A:HIS:HA	1:53:A:ALA:H	3	0.67
(1,391)	1:54:A:HIS:HA	1:53:A:ALA:H	10	0.67
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	15	0.67
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	15	0.67
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	15	0.67
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	15	0.67
(1,212)	1:96:A:ARG:H	1:92:A:CYS:HA	8	0.67
(2,363)	1:49:A:ILE:HB	1:49:A:ILE:H	2	0.66
(2,363)	1:49:A:ILE:HB	1:49:A:ILE:H	6	0.66
(2,363)	1:49:A:ILE:HB	1:49:A:ILE:H	11	0.66
(2,361)	1:61:A:VAL:HG21	1:64:A:ARG:H	19	0.66

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,330)	1:92:A:CYS:HA	1:93:A:SER:H	3	0.66
(1,923)	1:8:A:PHE:HB2	1:16:A:VAL:HA	6	0.66
(1,923)	1:8:A:PHE:HB2	1:16:A:VAL:HA	7	0.66
(1,923)	1:8:A:PHE:HB2	1:16:A:VAL:HA	9	0.66
(1,890)	1:81:A:GLY:HA2	1:63:A:TRP:HE1	10	0.66
(1,890)	1:81:A:GLY:HA2	1:63:A:TRP:HE1	10	0.66
(1,890)	1:81:A:GLY:HA3	1:63:A:TRP:HE1	10	0.66
(1,890)	1:81:A:GLY:HA3	1:63:A:TRP:HE1	10	0.66
(1,700)	1:69:A:ASN:HB2	1:69:A:ASN:H	9	0.66
(1,700)	1:69:A:ASN:HB3	1:69:A:ASN:H	9	0.66
(1,692)	1:8:A:PHE:HB2	1:8:A:PHE:H	15	0.66
(1,692)	1:8:A:PHE:HB3	1:8:A:PHE:H	15	0.66
(1,502)	1:34:A:GLU:HG2	1:34:A:GLU:H	8	0.66
(1,502)	1:34:A:GLU:HG3	1:34:A:GLU:H	8	0.66
(1,502)	1:34:A:GLU:HG2	1:34:A:GLU:H	9	0.66
(1,502)	1:34:A:GLU:HG3	1:34:A:GLU:H	9	0.66
(1,492)	1:22:A:CYS:H	1:24:A:GLY:H	5	0.66
(1,492)	1:22:A:CYS:H	1:24:A:GLY:H	20	0.66
(1,491)	1:22:A:CYS:H	1:24:A:GLY:H	5	0.66
(1,491)	1:22:A:CYS:H	1:24:A:GLY:H	20	0.66
(1,480)	1:10:A:CYS:HB2	1:10:A:CYS:H	17	0.66
(1,480)	1:10:A:CYS:HB3	1:10:A:CYS:H	17	0.66
(1,447)	1:71:A:CYS:HA	1:74:A:GLY:H	19	0.66
(1,391)	1:54:A:HIS:HA	1:53:A:ALA:H	18	0.66
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	2	0.66
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	2	0.66
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	2	0.66
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	2	0.66
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	3	0.66
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	3	0.66
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	3	0.66
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	3	0.66
(1,150)	1:104:A:CYS:H	1:106:A:GLY:H	5	0.66
(2,381)	1:85:A:CYS:HB3	1:90:A:PHE:H	16	0.65
(2,374)	1:25:A:ASP:HA	1:23:A:ASP:H	19	0.65
(2,337)	1:53:A:ALA:HB3	1:55:A:SER:H	8	0.65
(2,327)	1:64:A:ARG:HG2	1:71:A:CYS:H	3	0.65
(2,327)	1:68:A:GLU:HG2	1:71:A:CYS:H	5	0.65
(2,327)	1:68:A:GLU:HG2	1:71:A:CYS:H	10	0.65
(2,296)	1:113:A:GLY:HA2	1:117:A:LEU:H	18	0.65
(2,244)	1:45:A:ARG:HA	1:47:A:HIS:H	4	0.65
(2,223)	1:46:A:ILE:HB	1:45:A:ARG:H	5	0.65

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	4	0.65
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	4	0.65
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	4	0.65
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	4	0.65
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	4	0.65
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	4	0.65
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	4	0.65
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	4	0.65
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	4	0.65
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	4	0.65
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	4	0.65
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	4	0.65
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	4	0.65
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	4	0.65
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	4	0.65
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	4	0.65
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	4	0.65
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	4	0.65
(2,66)	1:5:A:GLU:H	1:7:A:ASP:H	5	0.65
(2,44)	1:83:A:ILE:HG22	1:97:A:CYS:H	2	0.65
(1,898)	1:57:A:GLN:HE22	1:71:A:CYS:H	3	0.65
(1,813)	1:107:A:GLN:HE21	1:108:A:ASP:HA	10	0.65
(1,721)	1:21:A:LYS:HG2	1:22:A:CYS:H	1	0.65
(1,721)	1:21:A:LYS:HG3	1:22:A:CYS:H	1	0.65
(1,708)	1:44:A:CYS:HB2	1:45:A:ARG:H	17	0.65
(1,708)	1:44:A:CYS:HB3	1:45:A:ARG:H	17	0.65
(1,700)	1:69:A:ASN:HB2	1:69:A:ASN:H	1	0.65
(1,700)	1:69:A:ASN:HB3	1:69:A:ASN:H	1	0.65
(1,686)	1:74:A:GLY:H	1:69:A:ASN:HD22	13	0.65
(1,634)	1:79:A:ASN:HD22	1:79:A:ASN:HA	8	0.65
(1,634)	1:79:A:ASN:HD22	1:79:A:ASN:HA	20	0.65
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	2	0.65
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	2	0.65
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	2	0.65
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	2	0.65
(1,502)	1:34:A:GLU:HG2	1:34:A:GLU:H	17	0.65
(1,502)	1:34:A:GLU:HG3	1:34:A:GLU:H	17	0.65
(1,492)	1:22:A:CYS:H	1:24:A:GLY:H	1	0.65
(1,492)	1:22:A:CYS:H	1:24:A:GLY:H	8	0.65
(1,492)	1:22:A:CYS:H	1:24:A:GLY:H	11	0.65
(1,492)	1:22:A:CYS:H	1:24:A:GLY:H	13	0.65
(1,491)	1:22:A:CYS:H	1:24:A:GLY:H	1	0.65

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,491)	1:22:A:CYS:H	1:24:A:GLY:H	8	0.65
(1,491)	1:22:A:CYS:H	1:24:A:GLY:H	11	0.65
(1,491)	1:22:A:CYS:H	1:24:A:GLY:H	13	0.65
(1,430)	1:69:A:ASN:HB2	1:69:A:ASN:H	14	0.65
(1,430)	1:69:A:ASN:HB3	1:69:A:ASN:H	14	0.65
(1,391)	1:54:A:HIS:HA	1:53:A:ALA:H	16	0.65
(1,391)	1:54:A:HIS:HA	1:53:A:ALA:H	20	0.65
(1,212)	1:96:A:ARG:H	1:92:A:CYS:HA	2	0.65
(1,212)	1:96:A:ARG:H	1:92:A:CYS:HA	16	0.65
(1,2)	1:112:A:ASP:H	1:113:A:GLY:H	5	0.65
(2,374)	1:25:A:ASP:HA	1:23:A:ASP:H	3	0.64
(2,363)	1:49:A:ILE:HB	1:49:A:ILE:H	17	0.64
(2,361)	1:61:A:VAL:HG21	1:64:A:ARG:H	18	0.64
(2,327)	1:64:A:ARG:HG2	1:71:A:CYS:H	13	0.64
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	17	0.64
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	17	0.64
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	17	0.64
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	17	0.64
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	17	0.64
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	17	0.64
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	17	0.64
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	17	0.64
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	17	0.64
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	17	0.64
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	17	0.64
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	17	0.64
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	17	0.64
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	17	0.64
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	17	0.64
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	17	0.64
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	17	0.64
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	17	0.64
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	17	0.64
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	17	0.64
(2,66)	1:5:A:GLU:H	1:7:A:ASP:H	1	0.64
(1,923)	1:8:A:PHE:HB2	1:16:A:VAL:HA	11	0.64
(1,700)	1:69:A:ASN:HB2	1:69:A:ASN:H	7	0.64
(1,700)	1:69:A:ASN:HB3	1:69:A:ASN:H	7	0.64
(1,692)	1:8:A:PHE:HB2	1:8:A:PHE:H	4	0.64
(1,692)	1:8:A:PHE:HB3	1:8:A:PHE:H	4	0.64
(1,687)	1:69:A:ASN:HD21	1:74:A:GLY:H	1	0.64
(1,687)	1:69:A:ASN:HD21	1:74:A:GLY:H	7	0.64
(1,687)	1:69:A:ASN:HD21	1:74:A:GLY:H	13	0.64
(1,686)	1:74:A:GLY:H	1:69:A:ASN:HD22	14	0.64

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,670)	1:107:A:GLN:HB2	1:105:A:ASN:HD22	9	0.64
(1,670)	1:107:A:GLN:HB2	1:105:A:ASN:HD22	9	0.64
(1,670)	1:107:A:GLN:HB3	1:105:A:ASN:HD22	9	0.64
(1,670)	1:107:A:GLN:HB3	1:105:A:ASN:HD22	9	0.64
(1,634)	1:79:A:ASN:HD22	1:79:A:ASN:HA	16	0.64
(1,584)	1:27:A:ASP:HB2	1:27:A:ASP:H	8	0.64
(1,584)	1:27:A:ASP:HB3	1:27:A:ASP:H	8	0.64
(1,584)	1:27:A:ASP:HB2	1:27:A:ASP:H	17	0.64
(1,584)	1:27:A:ASP:HB3	1:27:A:ASP:H	17	0.64
(1,583)	1:40:A:HIS:HA	1:38:A:GLN:H	15	0.64
(1,541)	1:115:A:ASP:HB2	1:116:A:GLU:H	20	0.64
(1,541)	1:115:A:ASP:HB3	1:116:A:GLU:H	20	0.64
(1,531)	1:71:A:CYS:HB2	1:71:A:CYS:H	17	0.64
(1,531)	1:71:A:CYS:HB3	1:71:A:CYS:H	17	0.64
(1,502)	1:34:A:GLU:HG2	1:34:A:GLU:H	12	0.64
(1,502)	1:34:A:GLU:HG3	1:34:A:GLU:H	12	0.64
(1,502)	1:34:A:GLU:HG2	1:34:A:GLU:H	20	0.64
(1,502)	1:34:A:GLU:HG3	1:34:A:GLU:H	20	0.64
(1,492)	1:22:A:CYS:H	1:24:A:GLY:H	18	0.64
(1,491)	1:22:A:CYS:H	1:24:A:GLY:H	18	0.64
(1,463)	1:71:A:CYS:HB2	1:78:A:GLU:H	12	0.64
(1,463)	1:71:A:CYS:HB3	1:78:A:GLU:H	12	0.64
(1,391)	1:54:A:HIS:HA	1:53:A:ALA:H	1	0.64
(1,391)	1:54:A:HIS:HA	1:53:A:ALA:H	9	0.64
(1,391)	1:54:A:HIS:HA	1:53:A:ALA:H	11	0.64
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	16	0.64
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	16	0.64
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	16	0.64
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	16	0.64
(1,212)	1:96:A:ARG:H	1:92:A:CYS:HA	3	0.64
(1,27)	1:118:A:ASP:H	1:117:A:LEU:H	19	0.64
(1,2)	1:112:A:ASP:H	1:113:A:GLY:H	19	0.64
(4,8)	1:8:A:PHE:O	1:16:A:VAL:H	7	0.63
(2,374)	1:25:A:ASP:HA	1:23:A:ASP:H	18	0.63
(2,374)	1:25:A:ASP:HA	1:23:A:ASP:H	20	0.63
(2,330)	1:92:A:CYS:HA	1:93:A:SER:H	18	0.63
(2,296)	1:114:A:SER:HB2	1:117:A:LEU:H	5	0.63
(2,207)	1:79:A:ASN:HB2	1:79:A:ASN:HD22	17	0.63
(1,923)	1:8:A:PHE:HB2	1:16:A:VAL:HA	15	0.63
(1,877)	1:22:A:CYS:HA	1:44:A:CYS:H	6	0.63
(1,723)	1:23:A:ASP:H	1:21:A:LYS:HA	4	0.63
(1,723)	1:23:A:ASP:H	1:21:A:LYS:HA	12	0.63

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,723)	1:23:A:ASP:H	1:21:A:LYS:HA	16	0.63
(1,708)	1:44:A:CYS:HB2	1:45:A:ARG:H	7	0.63
(1,708)	1:44:A:CYS:HB3	1:45:A:ARG:H	7	0.63
(1,700)	1:69:A:ASN:HB2	1:69:A:ASN:H	2	0.63
(1,700)	1:69:A:ASN:HB3	1:69:A:ASN:H	2	0.63
(1,687)	1:69:A:ASN:HD21	1:74:A:GLY:H	9	0.63
(1,492)	1:22:A:CYS:H	1:24:A:GLY:H	10	0.63
(1,491)	1:22:A:CYS:H	1:24:A:GLY:H	10	0.63
(1,459)	1:70:A:ASP:HA	1:76:A:ASP:H	10	0.63
(1,431)	1:72:A:ASP:H	1:70:A:ASP:H	14	0.63
(1,430)	1:69:A:ASN:HB2	1:69:A:ASN:H	18	0.63
(1,430)	1:69:A:ASN:HB3	1:69:A:ASN:H	18	0.63
(1,347)	1:31:A:GLY:H	1:28:A:CYS:H	19	0.63
(1,2)	1:112:A:ASP:H	1:113:A:GLY:H	17	0.63
(2,374)	1:25:A:ASP:HA	1:23:A:ASP:H	1	0.62
(2,374)	1:25:A:ASP:HA	1:23:A:ASP:H	2	0.62
(2,374)	1:25:A:ASP:HA	1:23:A:ASP:H	5	0.62
(2,374)	1:20:A:TRP:HA	1:23:A:ASP:H	8	0.62
(2,374)	1:25:A:ASP:HA	1:23:A:ASP:H	9	0.62
(2,374)	1:25:A:ASP:HA	1:23:A:ASP:H	11	0.62
(2,374)	1:25:A:ASP:HA	1:23:A:ASP:H	14	0.62
(2,361)	1:61:A:VAL:HG23	1:64:A:ARG:H	10	0.62
(2,359)	1:98:A:ILE:HD11	1:98:A:ILE:H	16	0.62
(2,323)	1:64:A:ARG:HG2	1:68:A:GLU:H	3	0.62
(2,296)	1:114:A:SER:HB3	1:117:A:LEU:H	10	0.62
(2,276)	1:43:A:THR:HA	1:57:A:GLN:H	18	0.62
(2,212)	1:88:A:ASP:H	1:86:A:SER:H	17	0.62
(2,207)	1:79:A:ASN:HB2	1:79:A:ASN:HD22	14	0.62
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	12	0.62
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	12	0.62
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	12	0.62
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	12	0.62
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	12	0.62
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	12	0.62
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	12	0.62
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	12	0.62
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	12	0.62
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	12	0.62
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	12	0.62
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	12	0.62
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	12	0.62
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	12	0.62

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	12	0.62
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	12	0.62
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	12	0.62
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	12	0.62
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	14	0.62
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	14	0.62
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	14	0.62
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	14	0.62
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	14	0.62
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	14	0.62
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	14	0.62
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	14	0.62
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	14	0.62
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	14	0.62
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	14	0.62
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	14	0.62
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	14	0.62
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	14	0.62
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	14	0.62
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	14	0.62
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	14	0.62
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	14	0.62
(2,52)	1:60:A:PRO:HD2	1:63:A:TRP:HE1	17	0.62
(2,25)	1:79:A:ASN:HD22	1:80:A:CYS:HA	16	0.62
(1,824)	1:118:A:ASP:H	1:116:A:GLU:H	9	0.62
(1,813)	1:107:A:GLN:HE21	1:108:A:ASP:HA	17	0.62
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	14	0.62
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	14	0.62
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	14	0.62
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	14	0.62
(1,723)	1:23:A:ASP:H	1:21:A:LYS:HA	6	0.62
(1,723)	1:23:A:ASP:H	1:21:A:LYS:HA	10	0.62
(1,686)	1:74:A:GLY:H	1:69:A:ASN:HD22	9	0.62
(1,642)	1:82:A:ASN:HA	1:82:A:ASN:HD22	4	0.62
(1,628)	1:71:A:CYS:HB2	1:57:A:GLN:HE22	6	0.62
(1,628)	1:71:A:CYS:HB3	1:57:A:GLN:HE22	6	0.62
(1,622)	1:12:A:ASN:HB2	1:12:A:ASN:HD21	1	0.62
(1,622)	1:12:A:ASN:HB3	1:12:A:ASN:HD21	1	0.62
(1,622)	1:12:A:ASN:HB2	1:12:A:ASN:HD21	2	0.62
(1,622)	1:12:A:ASN:HB3	1:12:A:ASN:HD21	2	0.62
(1,622)	1:12:A:ASN:HB2	1:12:A:ASN:HD21	3	0.62
(1,622)	1:12:A:ASN:HB3	1:12:A:ASN:HD21	3	0.62

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,622)	1:12:A:ASN:HB2	1:12:A:ASN:HD21	4	0.62
(1,622)	1:12:A:ASN:HB3	1:12:A:ASN:HD21	4	0.62
(1,622)	1:12:A:ASN:HB2	1:12:A:ASN:HD21	5	0.62
(1,622)	1:12:A:ASN:HB3	1:12:A:ASN:HD21	5	0.62
(1,622)	1:12:A:ASN:HB2	1:12:A:ASN:HD21	6	0.62
(1,622)	1:12:A:ASN:HB3	1:12:A:ASN:HD21	6	0.62
(1,622)	1:12:A:ASN:HB2	1:12:A:ASN:HD21	8	0.62
(1,622)	1:12:A:ASN:HB3	1:12:A:ASN:HD21	8	0.62
(1,622)	1:12:A:ASN:HB2	1:12:A:ASN:HD21	10	0.62
(1,622)	1:12:A:ASN:HB3	1:12:A:ASN:HD21	10	0.62
(1,622)	1:12:A:ASN:HB2	1:12:A:ASN:HD21	11	0.62
(1,622)	1:12:A:ASN:HB3	1:12:A:ASN:HD21	11	0.62
(1,622)	1:12:A:ASN:HB2	1:12:A:ASN:HD21	12	0.62
(1,622)	1:12:A:ASN:HB3	1:12:A:ASN:HD21	12	0.62
(1,622)	1:12:A:ASN:HB2	1:12:A:ASN:HD21	13	0.62
(1,622)	1:12:A:ASN:HB3	1:12:A:ASN:HD21	13	0.62
(1,622)	1:12:A:ASN:HB2	1:12:A:ASN:HD21	14	0.62
(1,622)	1:12:A:ASN:HB3	1:12:A:ASN:HD21	14	0.62
(1,622)	1:12:A:ASN:HB2	1:12:A:ASN:HD21	15	0.62
(1,622)	1:12:A:ASN:HB3	1:12:A:ASN:HD21	15	0.62
(1,622)	1:12:A:ASN:HB2	1:12:A:ASN:HD21	16	0.62
(1,622)	1:12:A:ASN:HB3	1:12:A:ASN:HD21	16	0.62
(1,622)	1:12:A:ASN:HB2	1:12:A:ASN:HD21	17	0.62
(1,622)	1:12:A:ASN:HB3	1:12:A:ASN:HD21	17	0.62
(1,622)	1:12:A:ASN:HB2	1:12:A:ASN:HD21	18	0.62
(1,622)	1:12:A:ASN:HB3	1:12:A:ASN:HD21	18	0.62
(1,622)	1:12:A:ASN:HB2	1:12:A:ASN:HD21	20	0.62
(1,622)	1:12:A:ASN:HB3	1:12:A:ASN:HD21	20	0.62
(1,502)	1:34:A:GLU:HG2	1:34:A:GLU:H	14	0.62
(1,502)	1:34:A:GLU:HG3	1:34:A:GLU:H	14	0.62
(1,499)	1:33:A:ASP:HB2	1:33:A:ASP:H	5	0.62
(1,499)	1:33:A:ASP:HB3	1:33:A:ASP:H	5	0.62
(1,499)	1:33:A:ASP:HB2	1:33:A:ASP:H	6	0.62
(1,499)	1:33:A:ASP:HB3	1:33:A:ASP:H	6	0.62
(1,492)	1:22:A:CYS:H	1:24:A:GLY:H	3	0.62
(1,491)	1:22:A:CYS:H	1:24:A:GLY:H	3	0.62
(1,391)	1:54:A:HIS:HA	1:53:A:ALA:H	5	0.62
(1,391)	1:54:A:HIS:HA	1:53:A:ALA:H	8	0.62
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	18	0.62
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	18	0.62
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	18	0.62
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	18	0.62

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,137)	1:109:A:ASP:H	1:113:A:GLY:HA2	6	0.62
(1,137)	1:109:A:ASP:H	1:113:A:GLY:HA3	6	0.62
(1,27)	1:118:A:ASP:H	1:117:A:LEU:H	1	0.62
(1,2)	1:112:A:ASP:H	1:113:A:GLY:H	14	0.62
(2,363)	1:49:A:ILE:HB	1:49:A:ILE:H	1	0.61
(2,330)	1:92:A:CYS:HA	1:93:A:SER:H	14	0.61
(2,264)	1:49:A:ILE:HB	1:50:A:SER:H	5	0.61
(2,264)	1:49:A:ILE:HB	1:50:A:SER:H	11	0.61
(2,212)	1:88:A:ASP:H	1:86:A:SER:H	3	0.61
(2,212)	1:88:A:ASP:H	1:86:A:SER:H	9	0.61
(2,212)	1:88:A:ASP:H	1:86:A:SER:H	15	0.61
(1,824)	1:118:A:ASP:H	1:116:A:GLU:H	10	0.61
(1,813)	1:107:A:GLN:HE21	1:108:A:ASP:HA	2	0.61
(1,721)	1:21:A:LYS:HG2	1:22:A:CYS:H	8	0.61
(1,721)	1:21:A:LYS:HG3	1:22:A:CYS:H	8	0.61
(1,708)	1:44:A:CYS:HB2	1:45:A:ARG:H	13	0.61
(1,708)	1:44:A:CYS:HB3	1:45:A:ARG:H	13	0.61
(1,700)	1:69:A:ASN:HB2	1:69:A:ASN:H	17	0.61
(1,700)	1:69:A:ASN:HB3	1:69:A:ASN:H	17	0.61
(1,700)	1:69:A:ASN:HB2	1:69:A:ASN:H	19	0.61
(1,700)	1:69:A:ASN:HB3	1:69:A:ASN:H	19	0.61
(1,687)	1:69:A:ASN:HD21	1:74:A:GLY:H	3	0.61
(1,622)	1:12:A:ASN:HB2	1:12:A:ASN:HD21	7	0.61
(1,622)	1:12:A:ASN:HB3	1:12:A:ASN:HD21	7	0.61
(1,622)	1:12:A:ASN:HB2	1:12:A:ASN:HD21	9	0.61
(1,622)	1:12:A:ASN:HB3	1:12:A:ASN:HD21	9	0.61
(1,622)	1:12:A:ASN:HB2	1:12:A:ASN:HD21	19	0.61
(1,622)	1:12:A:ASN:HB3	1:12:A:ASN:HD21	19	0.61
(1,584)	1:27:A:ASP:HB2	1:27:A:ASP:H	16	0.61
(1,584)	1:27:A:ASP:HB3	1:27:A:ASP:H	16	0.61
(1,555)	1:103:A:VAL:HG11	1:104:A:CYS:H	14	0.61
(1,555)	1:103:A:VAL:HG12	1:104:A:CYS:H	14	0.61
(1,555)	1:103:A:VAL:HG13	1:104:A:CYS:H	14	0.61
(1,555)	1:103:A:VAL:HG21	1:104:A:CYS:H	14	0.61
(1,555)	1:103:A:VAL:HG22	1:104:A:CYS:H	14	0.61
(1,555)	1:103:A:VAL:HG23	1:104:A:CYS:H	14	0.61
(1,555)	1:103:A:VAL:HG11	1:104:A:CYS:H	18	0.61
(1,555)	1:103:A:VAL:HG12	1:104:A:CYS:H	18	0.61
(1,555)	1:103:A:VAL:HG13	1:104:A:CYS:H	18	0.61
(1,555)	1:103:A:VAL:HG21	1:104:A:CYS:H	18	0.61
(1,555)	1:103:A:VAL:HG22	1:104:A:CYS:H	18	0.61
(1,555)	1:103:A:VAL:HG23	1:104:A:CYS:H	18	0.61

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,492)	1:22:A:CYS:H	1:24:A:GLY:H	4	0.61
(1,491)	1:22:A:CYS:H	1:24:A:GLY:H	4	0.61
(1,431)	1:72:A:ASP:H	1:70:A:ASP:H	18	0.61
(1,430)	1:69:A:ASN:HB2	1:69:A:ASN:H	4	0.61
(1,430)	1:69:A:ASN:HB3	1:69:A:ASN:H	4	0.61
(1,430)	1:69:A:ASN:HB2	1:69:A:ASN:H	6	0.61
(1,430)	1:69:A:ASN:HB3	1:69:A:ASN:H	6	0.61
(1,391)	1:54:A:HIS:HA	1:53:A:ALA:H	13	0.61
(1,346)	1:32:A:SER:H	1:31:A:GLY:H	19	0.61
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	8	0.61
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	8	0.61
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	8	0.61
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	8	0.61
(1,80)	1:44:A:CYS:HB2	1:45:A:ARG:H	5	0.61
(1,80)	1:44:A:CYS:HB3	1:45:A:ARG:H	5	0.61
(1,27)	1:118:A:ASP:H	1:117:A:LEU:H	2	0.61
(1,27)	1:118:A:ASP:H	1:117:A:LEU:H	8	0.61
(1,27)	1:118:A:ASP:H	1:117:A:LEU:H	10	0.61
(2,374)	1:25:A:ASP:HA	1:23:A:ASP:H	10	0.6
(2,311)	1:90:A:PHE:HB3	1:91:A:THR:H	1	0.6
(2,180)	1:11:A:ASN:HA	1:11:A:ASN:HD21	20	0.6
(2,66)	1:4:A:ALA:H	1:7:A:ASP:H	13	0.6
(2,66)	1:4:A:ALA:H	1:7:A:ASP:H	16	0.6
(2,52)	1:60:A:PRO:HD2	1:63:A:TRP:HE1	13	0.6
(2,46)	1:114:A:SER:HG	1:115:A:ASP:H	20	0.6
(2,25)	1:79:A:ASN:HD22	1:80:A:CYS:HA	7	0.6
(2,25)	1:79:A:ASN:HD22	1:80:A:CYS:HA	11	0.6
(1,898)	1:57:A:GLN:HE22	1:71:A:CYS:H	12	0.6
(1,849)	1:33:A:ASP:H	1:11:A:ASN:H	15	0.6
(1,824)	1:118:A:ASP:H	1:116:A:GLU:H	8	0.6
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG12	14	0.6
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG13	14	0.6
(1,723)	1:23:A:ASP:H	1:21:A:LYS:HA	7	0.6
(1,723)	1:23:A:ASP:H	1:21:A:LYS:HA	18	0.6
(1,686)	1:74:A:GLY:H	1:69:A:ASN:HD22	5	0.6
(1,634)	1:79:A:ASN:HD22	1:79:A:ASN:HA	7	0.6
(1,555)	1:103:A:VAL:HG11	1:104:A:CYS:H	11	0.6
(1,555)	1:103:A:VAL:HG12	1:104:A:CYS:H	11	0.6
(1,555)	1:103:A:VAL:HG13	1:104:A:CYS:H	11	0.6
(1,555)	1:103:A:VAL:HG21	1:104:A:CYS:H	11	0.6
(1,555)	1:103:A:VAL:HG22	1:104:A:CYS:H	11	0.6
(1,555)	1:103:A:VAL:HG23	1:104:A:CYS:H	11	0.6

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,531)	1:71:A:CYS:HB2	1:71:A:CYS:H	20	0.6
(1,531)	1:71:A:CYS:HB3	1:71:A:CYS:H	20	0.6
(1,502)	1:34:A:GLU:HG2	1:34:A:GLU:H	10	0.6
(1,502)	1:34:A:GLU:HG3	1:34:A:GLU:H	10	0.6
(1,502)	1:34:A:GLU:HG2	1:34:A:GLU:H	18	0.6
(1,502)	1:34:A:GLU:HG3	1:34:A:GLU:H	18	0.6
(1,492)	1:22:A:CYS:H	1:24:A:GLY:H	12	0.6
(1,491)	1:22:A:CYS:H	1:24:A:GLY:H	12	0.6
(1,463)	1:71:A:CYS:HB2	1:78:A:GLU:H	15	0.6
(1,463)	1:71:A:CYS:HB3	1:78:A:GLU:H	15	0.6
(1,431)	1:72:A:ASP:H	1:70:A:ASP:H	4	0.6
(1,430)	1:69:A:ASN:HB2	1:69:A:ASN:H	10	0.6
(1,430)	1:69:A:ASN:HB3	1:69:A:ASN:H	10	0.6
(1,430)	1:69:A:ASN:HB2	1:69:A:ASN:H	13	0.6
(1,430)	1:69:A:ASN:HB3	1:69:A:ASN:H	13	0.6
(1,430)	1:69:A:ASN:HB2	1:69:A:ASN:H	20	0.6
(1,430)	1:69:A:ASN:HB3	1:69:A:ASN:H	20	0.6
(1,391)	1:54:A:HIS:HA	1:53:A:ALA:H	6	0.6
(1,391)	1:54:A:HIS:HA	1:53:A:ALA:H	7	0.6
(1,212)	1:96:A:ARG:H	1:92:A:CYS:HA	19	0.6
(1,137)	1:109:A:ASP:H	1:113:A:GLY:HA2	3	0.6
(1,137)	1:109:A:ASP:H	1:113:A:GLY:HA3	3	0.6
(1,118)	1:115:A:ASP:H	1:113:A:GLY:H	10	0.6
(1,27)	1:118:A:ASP:H	1:117:A:LEU:H	3	0.6
(1,27)	1:118:A:ASP:H	1:117:A:LEU:H	16	0.6
(2,374)	1:25:A:ASP:HA	1:23:A:ASP:H	4	0.59
(2,374)	1:25:A:ASP:HA	1:23:A:ASP:H	15	0.59
(2,374)	1:25:A:ASP:HA	1:23:A:ASP:H	16	0.59
(2,330)	1:114:A:SER:HG	1:93:A:SER:H	7	0.59
(2,330)	1:92:A:CYS:HA	1:93:A:SER:H	20	0.59
(2,327)	1:64:A:ARG:HG2	1:71:A:CYS:H	9	0.59
(2,327)	1:68:A:GLU:HG3	1:71:A:CYS:H	15	0.59
(2,257)	1:33:A:ASP:HA	1:38:A:GLN:HE22	13	0.59
(2,207)	1:79:A:ASN:HB2	1:79:A:ASN:HD22	15	0.59
(2,193)	1:117:A:LEU:HD13	1:109:A:ASP:H	12	0.59
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	15	0.59
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	15	0.59
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	15	0.59
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	15	0.59
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	15	0.59
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	15	0.59
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	15	0.59

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	15	0.59
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	15	0.59
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	15	0.59
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	15	0.59
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	15	0.59
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	15	0.59
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	15	0.59
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	15	0.59
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	15	0.59
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	15	0.59
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	15	0.59
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	15	0.59
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	20	0.59
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	20	0.59
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	20	0.59
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	20	0.59
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	20	0.59
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	20	0.59
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	20	0.59
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	20	0.59
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	20	0.59
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	20	0.59
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	20	0.59
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	20	0.59
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	20	0.59
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	20	0.59
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	20	0.59
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	20	0.59
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	20	0.59
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	20	0.59
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	20	0.59
(2,180)	1:11:A:ASN:HA	1:11:A:ASN:HD21	11	0.59
(2,180)	1:11:A:ASN:HA	1:11:A:ASN:HD21	16	0.59
(2,166)	1:86:A:SER:HA	1:79:A:ASN:HD21	19	0.59
(2,166)	1:86:A:SER:HA	1:79:A:ASN:HD21	20	0.59
(1,824)	1:118:A:ASP:H	1:116:A:GLU:H	1	0.59
(1,803)	1:101:A:ASN:HD21	1:99:A:SER:H	5	0.59
(1,803)	1:101:A:ASN:HD21	1:99:A:SER:H	19	0.59
(1,772)	1:68:A:GLU:H	1:64:A:ARG:H	8	0.59
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD2	3	0.59
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD3	3	0.59
(1,688)	1:69:A:ASN:H	1:69:A:ASN:HD22	6	0.59
(1,687)	1:69:A:ASN:HD21	1:74:A:GLY:H	16	0.59
(1,634)	1:79:A:ASN:HD22	1:79:A:ASN:HA	19	0.59

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,583)	1:40:A:HIS:HA	1:38:A:GLN:H	18	0.59
(1,555)	1:103:A:VAL:HG11	1:104:A:CYS:H	12	0.59
(1,555)	1:103:A:VAL:HG12	1:104:A:CYS:H	12	0.59
(1,555)	1:103:A:VAL:HG13	1:104:A:CYS:H	12	0.59
(1,555)	1:103:A:VAL:HG21	1:104:A:CYS:H	12	0.59
(1,555)	1:103:A:VAL:HG22	1:104:A:CYS:H	12	0.59
(1,555)	1:103:A:VAL:HG23	1:104:A:CYS:H	12	0.59
(1,502)	1:34:A:GLU:HG2	1:34:A:GLU:H	4	0.59
(1,502)	1:34:A:GLU:HG3	1:34:A:GLU:H	4	0.59
(1,502)	1:34:A:GLU:HG2	1:34:A:GLU:H	15	0.59
(1,502)	1:34:A:GLU:HG3	1:34:A:GLU:H	15	0.59
(1,459)	1:70:A:ASP:HA	1:76:A:ASP:H	13	0.59
(1,430)	1:69:A:ASN:HB2	1:69:A:ASN:H	3	0.59
(1,430)	1:69:A:ASN:HB3	1:69:A:ASN:H	3	0.59
(1,430)	1:69:A:ASN:HB2	1:69:A:ASN:H	12	0.59
(1,430)	1:69:A:ASN:HB3	1:69:A:ASN:H	12	0.59
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	20	0.59
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	20	0.59
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	20	0.59
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	20	0.59
(1,212)	1:96:A:ARG:H	1:92:A:CYS:HA	5	0.59
(1,212)	1:96:A:ARG:H	1:92:A:CYS:HA	9	0.59
(1,118)	1:115:A:ASP:H	1:113:A:GLY:H	1	0.59
(1,58)	1:66:A:ASP:H	1:65:A:CYS:H	12	0.59
(1,27)	1:118:A:ASP:H	1:117:A:LEU:H	13	0.59
(2,298)	1:28:A:CYS:HB2	1:14:A:GLN:HE22	1	0.58
(2,296)	1:113:A:GLY:HA2	1:117:A:LEU:H	12	0.58
(2,264)	1:49:A:ILE:HB	1:50:A:SER:H	6	0.58
(2,264)	1:49:A:ILE:HB	1:50:A:SER:H	13	0.58
(2,31)	1:59:A:ILE:HD12	1:71:A:CYS:H	2	0.58
(2,25)	1:79:A:ASN:HD22	1:80:A:CYS:HA	3	0.58
(1,783)	1:71:A:CYS:HB2	1:74:A:GLY:H	7	0.58
(1,783)	1:71:A:CYS:HB3	1:74:A:GLY:H	7	0.58
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG12	16	0.58
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG13	16	0.58
(1,723)	1:23:A:ASP:H	1:21:A:LYS:HA	13	0.58
(1,723)	1:23:A:ASP:H	1:21:A:LYS:HA	19	0.58
(1,721)	1:21:A:LYS:HG2	1:22:A:CYS:H	5	0.58
(1,721)	1:21:A:LYS:HG3	1:22:A:CYS:H	5	0.58
(1,693)	1:21:A:LYS:HD2	1:21:A:LYS:H	5	0.58
(1,693)	1:21:A:LYS:HD3	1:21:A:LYS:H	5	0.58
(1,687)	1:69:A:ASN:HD21	1:74:A:GLY:H	11	0.58

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,634)	1:79:A:ASN:HD22	1:79:A:ASN:HA	3	0.58
(1,587)	1:14:A:GLN:H	1:12:A:ASN:H	15	0.58
(1,543)	1:112:A:ASP:HB2	1:114:A:SER:H	8	0.58
(1,543)	1:112:A:ASP:HB3	1:114:A:SER:H	8	0.58
(1,492)	1:22:A:CYS:H	1:24:A:GLY:H	14	0.58
(1,492)	1:22:A:CYS:H	1:24:A:GLY:H	15	0.58
(1,491)	1:22:A:CYS:H	1:24:A:GLY:H	14	0.58
(1,491)	1:22:A:CYS:H	1:24:A:GLY:H	15	0.58
(1,430)	1:69:A:ASN:HB2	1:69:A:ASN:H	8	0.58
(1,430)	1:69:A:ASN:HB3	1:69:A:ASN:H	8	0.58
(1,430)	1:69:A:ASN:HB2	1:69:A:ASN:H	11	0.58
(1,430)	1:69:A:ASN:HB3	1:69:A:ASN:H	11	0.58
(1,430)	1:69:A:ASN:HB2	1:69:A:ASN:H	16	0.58
(1,430)	1:69:A:ASN:HB3	1:69:A:ASN:H	16	0.58
(1,391)	1:54:A:HIS:HA	1:53:A:ALA:H	17	0.58
(1,371)	1:44:A:CYS:HA	1:45:A:ARG:H	9	0.58
(1,80)	1:44:A:CYS:HB2	1:45:A:ARG:H	1	0.58
(1,80)	1:44:A:CYS:HB3	1:45:A:ARG:H	1	0.58
(1,58)	1:66:A:ASP:H	1:65:A:CYS:H	19	0.58
(1,27)	1:118:A:ASP:H	1:117:A:LEU:H	7	0.58
(2,337)	1:53:A:ALA:HB3	1:55:A:SER:H	9	0.57
(2,307)	1:60:A:PRO:HB2	1:63:A:TRP:H	10	0.57
(2,298)	1:28:A:CYS:HB2	1:14:A:GLN:HE22	2	0.57
(2,264)	1:49:A:ILE:HB	1:50:A:SER:H	2	0.57
(2,264)	1:49:A:ILE:HB	1:50:A:SER:H	7	0.57
(2,212)	1:88:A:ASP:H	1:86:A:SER:H	1	0.57
(2,212)	1:88:A:ASP:H	1:86:A:SER:H	5	0.57
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	1	0.57
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	1	0.57
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	1	0.57
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	1	0.57
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	1	0.57
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	1	0.57
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	1	0.57
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	1	0.57
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	1	0.57
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	1	0.57
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	1	0.57
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	1	0.57
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	1	0.57
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	1	0.57
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	1	0.57

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	1	0.57
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	1	0.57
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	1	0.57
(2,180)	1:11:A:ASN:HA	1:11:A:ASN:HD21	13	0.57
(2,168)	1:38:A:GLN:HG2	1:38:A:GLN:H	5	0.57
(2,25)	1:79:A:ASN:HD22	1:80:A:CYS:HA	5	0.57
(1,909)	1:43:A:THR:HG21	1:46:A:ILE:H	16	0.57
(1,807)	1:98:A:ILE:HG12	1:103:A:VAL:H	12	0.57
(1,807)	1:98:A:ILE:HG13	1:103:A:VAL:H	12	0.57
(1,772)	1:68:A:GLU:H	1:64:A:ARG:H	12	0.57
(1,772)	1:68:A:GLU:H	1:64:A:ARG:H	15	0.57
(1,750)	1:57:A:GLN:HB2	1:52:A:GLY:H	20	0.57
(1,750)	1:57:A:GLN:HB2	1:52:A:GLY:H	20	0.57
(1,750)	1:57:A:GLN:HB3	1:52:A:GLY:H	20	0.57
(1,750)	1:57:A:GLN:HB3	1:52:A:GLY:H	20	0.57
(1,723)	1:23:A:ASP:H	1:21:A:LYS:HA	11	0.57
(1,723)	1:23:A:ASP:H	1:21:A:LYS:HA	14	0.57
(1,723)	1:23:A:ASP:H	1:21:A:LYS:HA	15	0.57
(1,708)	1:44:A:CYS:HB2	1:45:A:ARG:H	2	0.57
(1,708)	1:44:A:CYS:HB3	1:45:A:ARG:H	2	0.57
(1,687)	1:69:A:ASN:HD21	1:74:A:GLY:H	14	0.57
(1,634)	1:79:A:ASN:HD22	1:79:A:ASN:HA	1	0.57
(1,587)	1:14:A:GLN:H	1:12:A:ASN:H	14	0.57
(1,583)	1:40:A:HIS:HA	1:38:A:GLN:H	2	0.57
(1,583)	1:40:A:HIS:HA	1:38:A:GLN:H	14	0.57
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	6	0.57
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	6	0.57
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	6	0.57
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	6	0.57
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	17	0.57
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	17	0.57
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	17	0.57
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	17	0.57
(1,502)	1:34:A:GLU:HG2	1:34:A:GLU:H	3	0.57
(1,502)	1:34:A:GLU:HG3	1:34:A:GLU:H	3	0.57
(1,430)	1:69:A:ASN:HB2	1:69:A:ASN:H	5	0.57
(1,430)	1:69:A:ASN:HB3	1:69:A:ASN:H	5	0.57
(1,430)	1:69:A:ASN:HB2	1:69:A:ASN:H	15	0.57
(1,430)	1:69:A:ASN:HB3	1:69:A:ASN:H	15	0.57
(1,391)	1:54:A:HIS:HA	1:53:A:ALA:H	2	0.57
(1,298)	1:14:A:GLN:H	1:11:A:ASN:H	9	0.57
(1,212)	1:96:A:ARG:H	1:92:A:CYS:HA	11	0.57

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:118:A:ASP:H	1:117:A:LEU:H	4	0.57
(1,2)	1:112:A:ASP:H	1:113:A:GLY:H	13	0.57
(2,374)	1:25:A:ASP:HA	1:23:A:ASP:H	6	0.56
(2,374)	1:25:A:ASP:HA	1:23:A:ASP:H	12	0.56
(2,337)	1:53:A:ALA:HB2	1:55:A:SER:H	19	0.56
(2,323)	1:64:A:ARG:HG2	1:68:A:GLU:H	19	0.56
(2,323)	1:64:A:ARG:HG2	1:68:A:GLU:H	20	0.56
(2,264)	1:49:A:ILE:HB	1:50:A:SER:H	9	0.56
(2,241)	1:12:A:ASN:HD22	1:12:A:ASN:HD21	1	0.56
(2,241)	1:12:A:ASN:HD22	1:12:A:ASN:HD21	2	0.56
(2,241)	1:12:A:ASN:HD22	1:12:A:ASN:HD21	3	0.56
(2,241)	1:12:A:ASN:HD22	1:12:A:ASN:HD21	4	0.56
(2,241)	1:12:A:ASN:HD22	1:12:A:ASN:HD21	5	0.56
(2,241)	1:12:A:ASN:HD22	1:12:A:ASN:HD21	6	0.56
(2,241)	1:12:A:ASN:HD22	1:12:A:ASN:HD21	7	0.56
(2,241)	1:12:A:ASN:HD22	1:12:A:ASN:HD21	8	0.56
(2,241)	1:12:A:ASN:HD22	1:12:A:ASN:HD21	9	0.56
(2,241)	1:12:A:ASN:HD22	1:12:A:ASN:HD21	10	0.56
(2,241)	1:12:A:ASN:HD22	1:12:A:ASN:HD21	11	0.56
(2,241)	1:12:A:ASN:HD22	1:12:A:ASN:HD21	12	0.56
(2,241)	1:12:A:ASN:HD22	1:12:A:ASN:HD21	13	0.56
(2,241)	1:12:A:ASN:HD22	1:12:A:ASN:HD21	14	0.56
(2,241)	1:12:A:ASN:HD22	1:12:A:ASN:HD21	15	0.56
(2,241)	1:12:A:ASN:HD22	1:12:A:ASN:HD21	16	0.56
(2,241)	1:12:A:ASN:HD22	1:12:A:ASN:HD21	17	0.56
(2,241)	1:12:A:ASN:HD22	1:12:A:ASN:HD21	18	0.56
(2,241)	1:12:A:ASN:HD22	1:12:A:ASN:HD21	20	0.56
(2,207)	1:79:A:ASN:HB2	1:79:A:ASN:HD22	12	0.56
(2,66)	1:4:A:ALA:H	1:7:A:ASP:H	7	0.56
(1,898)	1:57:A:GLN:HE22	1:71:A:CYS:H	15	0.56
(1,881)	1:48:A:GLU:H	1:45:A:ARG:H	4	0.56
(1,879)	1:48:A:GLU:H	1:45:A:ARG:H	4	0.56
(1,850)	1:12:A:ASN:H	1:11:A:ASN:HD22	2	0.56
(1,723)	1:23:A:ASP:H	1:21:A:LYS:HA	3	0.56
(1,723)	1:23:A:ASP:H	1:21:A:LYS:HA	8	0.56
(1,723)	1:23:A:ASP:H	1:21:A:LYS:HA	9	0.56
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD2	20	0.56
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD3	20	0.56
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG2	15	0.56
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG3	15	0.56
(1,687)	1:69:A:ASN:HD21	1:74:A:GLY:H	18	0.56
(1,686)	1:74:A:GLY:H	1:69:A:ASN:HD22	15	0.56

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,555)	1:103:A:VAL:HG11	1:104:A:CYS:H	13	0.56
(1,555)	1:103:A:VAL:HG12	1:104:A:CYS:H	13	0.56
(1,555)	1:103:A:VAL:HG13	1:104:A:CYS:H	13	0.56
(1,555)	1:103:A:VAL:HG21	1:104:A:CYS:H	13	0.56
(1,555)	1:103:A:VAL:HG22	1:104:A:CYS:H	13	0.56
(1,555)	1:103:A:VAL:HG23	1:104:A:CYS:H	13	0.56
(1,555)	1:103:A:VAL:HG11	1:104:A:CYS:H	15	0.56
(1,555)	1:103:A:VAL:HG12	1:104:A:CYS:H	15	0.56
(1,555)	1:103:A:VAL:HG13	1:104:A:CYS:H	15	0.56
(1,555)	1:103:A:VAL:HG21	1:104:A:CYS:H	15	0.56
(1,555)	1:103:A:VAL:HG22	1:104:A:CYS:H	15	0.56
(1,555)	1:103:A:VAL:HG23	1:104:A:CYS:H	15	0.56
(1,555)	1:103:A:VAL:HG11	1:104:A:CYS:H	16	0.56
(1,555)	1:103:A:VAL:HG12	1:104:A:CYS:H	16	0.56
(1,555)	1:103:A:VAL:HG13	1:104:A:CYS:H	16	0.56
(1,555)	1:103:A:VAL:HG21	1:104:A:CYS:H	16	0.56
(1,555)	1:103:A:VAL:HG22	1:104:A:CYS:H	16	0.56
(1,555)	1:103:A:VAL:HG23	1:104:A:CYS:H	16	0.56
(1,543)	1:112:A:ASP:HB2	1:114:A:SER:H	15	0.56
(1,543)	1:112:A:ASP:HB3	1:114:A:SER:H	15	0.56
(1,531)	1:71:A:CYS:HB2	1:71:A:CYS:H	5	0.56
(1,531)	1:71:A:CYS:HB3	1:71:A:CYS:H	5	0.56
(1,531)	1:71:A:CYS:HB2	1:71:A:CYS:H	11	0.56
(1,531)	1:71:A:CYS:HB3	1:71:A:CYS:H	11	0.56
(1,502)	1:34:A:GLU:HG2	1:34:A:GLU:H	5	0.56
(1,502)	1:34:A:GLU:HG3	1:34:A:GLU:H	5	0.56
(1,447)	1:71:A:CYS:HA	1:74:A:GLY:H	7	0.56
(1,430)	1:69:A:ASN:HB2	1:69:A:ASN:H	9	0.56
(1,430)	1:69:A:ASN:HB3	1:69:A:ASN:H	9	0.56
(1,371)	1:44:A:CYS:HA	1:45:A:ARG:H	6	0.56
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB2	1	0.56
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB3	1	0.56
(1,289)	1:8:A:PHE:HA	1:8:A:PHE:H	11	0.56
(1,289)	1:8:A:PHE:HA	1:8:A:PHE:H	16	0.56
(1,212)	1:96:A:ARG:H	1:92:A:CYS:HA	10	0.56
(1,58)	1:66:A:ASP:H	1:65:A:CYS:H	3	0.56
(1,58)	1:66:A:ASP:H	1:65:A:CYS:H	4	0.56
(1,58)	1:66:A:ASP:H	1:65:A:CYS:H	16	0.56
(1,58)	1:66:A:ASP:H	1:65:A:CYS:H	20	0.56
(1,2)	1:112:A:ASP:H	1:113:A:GLY:H	2	0.56
(4,8)	1:8:A:PHE:O	1:16:A:VAL:H	10	0.55
(2,374)	1:25:A:ASP:HA	1:23:A:ASP:H	7	0.55

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,374)	1:25:A:ASP:HA	1:23:A:ASP:H	13	0.55
(2,323)	1:64:A:ARG:HG2	1:68:A:GLU:H	2	0.55
(2,241)	1:12:A:ASN:HD22	1:12:A:ASN:HD21	19	0.55
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	5	0.55
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	5	0.55
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	5	0.55
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	5	0.55
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	5	0.55
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	5	0.55
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	5	0.55
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	5	0.55
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	5	0.55
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	5	0.55
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	5	0.55
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	5	0.55
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	5	0.55
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	5	0.55
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	5	0.55
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	5	0.55
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	5	0.55
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	5	0.55
(2,66)	1:4:A:ALA:H	1:7:A:ASP:H	2	0.55
(2,66)	1:4:A:ALA:H	1:7:A:ASP:H	8	0.55
(2,66)	1:4:A:ALA:H	1:7:A:ASP:H	14	0.55
(2,25)	1:79:A:ASN:HD22	1:80:A:CYS:HA	12	0.55
(2,25)	1:79:A:ASN:HD22	1:80:A:CYS:HA	20	0.55
(1,877)	1:22:A:CYS:HA	1:44:A:CYS:H	18	0.55
(1,850)	1:12:A:ASN:H	1:11:A:ASN:HD22	7	0.55
(1,803)	1:101:A:ASN:HD21	1:99:A:SER:H	17	0.55
(1,794)	1:82:A:ASN:HD22	1:94:A:SER:H	17	0.55
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	12	0.55
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	12	0.55
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	12	0.55
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	12	0.55
(1,723)	1:23:A:ASP:H	1:21:A:LYS:HA	2	0.55
(1,721)	1:21:A:LYS:HG2	1:22:A:CYS:H	9	0.55
(1,721)	1:21:A:LYS:HG3	1:22:A:CYS:H	9	0.55
(1,721)	1:21:A:LYS:HG2	1:22:A:CYS:H	14	0.55
(1,721)	1:21:A:LYS:HG3	1:22:A:CYS:H	14	0.55
(1,721)	1:21:A:LYS:HG2	1:22:A:CYS:H	20	0.55
(1,721)	1:21:A:LYS:HG3	1:22:A:CYS:H	20	0.55
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD2	18	0.55

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD3	18	0.55
(1,688)	1:69:A:ASN:H	1:69:A:ASN:HD22	8	0.55
(1,587)	1:14:A:GLN:H	1:12:A:ASN:H	10	0.55
(1,583)	1:40:A:HIS:HA	1:38:A:GLN:H	5	0.55
(1,583)	1:40:A:HIS:HA	1:38:A:GLN:H	6	0.55
(1,555)	1:103:A:VAL:HG11	1:104:A:CYS:H	9	0.55
(1,555)	1:103:A:VAL:HG12	1:104:A:CYS:H	9	0.55
(1,555)	1:103:A:VAL:HG13	1:104:A:CYS:H	9	0.55
(1,555)	1:103:A:VAL:HG21	1:104:A:CYS:H	9	0.55
(1,555)	1:103:A:VAL:HG22	1:104:A:CYS:H	9	0.55
(1,555)	1:103:A:VAL:HG23	1:104:A:CYS:H	9	0.55
(1,534)	1:77:A:GLU:HB2	1:77:A:GLU:H	6	0.55
(1,534)	1:77:A:GLU:HB3	1:77:A:GLU:H	6	0.55
(1,531)	1:71:A:CYS:HB2	1:71:A:CYS:H	9	0.55
(1,531)	1:71:A:CYS:HB3	1:71:A:CYS:H	9	0.55
(1,529)	1:59:A:ILE:HD11	1:70:A:ASP:H	18	0.55
(1,529)	1:59:A:ILE:HD12	1:70:A:ASP:H	18	0.55
(1,529)	1:59:A:ILE:HD13	1:70:A:ASP:H	18	0.55
(1,480)	1:10:A:CYS:HB2	1:10:A:CYS:H	5	0.55
(1,480)	1:10:A:CYS:HB3	1:10:A:CYS:H	5	0.55
(1,480)	1:10:A:CYS:HB2	1:10:A:CYS:H	10	0.55
(1,480)	1:10:A:CYS:HB3	1:10:A:CYS:H	10	0.55
(1,480)	1:10:A:CYS:HB2	1:10:A:CYS:H	14	0.55
(1,480)	1:10:A:CYS:HB3	1:10:A:CYS:H	14	0.55
(1,459)	1:70:A:ASP:HA	1:76:A:ASP:H	15	0.55
(1,447)	1:71:A:CYS:HA	1:74:A:GLY:H	1	0.55
(1,430)	1:69:A:ASN:HB2	1:69:A:ASN:H	1	0.55
(1,430)	1:69:A:ASN:HB3	1:69:A:ASN:H	1	0.55
(1,371)	1:44:A:CYS:HA	1:45:A:ARG:H	12	0.55
(1,371)	1:44:A:CYS:HA	1:45:A:ARG:H	16	0.55
(1,371)	1:44:A:CYS:HA	1:45:A:ARG:H	20	0.55
(1,289)	1:8:A:PHE:HA	1:8:A:PHE:H	14	0.55
(1,134)	1:110:A:CYS:H	1:109:A:ASP:HB2	17	0.55
(1,134)	1:110:A:CYS:H	1:109:A:ASP:HB2	17	0.55
(1,134)	1:110:A:CYS:H	1:109:A:ASP:HB3	17	0.55
(1,134)	1:110:A:CYS:H	1:109:A:ASP:HB3	17	0.55
(1,80)	1:44:A:CYS:HB2	1:45:A:ARG:H	17	0.55
(1,80)	1:44:A:CYS:HB3	1:45:A:ARG:H	17	0.55
(1,58)	1:66:A:ASP:H	1:65:A:CYS:H	1	0.55
(1,58)	1:66:A:ASP:H	1:65:A:CYS:H	5	0.55
(1,58)	1:66:A:ASP:H	1:65:A:CYS:H	7	0.55
(1,58)	1:66:A:ASP:H	1:65:A:CYS:H	11	0.55

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:66:A:ASP:H	1:65:A:CYS:H	18	0.55
(1,2)	1:112:A:ASP:H	1:113:A:GLY:H	10	0.55
(2,363)	1:49:A:ILE:HB	1:49:A:ILE:H	15	0.54
(2,330)	1:92:A:CYS:HA	1:93:A:SER:H	12	0.54
(2,327)	1:68:A:GLU:HG2	1:71:A:CYS:H	17	0.54
(2,311)	1:90:A:PHE:HB2	1:91:A:THR:H	19	0.54
(2,296)	1:114:A:SER:HB3	1:117:A:LEU:H	1	0.54
(2,296)	1:114:A:SER:HB2	1:117:A:LEU:H	17	0.54
(2,264)	1:49:A:ILE:HB	1:50:A:SER:H	1	0.54
(2,264)	1:49:A:ILE:HB	1:50:A:SER:H	16	0.54
(2,264)	1:49:A:ILE:HB	1:50:A:SER:H	17	0.54
(2,264)	1:49:A:ILE:HB	1:50:A:SER:H	20	0.54
(2,212)	1:88:A:ASP:H	1:86:A:SER:H	7	0.54
(2,168)	1:38:A:GLN:HG3	1:38:A:GLN:H	19	0.54
(1,888)	1:49:A:ILE:HA	1:61:A:VAL:H	8	0.54
(1,888)	1:49:A:ILE:HA	1:61:A:VAL:H	18	0.54
(1,772)	1:68:A:GLU:H	1:64:A:ARG:H	4	0.54
(1,745)	1:48:A:GLU:HB2	1:49:A:ILE:H	11	0.54
(1,745)	1:48:A:GLU:HB3	1:49:A:ILE:H	11	0.54
(1,723)	1:23:A:ASP:H	1:21:A:LYS:HA	17	0.54
(1,723)	1:23:A:ASP:H	1:21:A:LYS:HA	20	0.54
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD2	15	0.54
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD3	15	0.54
(1,693)	1:21:A:LYS:HD2	1:21:A:LYS:H	6	0.54
(1,693)	1:21:A:LYS:HD3	1:21:A:LYS:H	6	0.54
(1,687)	1:69:A:ASN:HD21	1:74:A:GLY:H	5	0.54
(1,687)	1:69:A:ASN:HD21	1:74:A:GLY:H	10	0.54
(1,634)	1:79:A:ASN:HD22	1:79:A:ASN:HA	5	0.54
(1,634)	1:79:A:ASN:HD22	1:79:A:ASN:HA	9	0.54
(1,608)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	19	0.54
(1,608)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	19	0.54
(1,583)	1:40:A:HIS:HA	1:38:A:GLN:H	12	0.54
(1,583)	1:40:A:HIS:HA	1:38:A:GLN:H	13	0.54
(1,583)	1:40:A:HIS:HA	1:38:A:GLN:H	20	0.54
(1,543)	1:112:A:ASP:HB2	1:114:A:SER:H	11	0.54
(1,543)	1:112:A:ASP:HB3	1:114:A:SER:H	11	0.54
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	8	0.54
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	8	0.54
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	8	0.54
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	8	0.54
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	11	0.54
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	11	0.54

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	11	0.54
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	11	0.54
(1,509)	1:46:A:ILE:HA	1:46:A:ILE:H	5	0.54
(1,509)	1:46:A:ILE:HA	1:46:A:ILE:H	9	0.54
(1,509)	1:46:A:ILE:HA	1:46:A:ILE:H	16	0.54
(1,509)	1:46:A:ILE:HA	1:46:A:ILE:H	17	0.54
(1,509)	1:46:A:ILE:HA	1:46:A:ILE:H	18	0.54
(1,509)	1:46:A:ILE:HA	1:46:A:ILE:H	20	0.54
(1,480)	1:10:A:CYS:HB2	1:10:A:CYS:H	1	0.54
(1,480)	1:10:A:CYS:HB3	1:10:A:CYS:H	1	0.54
(1,480)	1:10:A:CYS:HB2	1:10:A:CYS:H	19	0.54
(1,480)	1:10:A:CYS:HB3	1:10:A:CYS:H	19	0.54
(1,454)	1:78:A:GLU:HG2	1:76:A:ASP:H	4	0.54
(1,454)	1:78:A:GLU:HG3	1:76:A:ASP:H	4	0.54
(1,454)	1:78:A:GLU:HG2	1:76:A:ASP:H	17	0.54
(1,454)	1:78:A:GLU:HG3	1:76:A:ASP:H	17	0.54
(1,446)	1:73:A:SER:H	1:74:A:GLY:H	6	0.54
(1,430)	1:69:A:ASN:HB2	1:69:A:ASN:H	7	0.54
(1,430)	1:69:A:ASN:HB3	1:69:A:ASN:H	7	0.54
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB1	8	0.54
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB2	8	0.54
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB3	8	0.54
(1,371)	1:44:A:CYS:HA	1:45:A:ARG:H	4	0.54
(1,371)	1:44:A:CYS:HA	1:45:A:ARG:H	15	0.54
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	17	0.54
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	17	0.54
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	17	0.54
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	17	0.54
(1,289)	1:8:A:PHE:HA	1:8:A:PHE:H	7	0.54
(1,289)	1:8:A:PHE:HA	1:8:A:PHE:H	10	0.54
(1,174)	1:103:A:VAL:H	1:101:A:ASN:HB2	7	0.54
(1,174)	1:103:A:VAL:H	1:101:A:ASN:HB3	7	0.54
(1,137)	1:109:A:ASP:H	1:113:A:GLY:HA2	4	0.54
(1,137)	1:109:A:ASP:H	1:113:A:GLY:HA3	4	0.54
(1,137)	1:109:A:ASP:H	1:113:A:GLY:HA2	7	0.54
(1,137)	1:109:A:ASP:H	1:113:A:GLY:HA3	7	0.54
(1,119)	1:112:A:ASP:H	1:115:A:ASP:H	3	0.54
(1,118)	1:115:A:ASP:H	1:113:A:GLY:H	14	0.54
(1,58)	1:66:A:ASP:H	1:65:A:CYS:H	9	0.54
(1,2)	1:112:A:ASP:H	1:113:A:GLY:H	1	0.54
(4,8)	1:8:A:PHE:O	1:16:A:VAL:H	2	0.53
(2,337)	1:53:A:ALA:HB3	1:55:A:SER:H	3	0.53

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,323)	1:64:A:ARG:HG2	1:68:A:GLU:H	9	0.53
(2,302)	1:119:A:CYS:HA	1:120:A:ALA:H	11	0.53
(2,207)	1:79:A:ASN:HB2	1:79:A:ASN:HD22	18	0.53
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	9	0.53
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	9	0.53
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	9	0.53
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	9	0.53
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	9	0.53
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	9	0.53
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	9	0.53
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	9	0.53
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	9	0.53
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	9	0.53
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	9	0.53
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	9	0.53
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	9	0.53
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	9	0.53
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	9	0.53
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	9	0.53
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	9	0.53
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	9	0.53
(2,180)	1:11:A:ASN:HA	1:11:A:ASN:HD21	7	0.53
(2,180)	1:11:A:ASN:HA	1:11:A:ASN:HD21	19	0.53
(1,923)	1:8:A:PHE:HB2	1:16:A:VAL:HA	16	0.53
(1,850)	1:12:A:ASN:H	1:11:A:ASN:HD22	1	0.53
(1,797)	1:91:A:THR:HG21	1:96:A:ARG:H	1	0.53
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	19	0.53
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	19	0.53
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	19	0.53
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	19	0.53
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG12	18	0.53
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG13	18	0.53
(1,721)	1:21:A:LYS:HG2	1:22:A:CYS:H	6	0.53
(1,721)	1:21:A:LYS:HG3	1:22:A:CYS:H	6	0.53
(1,721)	1:21:A:LYS:HG2	1:22:A:CYS:H	12	0.53
(1,721)	1:21:A:LYS:HG3	1:22:A:CYS:H	12	0.53
(1,711)	1:10:A:CYS:HB2	1:11:A:ASN:H	11	0.53
(1,711)	1:10:A:CYS:HB3	1:11:A:ASN:H	11	0.53
(1,711)	1:10:A:CYS:HB2	1:11:A:ASN:H	13	0.53
(1,711)	1:10:A:CYS:HB3	1:11:A:ASN:H	13	0.53
(1,687)	1:69:A:ASN:HD21	1:74:A:GLY:H	4	0.53
(1,670)	1:107:A:GLN:HB2	1:105:A:ASN:HD22	11	0.53

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,670)	1:107:A:GLN:HB2	1:105:A:ASN:HD22	11	0.53
(1,670)	1:107:A:GLN:HB3	1:105:A:ASN:HD22	11	0.53
(1,670)	1:107:A:GLN:HB3	1:105:A:ASN:HD22	11	0.53
(1,642)	1:82:A:ASN:HA	1:82:A:ASN:HD22	10	0.53
(1,634)	1:79:A:ASN:HD22	1:79:A:ASN:HA	6	0.53
(1,634)	1:79:A:ASN:HD22	1:79:A:ASN:HA	10	0.53
(1,634)	1:79:A:ASN:HD22	1:79:A:ASN:HA	11	0.53
(1,634)	1:79:A:ASN:HD22	1:79:A:ASN:HA	13	0.53
(1,587)	1:14:A:GLN:H	1:12:A:ASN:H	4	0.53
(1,587)	1:14:A:GLN:H	1:12:A:ASN:H	6	0.53
(1,531)	1:71:A:CYS:HB2	1:71:A:CYS:H	13	0.53
(1,531)	1:71:A:CYS:HB3	1:71:A:CYS:H	13	0.53
(1,531)	1:71:A:CYS:HB2	1:71:A:CYS:H	16	0.53
(1,531)	1:71:A:CYS:HB3	1:71:A:CYS:H	16	0.53
(1,509)	1:46:A:ILE:HA	1:46:A:ILE:H	1	0.53
(1,509)	1:46:A:ILE:HA	1:46:A:ILE:H	2	0.53
(1,509)	1:46:A:ILE:HA	1:46:A:ILE:H	6	0.53
(1,509)	1:46:A:ILE:HA	1:46:A:ILE:H	8	0.53
(1,509)	1:46:A:ILE:HA	1:46:A:ILE:H	13	0.53
(1,447)	1:71:A:CYS:HA	1:74:A:GLY:H	9	0.53
(1,430)	1:69:A:ASN:HB2	1:69:A:ASN:H	2	0.53
(1,430)	1:69:A:ASN:HB3	1:69:A:ASN:H	2	0.53
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	3	0.53
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	3	0.53
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	3	0.53
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	3	0.53
(1,289)	1:8:A:PHE:HA	1:8:A:PHE:H	4	0.53
(1,80)	1:44:A:CYS:HB2	1:45:A:ARG:H	7	0.53
(1,80)	1:44:A:CYS:HB3	1:45:A:ARG:H	7	0.53
(1,58)	1:66:A:ASP:H	1:65:A:CYS:H	10	0.53
(1,58)	1:66:A:ASP:H	1:65:A:CYS:H	14	0.53
(1,27)	1:118:A:ASP:H	1:117:A:LEU:H	9	0.53
(1,2)	1:112:A:ASP:H	1:113:A:GLY:H	18	0.53
(1,2)	1:112:A:ASP:H	1:113:A:GLY:H	20	0.53
(2,327)	1:64:A:ARG:HG2	1:71:A:CYS:H	20	0.52
(2,323)	1:64:A:ARG:HG2	1:68:A:GLU:H	7	0.52
(2,323)	1:64:A:ARG:HG2	1:68:A:GLU:H	13	0.52
(2,264)	1:49:A:ILE:HB	1:50:A:SER:H	19	0.52
(2,212)	1:88:A:ASP:H	1:86:A:SER:H	11	0.52
(2,200)	1:77:A:GLU:HG3	1:76:A:ASP:H	3	0.52
(2,200)	1:77:A:GLU:HG3	1:76:A:ASP:H	11	0.52
(2,98)	1:28:A:CYS:HB3	1:11:A:ASN:H	19	0.52

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,83)	1:35:A:SER:HB3	1:38:A:GLN:H	4	0.52
(2,25)	1:79:A:ASN:HD22	1:80:A:CYS:HA	19	0.52
(1,911)	1:57:A:GLN:HE21	1:71:A:CYS:H	2	0.52
(1,819)	1:112:A:ASP:HB2	1:115:A:ASP:H	11	0.52
(1,819)	1:112:A:ASP:HB3	1:115:A:ASP:H	11	0.52
(1,766)	1:48:A:GLU:HB2	1:58:A:CYS:H	8	0.52
(1,766)	1:48:A:GLU:HB3	1:58:A:CYS:H	8	0.52
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD2	5	0.52
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD3	5	0.52
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD2	7	0.52
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD3	7	0.52
(1,608)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	12	0.52
(1,608)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	12	0.52
(1,587)	1:14:A:GLN:H	1:12:A:ASN:H	5	0.52
(1,587)	1:14:A:GLN:H	1:12:A:ASN:H	8	0.52
(1,587)	1:14:A:GLN:H	1:12:A:ASN:H	12	0.52
(1,583)	1:40:A:HIS:HA	1:38:A:GLN:H	7	0.52
(1,555)	1:103:A:VAL:HG11	1:104:A:CYS:H	20	0.52
(1,555)	1:103:A:VAL:HG12	1:104:A:CYS:H	20	0.52
(1,555)	1:103:A:VAL:HG13	1:104:A:CYS:H	20	0.52
(1,555)	1:103:A:VAL:HG21	1:104:A:CYS:H	20	0.52
(1,555)	1:103:A:VAL:HG22	1:104:A:CYS:H	20	0.52
(1,555)	1:103:A:VAL:HG23	1:104:A:CYS:H	20	0.52
(1,551)	1:104:A:CYS:HB2	1:104:A:CYS:H	19	0.52
(1,551)	1:104:A:CYS:HB3	1:104:A:CYS:H	19	0.52
(1,550)	1:104:A:CYS:HB2	1:104:A:CYS:H	19	0.52
(1,550)	1:104:A:CYS:HB3	1:104:A:CYS:H	19	0.52
(1,543)	1:112:A:ASP:HB2	1:114:A:SER:H	12	0.52
(1,543)	1:112:A:ASP:HB3	1:114:A:SER:H	12	0.52
(1,526)	1:64:A:ARG:H	1:67:A:GLY:H	15	0.52
(1,509)	1:46:A:ILE:HA	1:46:A:ILE:H	7	0.52
(1,459)	1:70:A:ASP:HA	1:76:A:ASP:H	8	0.52
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	4	0.52
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	4	0.52
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	4	0.52
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	4	0.52
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	5	0.52
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	5	0.52
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	5	0.52
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	9	0.52
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	9	0.52

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	9	0.52
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	9	0.52
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	16	0.52
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	16	0.52
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	16	0.52
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	16	0.52
(1,298)	1:14:A:GLN:H	1:11:A:ASN:H	6	0.52
(1,298)	1:14:A:GLN:H	1:11:A:ASN:H	12	0.52
(1,289)	1:8:A:PHE:HA	1:8:A:PHE:H	6	0.52
(1,289)	1:8:A:PHE:HA	1:8:A:PHE:H	9	0.52
(1,212)	1:96:A:ARG:H	1:92:A:CYS:HA	12	0.52
(1,73)	1:65:A:CYS:HB2	1:65:A:CYS:H	5	0.52
(1,73)	1:65:A:CYS:HB3	1:65:A:CYS:H	5	0.52
(1,73)	1:65:A:CYS:HB2	1:65:A:CYS:H	20	0.52
(1,73)	1:65:A:CYS:HB3	1:65:A:CYS:H	20	0.52
(1,2)	1:112:A:ASP:H	1:113:A:GLY:H	11	0.52
(1,2)	1:112:A:ASP:H	1:113:A:GLY:H	12	0.52
(4,8)	1:8:A:PHE:O	1:16:A:VAL:H	11	0.51
(2,331)	1:101:A:ASN:H	1:99:A:SER:H	19	0.51
(2,323)	1:64:A:ARG:HG2	1:68:A:GLU:H	17	0.51
(2,322)	1:70:A:ASP:HB2	1:71:A:CYS:H	8	0.51
(2,276)	1:43:A:THR:HA	1:57:A:GLN:H	3	0.51
(2,212)	1:88:A:ASP:H	1:86:A:SER:H	2	0.51
(2,212)	1:88:A:ASP:H	1:86:A:SER:H	12	0.51
(2,212)	1:88:A:ASP:H	1:86:A:SER:H	13	0.51
(2,207)	1:79:A:ASN:HB2	1:79:A:ASN:HD22	2	0.51
(2,207)	1:79:A:ASN:HB2	1:79:A:ASN:HD22	13	0.51
(2,168)	1:38:A:GLN:HG2	1:38:A:GLN:H	4	0.51
(2,166)	1:86:A:SER:HA	1:79:A:ASN:HD21	16	0.51
(2,44)	1:83:A:ILE:HG23	1:97:A:CYS:H	9	0.51
(2,25)	1:79:A:ASN:HD22	1:80:A:CYS:HA	8	0.51
(1,888)	1:49:A:ILE:HA	1:61:A:VAL:H	12	0.51
(1,878)	1:48:A:GLU:HB2	1:45:A:ARG:H	3	0.51
(1,878)	1:48:A:GLU:HB3	1:45:A:ARG:H	3	0.51
(1,856)	1:14:A:GLN:H	1:12:A:ASN:HD22	4	0.51
(1,850)	1:12:A:ASN:H	1:11:A:ASN:HD22	19	0.51
(1,819)	1:112:A:ASP:HB2	1:115:A:ASP:H	18	0.51
(1,819)	1:112:A:ASP:HB3	1:115:A:ASP:H	18	0.51
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	4	0.51
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	4	0.51
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	4	0.51
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	4	0.51

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	15	0.51
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	15	0.51
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	15	0.51
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	15	0.51
(1,723)	1:23:A:ASP:H	1:21:A:LYS:HA	1	0.51
(1,721)	1:21:A:LYS:HG2	1:22:A:CYS:H	18	0.51
(1,721)	1:21:A:LYS:HG3	1:22:A:CYS:H	18	0.51
(1,711)	1:10:A:CYS:HB2	1:11:A:ASN:H	20	0.51
(1,711)	1:10:A:CYS:HB3	1:11:A:ASN:H	20	0.51
(1,706)	1:45:A:ARG:HB2	1:45:A:ARG:H	5	0.51
(1,706)	1:45:A:ARG:HB3	1:45:A:ARG:H	5	0.51
(1,635)	1:78:A:GLU:HB2	1:79:A:ASN:HD21	8	0.51
(1,635)	1:78:A:GLU:HB2	1:79:A:ASN:HD21	8	0.51
(1,635)	1:78:A:GLU:HB3	1:79:A:ASN:HD21	8	0.51
(1,635)	1:78:A:GLU:HB3	1:79:A:ASN:HD21	8	0.51
(1,586)	1:69:A:ASN:HA	1:64:A:ARG:H	6	0.51
(1,543)	1:112:A:ASP:HB2	1:114:A:SER:H	10	0.51
(1,543)	1:112:A:ASP:HB3	1:114:A:SER:H	10	0.51
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	3	0.51
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	3	0.51
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	3	0.51
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	3	0.51
(1,509)	1:46:A:ILE:HA	1:46:A:ILE:H	19	0.51
(1,486)	1:7:A:ASP:HA	1:19:A:ARG:H	9	0.51
(1,486)	1:7:A:ASP:HA	1:19:A:ARG:H	11	0.51
(1,480)	1:10:A:CYS:HB2	1:10:A:CYS:H	2	0.51
(1,480)	1:10:A:CYS:HB3	1:10:A:CYS:H	2	0.51
(1,480)	1:10:A:CYS:HB2	1:10:A:CYS:H	18	0.51
(1,480)	1:10:A:CYS:HB3	1:10:A:CYS:H	18	0.51
(1,430)	1:69:A:ASN:HB2	1:69:A:ASN:H	17	0.51
(1,430)	1:69:A:ASN:HB3	1:69:A:ASN:H	17	0.51
(1,430)	1:69:A:ASN:HB2	1:69:A:ASN:H	19	0.51
(1,430)	1:69:A:ASN:HB3	1:69:A:ASN:H	19	0.51
(1,371)	1:44:A:CYS:HA	1:45:A:ARG:H	11	0.51
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	11	0.51
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	11	0.51
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	11	0.51
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	11	0.51
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB2	10	0.51
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB3	10	0.51
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB2	16	0.51
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB3	16	0.51

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,289)	1:8:A:PHE:HA	1:8:A:PHE:H	12	0.51
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB2	1	0.51
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB3	1	0.51
(1,118)	1:115:A:ASP:H	1:113:A:GLY:H	15	0.51
(1,81)	1:28:A:CYS:HA	1:33:A:ASP:H	7	0.51
(1,80)	1:44:A:CYS:HB2	1:45:A:ARG:H	13	0.51
(1,80)	1:44:A:CYS:HB3	1:45:A:ARG:H	13	0.51
(1,60)	1:56:A:THR:H	1:57:A:GLN:H	1	0.51
(1,58)	1:66:A:ASP:H	1:65:A:CYS:H	8	0.51
(1,27)	1:118:A:ASP:H	1:117:A:LEU:H	6	0.51
(2,330)	1:92:A:CYS:HA	1:93:A:SER:H	11	0.5
(2,330)	1:92:A:CYS:HA	1:93:A:SER:H	13	0.5
(2,323)	1:64:A:ARG:HG2	1:68:A:GLU:H	16	0.5
(2,296)	1:114:A:SER:HB3	1:117:A:LEU:H	8	0.5
(2,296)	1:113:A:GLY:HA2	1:117:A:LEU:H	15	0.5
(2,281)	1:10:A:CYS:HA	1:11:A:ASN:HD22	17	0.5
(2,264)	1:49:A:ILE:HB	1:50:A:SER:H	14	0.5
(2,244)	1:45:A:ARG:HA	1:47:A:HIS:H	12	0.5
(2,212)	1:88:A:ASP:H	1:86:A:SER:H	4	0.5
(2,207)	1:79:A:ASN:HB2	1:79:A:ASN:HD22	4	0.5
(2,200)	1:77:A:GLU:HG3	1:76:A:ASP:H	9	0.5
(2,114)	1:16:A:VAL:HG11	1:16:A:VAL:H	11	0.5
(2,114)	1:16:A:VAL:HG12	1:16:A:VAL:H	11	0.5
(2,114)	1:16:A:VAL:HG13	1:16:A:VAL:H	11	0.5
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	11	0.5
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	11	0.5
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	11	0.5
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	11	0.5
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	11	0.5
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	11	0.5
(1,890)	1:81:A:GLY:HA2	1:63:A:TRP:HE1	6	0.5
(1,890)	1:81:A:GLY:HA2	1:63:A:TRP:HE1	6	0.5
(1,890)	1:81:A:GLY:HA3	1:63:A:TRP:HE1	6	0.5
(1,890)	1:81:A:GLY:HA3	1:63:A:TRP:HE1	6	0.5
(1,888)	1:49:A:ILE:HA	1:61:A:VAL:H	3	0.5
(1,888)	1:49:A:ILE:HA	1:61:A:VAL:H	19	0.5
(1,862)	1:21:A:LYS:HE2	1:19:A:ARG:H	9	0.5
(1,862)	1:21:A:LYS:HE3	1:19:A:ARG:H	9	0.5
(1,849)	1:33:A:ASP:H	1:11:A:ASN:H	19	0.5
(1,819)	1:112:A:ASP:HB2	1:115:A:ASP:H	15	0.5
(1,819)	1:112:A:ASP:HB3	1:115:A:ASP:H	15	0.5
(1,807)	1:98:A:ILE:HG12	1:103:A:VAL:H	18	0.5

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,807)	1:98:A:ILE:HG13	1:103:A:VAL:H	18	0.5
(1,806)	1:101:A:ASN:HD21	1:102:A:PHE:H	2	0.5
(1,801)	1:102:A:PHE:HB2	1:98:A:ILE:H	10	0.5
(1,801)	1:102:A:PHE:HB3	1:98:A:ILE:H	10	0.5
(1,799)	1:85:A:CYS:HA	1:97:A:CYS:H	9	0.5
(1,786)	1:71:A:CYS:H	1:76:A:ASP:H	10	0.5
(1,772)	1:68:A:GLU:H	1:64:A:ARG:H	10	0.5
(1,723)	1:23:A:ASP:H	1:21:A:LYS:HA	5	0.5
(1,721)	1:21:A:LYS:HG2	1:22:A:CYS:H	3	0.5
(1,721)	1:21:A:LYS:HG3	1:22:A:CYS:H	3	0.5
(1,711)	1:10:A:CYS:HB2	1:11:A:ASN:H	16	0.5
(1,711)	1:10:A:CYS:HB3	1:11:A:ASN:H	16	0.5
(1,706)	1:45:A:ARG:HB2	1:45:A:ARG:H	16	0.5
(1,706)	1:45:A:ARG:HB3	1:45:A:ARG:H	16	0.5
(1,693)	1:21:A:LYS:HD2	1:21:A:LYS:H	16	0.5
(1,693)	1:21:A:LYS:HD3	1:21:A:LYS:H	16	0.5
(1,693)	1:21:A:LYS:HD2	1:21:A:LYS:H	17	0.5
(1,693)	1:21:A:LYS:HD3	1:21:A:LYS:H	17	0.5
(1,667)	1:107:A:GLN:HG2	1:105:A:ASN:HD22	17	0.5
(1,667)	1:107:A:GLN:HG2	1:105:A:ASN:HD22	17	0.5
(1,667)	1:107:A:GLN:HG3	1:105:A:ASN:HD22	17	0.5
(1,667)	1:107:A:GLN:HG3	1:105:A:ASN:HD22	17	0.5
(1,654)	1:107:A:GLN:HB2	1:107:A:GLN:HE22	11	0.5
(1,654)	1:107:A:GLN:HB2	1:107:A:GLN:HE22	11	0.5
(1,654)	1:107:A:GLN:HB3	1:107:A:GLN:HE22	11	0.5
(1,654)	1:107:A:GLN:HB3	1:107:A:GLN:HE22	11	0.5
(1,654)	1:107:A:GLN:HB2	1:107:A:GLN:HE22	13	0.5
(1,654)	1:107:A:GLN:HB2	1:107:A:GLN:HE22	13	0.5
(1,654)	1:107:A:GLN:HB3	1:107:A:GLN:HE22	13	0.5
(1,654)	1:107:A:GLN:HB3	1:107:A:GLN:HE22	13	0.5
(1,642)	1:82:A:ASN:HA	1:82:A:ASN:HD22	8	0.5
(1,636)	1:78:A:GLU:HB2	1:79:A:ASN:HD22	12	0.5
(1,636)	1:78:A:GLU:HB2	1:79:A:ASN:HD22	12	0.5
(1,636)	1:78:A:GLU:HB3	1:79:A:ASN:HD22	12	0.5
(1,636)	1:78:A:GLU:HB3	1:79:A:ASN:HD22	12	0.5
(1,634)	1:79:A:ASN:HD22	1:79:A:ASN:HA	4	0.5
(1,608)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	7	0.5
(1,608)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	7	0.5
(1,608)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	16	0.5
(1,608)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	16	0.5
(1,587)	1:14:A:GLN:H	1:12:A:ASN:H	3	0.5
(1,587)	1:14:A:GLN:H	1:12:A:ASN:H	18	0.5

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,583)	1:40:A:HIS:HA	1:38:A:GLN:H	11	0.5
(1,531)	1:71:A:CYS:HB2	1:71:A:CYS:H	1	0.5
(1,531)	1:71:A:CYS:HB3	1:71:A:CYS:H	1	0.5
(1,531)	1:71:A:CYS:HB2	1:71:A:CYS:H	3	0.5
(1,531)	1:71:A:CYS:HB3	1:71:A:CYS:H	3	0.5
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	13	0.5
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	13	0.5
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	13	0.5
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	13	0.5
(1,509)	1:46:A:ILE:HA	1:46:A:ILE:H	11	0.5
(1,486)	1:7:A:ASP:HA	1:19:A:ARG:H	10	0.5
(1,480)	1:10:A:CYS:HB2	1:10:A:CYS:H	3	0.5
(1,480)	1:10:A:CYS:HB3	1:10:A:CYS:H	3	0.5
(1,480)	1:10:A:CYS:HB2	1:10:A:CYS:H	6	0.5
(1,480)	1:10:A:CYS:HB3	1:10:A:CYS:H	6	0.5
(1,480)	1:10:A:CYS:HB2	1:10:A:CYS:H	8	0.5
(1,480)	1:10:A:CYS:HB3	1:10:A:CYS:H	8	0.5
(1,480)	1:10:A:CYS:HB2	1:10:A:CYS:H	15	0.5
(1,480)	1:10:A:CYS:HB3	1:10:A:CYS:H	15	0.5
(1,371)	1:44:A:CYS:HA	1:45:A:ARG:H	18	0.5
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB2	1	0.5
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB3	1	0.5
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB2	4	0.5
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB3	4	0.5
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB2	5	0.5
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB3	5	0.5
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB2	9	0.5
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB3	9	0.5
(1,346)	1:32:A:SER:H	1:31:A:GLY:H	12	0.5
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB2	12	0.5
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB3	12	0.5
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB2	10	0.5
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB3	10	0.5
(1,118)	1:115:A:ASP:H	1:113:A:GLY:H	20	0.5
(1,85)	1:21:A:LYS:HG2	1:22:A:CYS:H	10	0.5
(1,85)	1:21:A:LYS:HG3	1:22:A:CYS:H	10	0.5
(1,85)	1:21:A:LYS:HG2	1:22:A:CYS:H	11	0.5
(1,85)	1:21:A:LYS:HG3	1:22:A:CYS:H	11	0.5
(1,73)	1:65:A:CYS:HB2	1:65:A:CYS:H	16	0.5
(1,73)	1:65:A:CYS:HB3	1:65:A:CYS:H	16	0.5
(1,58)	1:66:A:ASP:H	1:65:A:CYS:H	15	0.5
(1,27)	1:118:A:ASP:H	1:117:A:LEU:H	20	0.5

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2)	1:112:A:ASP:H	1:113:A:GLY:H	8	0.5
(1,2)	1:112:A:ASP:H	1:113:A:GLY:H	15	0.5
(4,8)	1:8:A:PHE:O	1:16:A:VAL:H	13	0.49
(2,381)	1:100:A:ARG:HD3	1:90:A:PHE:H	8	0.49
(2,381)	1:100:A:ARG:HD3	1:90:A:PHE:H	18	0.49
(2,313)	1:17:A:PRO:HB2	1:20:A:TRP:H	4	0.49
(2,276)	1:43:A:THR:HA	1:57:A:GLN:H	15	0.49
(2,264)	1:49:A:ILE:HB	1:50:A:SER:H	3	0.49
(2,244)	1:45:A:ARG:HA	1:47:A:HIS:H	15	0.49
(2,207)	1:79:A:ASN:HB2	1:79:A:ASN:HD22	9	0.49
(2,90)	1:60:A:PRO:HB2	1:63:A:TRP:HE1	1	0.49
(1,923)	1:8:A:PHE:HB2	1:16:A:VAL:HA	14	0.49
(1,896)	1:64:A:ARG:H	1:66:A:ASP:H	15	0.49
(1,888)	1:49:A:ILE:HA	1:61:A:VAL:H	4	0.49
(1,878)	1:48:A:GLU:HB2	1:45:A:ARG:H	19	0.49
(1,878)	1:48:A:GLU:HB3	1:45:A:ARG:H	19	0.49
(1,859)	1:3:A:CYS:HB2	1:18:A:SER:H	12	0.49
(1,859)	1:3:A:CYS:HB3	1:18:A:SER:H	12	0.49
(1,856)	1:14:A:GLN:H	1:12:A:ASN:HD22	18	0.49
(1,850)	1:12:A:ASN:H	1:11:A:ASN:HD22	13	0.49
(1,819)	1:112:A:ASP:HB2	1:115:A:ASP:H	12	0.49
(1,819)	1:112:A:ASP:HB3	1:115:A:ASP:H	12	0.49
(1,799)	1:85:A:CYS:HA	1:97:A:CYS:H	5	0.49
(1,772)	1:68:A:GLU:H	1:64:A:ARG:H	14	0.49
(1,766)	1:48:A:GLU:HB2	1:58:A:CYS:H	2	0.49
(1,766)	1:48:A:GLU:HB3	1:58:A:CYS:H	2	0.49
(1,721)	1:21:A:LYS:HG2	1:22:A:CYS:H	4	0.49
(1,721)	1:21:A:LYS:HG3	1:22:A:CYS:H	4	0.49
(1,721)	1:21:A:LYS:HG2	1:22:A:CYS:H	15	0.49
(1,721)	1:21:A:LYS:HG3	1:22:A:CYS:H	15	0.49
(1,711)	1:10:A:CYS:HB2	1:11:A:ASN:H	7	0.49
(1,711)	1:10:A:CYS:HB3	1:11:A:ASN:H	7	0.49
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD2	8	0.49
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD3	8	0.49
(1,685)	1:107:A:GLN:HG2	1:107:A:GLN:HE21	10	0.49
(1,685)	1:107:A:GLN:HG2	1:107:A:GLN:HE21	10	0.49
(1,685)	1:107:A:GLN:HG3	1:107:A:GLN:HE21	10	0.49
(1,685)	1:107:A:GLN:HG3	1:107:A:GLN:HE21	10	0.49
(1,685)	1:107:A:GLN:HG2	1:107:A:GLN:HE21	17	0.49
(1,685)	1:107:A:GLN:HG2	1:107:A:GLN:HE21	17	0.49
(1,685)	1:107:A:GLN:HG3	1:107:A:GLN:HE21	17	0.49
(1,685)	1:107:A:GLN:HG3	1:107:A:GLN:HE21	17	0.49

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD2	10	0.49
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD3	10	0.49
(1,670)	1:107:A:GLN:HB2	1:105:A:ASN:HD22	20	0.49
(1,670)	1:107:A:GLN:HB2	1:105:A:ASN:HD22	20	0.49
(1,670)	1:107:A:GLN:HB3	1:105:A:ASN:HD22	20	0.49
(1,670)	1:107:A:GLN:HB3	1:105:A:ASN:HD22	20	0.49
(1,583)	1:40:A:HIS:HA	1:38:A:GLN:H	4	0.49
(1,583)	1:40:A:HIS:HA	1:38:A:GLN:H	9	0.49
(1,583)	1:40:A:HIS:HA	1:38:A:GLN:H	17	0.49
(1,583)	1:40:A:HIS:HA	1:38:A:GLN:H	19	0.49
(1,543)	1:112:A:ASP:HB2	1:114:A:SER:H	5	0.49
(1,543)	1:112:A:ASP:HB3	1:114:A:SER:H	5	0.49
(1,543)	1:112:A:ASP:HB2	1:114:A:SER:H	17	0.49
(1,543)	1:112:A:ASP:HB3	1:114:A:SER:H	17	0.49
(1,531)	1:71:A:CYS:HB2	1:71:A:CYS:H	19	0.49
(1,531)	1:71:A:CYS:HB3	1:71:A:CYS:H	19	0.49
(1,436)	1:73:A:SER:H	1:72:A:ASP:H	4	0.49
(1,371)	1:44:A:CYS:HA	1:45:A:ARG:H	14	0.49
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	1	0.49
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	1	0.49
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	1	0.49
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	1	0.49
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB2	19	0.49
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB3	19	0.49
(1,335)	1:45:A:ARG:HD2	1:24:A:GLY:H	11	0.49
(1,335)	1:45:A:ARG:HD3	1:24:A:GLY:H	11	0.49
(1,298)	1:14:A:GLN:H	1:11:A:ASN:H	8	0.49
(1,289)	1:8:A:PHE:HA	1:8:A:PHE:H	2	0.49
(1,212)	1:96:A:ARG:H	1:92:A:CYS:HA	20	0.49
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB2	8	0.49
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB3	8	0.49
(1,97)	1:98:A:ILE:HD11	1:99:A:SER:H	3	0.49
(1,97)	1:98:A:ILE:HD12	1:99:A:SER:H	3	0.49
(1,97)	1:98:A:ILE:HD13	1:99:A:SER:H	3	0.49
(1,73)	1:65:A:CYS:HB2	1:65:A:CYS:H	1	0.49
(1,73)	1:65:A:CYS:HB3	1:65:A:CYS:H	1	0.49
(1,60)	1:56:A:THR:H	1:57:A:GLN:H	18	0.49
(1,27)	1:118:A:ASP:H	1:117:A:LEU:H	17	0.49
(2,371)	1:83:A:ILE:HD13	1:83:A:ILE:H	20	0.48
(2,363)	1:49:A:ILE:HB	1:49:A:ILE:H	8	0.48
(2,330)	1:92:A:CYS:HA	1:93:A:SER:H	15	0.48
(2,207)	1:79:A:ASN:HB2	1:79:A:ASN:HD22	6	0.48

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,207)	1:79:A:ASN:HB2	1:79:A:ASN:HD22	10	0.48
(2,207)	1:79:A:ASN:HB2	1:79:A:ASN:HD22	11	0.48
(2,200)	1:87:A:PRO:HG3	1:76:A:ASP:H	6	0.48
(2,159)	1:39:A:CYS:HB3	1:43:A:THR:H	8	0.48
(2,98)	1:28:A:CYS:HB3	1:11:A:ASN:H	8	0.48
(2,72)	1:112:A:ASP:HB3	1:113:A:GLY:H	2	0.48
(2,39)	1:117:A:LEU:HD11	1:115:A:ASP:H	5	0.48
(1,909)	1:43:A:THR:HG23	1:46:A:ILE:H	12	0.48
(1,896)	1:64:A:ARG:H	1:66:A:ASP:H	18	0.48
(1,881)	1:48:A:GLU:H	1:45:A:ARG:H	18	0.48
(1,879)	1:48:A:GLU:H	1:45:A:ARG:H	18	0.48
(1,862)	1:21:A:LYS:HE2	1:19:A:ARG:H	14	0.48
(1,862)	1:21:A:LYS:HE3	1:19:A:ARG:H	14	0.48
(1,856)	1:14:A:GLN:H	1:12:A:ASN:HD22	14	0.48
(1,833)	1:42:A:ARG:HG2	1:41:A:MET:H	13	0.48
(1,833)	1:42:A:ARG:HG2	1:41:A:MET:H	13	0.48
(1,833)	1:42:A:ARG:HG3	1:41:A:MET:H	13	0.48
(1,833)	1:42:A:ARG:HG3	1:41:A:MET:H	13	0.48
(1,803)	1:101:A:ASN:HD21	1:99:A:SER:H	10	0.48
(1,800)	1:85:A:CYS:HB2	1:98:A:ILE:H	15	0.48
(1,800)	1:85:A:CYS:HB3	1:98:A:ILE:H	15	0.48
(1,799)	1:85:A:CYS:HA	1:97:A:CYS:H	19	0.48
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG21	11	0.48
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG22	11	0.48
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG23	11	0.48
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	8	0.48
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	8	0.48
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	8	0.48
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	8	0.48
(1,750)	1:57:A:GLN:HB2	1:52:A:GLY:H	10	0.48
(1,750)	1:57:A:GLN:HB2	1:52:A:GLY:H	10	0.48
(1,750)	1:57:A:GLN:HB3	1:52:A:GLY:H	10	0.48
(1,750)	1:57:A:GLN:HB3	1:52:A:GLY:H	10	0.48
(1,721)	1:21:A:LYS:HG2	1:22:A:CYS:H	2	0.48
(1,721)	1:21:A:LYS:HG3	1:22:A:CYS:H	2	0.48
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD2	9	0.48
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD3	9	0.48
(1,706)	1:45:A:ARG:HB2	1:45:A:ARG:H	6	0.48
(1,706)	1:45:A:ARG:HB3	1:45:A:ARG:H	6	0.48
(1,706)	1:45:A:ARG:HB2	1:45:A:ARG:H	11	0.48
(1,706)	1:45:A:ARG:HB3	1:45:A:ARG:H	11	0.48
(1,685)	1:107:A:GLN:HG2	1:107:A:GLN:HE21	2	0.48

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,685)	1:107:A:GLN:HG2	1:107:A:GLN:HE21	2	0.48
(1,685)	1:107:A:GLN:HG3	1:107:A:GLN:HE21	2	0.48
(1,685)	1:107:A:GLN:HG3	1:107:A:GLN:HE21	2	0.48
(1,657)	1:105:A:ASN:HA	1:105:A:ASN:HD22	2	0.48
(1,657)	1:105:A:ASN:HA	1:105:A:ASN:HD22	4	0.48
(1,657)	1:105:A:ASN:HA	1:105:A:ASN:HD22	6	0.48
(1,657)	1:105:A:ASN:HA	1:105:A:ASN:HD22	17	0.48
(1,654)	1:107:A:GLN:HB2	1:107:A:GLN:HE22	20	0.48
(1,654)	1:107:A:GLN:HB2	1:107:A:GLN:HE22	20	0.48
(1,654)	1:107:A:GLN:HB3	1:107:A:GLN:HE22	20	0.48
(1,654)	1:107:A:GLN:HB3	1:107:A:GLN:HE22	20	0.48
(1,634)	1:79:A:ASN:HD22	1:79:A:ASN:HA	2	0.48
(1,608)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	3	0.48
(1,608)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	3	0.48
(1,608)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	4	0.48
(1,608)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	4	0.48
(1,608)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	11	0.48
(1,608)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	11	0.48
(1,596)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	10	0.48
(1,596)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	10	0.48
(1,587)	1:14:A:GLN:H	1:12:A:ASN:H	9	0.48
(1,543)	1:112:A:ASP:HB2	1:114:A:SER:H	20	0.48
(1,543)	1:112:A:ASP:HB3	1:114:A:SER:H	20	0.48
(1,463)	1:71:A:CYS:HB2	1:78:A:GLU:H	18	0.48
(1,463)	1:71:A:CYS:HB3	1:78:A:GLU:H	18	0.48
(1,436)	1:73:A:SER:H	1:72:A:ASP:H	12	0.48
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	6	0.48
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	6	0.48
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	6	0.48
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	6	0.48
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB2	14	0.48
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB3	14	0.48
(1,289)	1:8:A:PHE:HA	1:8:A:PHE:H	19	0.48
(1,174)	1:103:A:VAL:H	1:101:A:ASN:HB2	10	0.48
(1,174)	1:103:A:VAL:H	1:101:A:ASN:HB3	10	0.48
(1,119)	1:112:A:ASP:H	1:115:A:ASP:H	6	0.48
(1,118)	1:115:A:ASP:H	1:113:A:GLY:H	8	0.48
(1,85)	1:21:A:LYS:HG2	1:22:A:CYS:H	13	0.48
(1,85)	1:21:A:LYS:HG3	1:22:A:CYS:H	13	0.48
(1,81)	1:28:A:CYS:HA	1:33:A:ASP:H	9	0.48
(1,58)	1:66:A:ASP:H	1:65:A:CYS:H	17	0.48
(1,27)	1:118:A:ASP:H	1:117:A:LEU:H	5	0.48

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,27)	1:118:A:ASP:H	1:117:A:LEU:H	14	0.48
(4,8)	1:8:A:PHE:O	1:16:A:VAL:H	9	0.47
(2,381)	1:100:A:ARG:HD3	1:90:A:PHE:H	13	0.47
(2,359)	1:98:A:ILE:HD13	1:98:A:ILE:H	15	0.47
(2,323)	1:64:A:ARG:HG2	1:68:A:GLU:H	1	0.47
(2,323)	1:64:A:ARG:HG2	1:68:A:GLU:H	11	0.47
(2,257)	1:33:A:ASP:HA	1:38:A:GLN:HE22	20	0.47
(2,212)	1:88:A:ASP:H	1:86:A:SER:H	19	0.47
(2,207)	1:79:A:ASN:HB2	1:79:A:ASN:HD22	5	0.47
(2,164)	1:14:A:GLN:HB2	1:14:A:GLN:H	17	0.47
(2,164)	1:14:A:GLN:HB3	1:14:A:GLN:H	17	0.47
(2,66)	1:5:A:GLU:H	1:7:A:ASP:H	3	0.47
(2,49)	1:35:A:SER:HB3	1:39:A:CYS:H	13	0.47
(2,46)	1:114:A:SER:HG	1:115:A:ASP:H	10	0.47
(2,11)	1:109:A:ASP:HA	1:113:A:GLY:H	14	0.47
(1,881)	1:48:A:GLU:H	1:45:A:ARG:H	10	0.47
(1,881)	1:48:A:GLU:H	1:45:A:ARG:H	12	0.47
(1,879)	1:48:A:GLU:H	1:45:A:ARG:H	10	0.47
(1,879)	1:48:A:GLU:H	1:45:A:ARG:H	12	0.47
(1,877)	1:22:A:CYS:HA	1:44:A:CYS:H	11	0.47
(1,859)	1:3:A:CYS:HB2	1:18:A:SER:H	14	0.47
(1,859)	1:3:A:CYS:HB3	1:18:A:SER:H	14	0.47
(1,856)	1:14:A:GLN:H	1:12:A:ASN:HD22	15	0.47
(1,824)	1:118:A:ASP:H	1:116:A:GLU:H	2	0.47
(1,824)	1:118:A:ASP:H	1:116:A:GLU:H	19	0.47
(1,807)	1:98:A:ILE:HG12	1:103:A:VAL:H	11	0.47
(1,807)	1:98:A:ILE:HG13	1:103:A:VAL:H	11	0.47
(1,803)	1:101:A:ASN:HD21	1:99:A:SER:H	1	0.47
(1,786)	1:71:A:CYS:H	1:76:A:ASP:H	8	0.47
(1,784)	1:71:A:CYS:HB2	1:76:A:ASP:H	8	0.47
(1,784)	1:71:A:CYS:HB3	1:76:A:ASP:H	8	0.47
(1,772)	1:68:A:GLU:H	1:64:A:ARG:H	18	0.47
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG12	4	0.47
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG13	4	0.47
(1,721)	1:21:A:LYS:HG2	1:22:A:CYS:H	16	0.47
(1,721)	1:21:A:LYS:HG3	1:22:A:CYS:H	16	0.47
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD2	17	0.47
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD3	17	0.47
(1,696)	1:44:A:CYS:HB2	1:34:A:GLU:H	2	0.47
(1,696)	1:44:A:CYS:HB3	1:34:A:GLU:H	2	0.47
(1,686)	1:74:A:GLY:H	1:69:A:ASN:HD22	20	0.47
(1,670)	1:107:A:GLN:HB2	1:105:A:ASN:HD22	13	0.47

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,670)	1:107:A:GLN:HB2	1:105:A:ASN:HD22	13	0.47
(1,670)	1:107:A:GLN:HB3	1:105:A:ASN:HD22	13	0.47
(1,670)	1:107:A:GLN:HB3	1:105:A:ASN:HD22	13	0.47
(1,667)	1:107:A:GLN:HG2	1:105:A:ASN:HD22	16	0.47
(1,667)	1:107:A:GLN:HG2	1:105:A:ASN:HD22	16	0.47
(1,667)	1:107:A:GLN:HG3	1:105:A:ASN:HD22	16	0.47
(1,667)	1:107:A:GLN:HG3	1:105:A:ASN:HD22	16	0.47
(1,657)	1:105:A:ASN:HA	1:105:A:ASN:HD22	3	0.47
(1,657)	1:105:A:ASN:HA	1:105:A:ASN:HD22	9	0.47
(1,657)	1:105:A:ASN:HA	1:105:A:ASN:HD22	19	0.47
(1,634)	1:79:A:ASN:HD22	1:79:A:ASN:HA	14	0.47
(1,608)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	8	0.47
(1,608)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	8	0.47
(1,608)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	15	0.47
(1,608)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	15	0.47
(1,596)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	6	0.47
(1,596)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	6	0.47
(1,543)	1:112:A:ASP:HB2	1:114:A:SER:H	18	0.47
(1,543)	1:112:A:ASP:HB3	1:114:A:SER:H	18	0.47
(1,534)	1:77:A:GLU:HB2	1:77:A:GLU:H	4	0.47
(1,534)	1:77:A:GLU:HB3	1:77:A:GLU:H	4	0.47
(1,534)	1:77:A:GLU:HB2	1:77:A:GLU:H	10	0.47
(1,534)	1:77:A:GLU:HB3	1:77:A:GLU:H	10	0.47
(1,534)	1:77:A:GLU:HB2	1:77:A:GLU:H	18	0.47
(1,534)	1:77:A:GLU:HB3	1:77:A:GLU:H	18	0.47
(1,531)	1:71:A:CYS:HB2	1:71:A:CYS:H	12	0.47
(1,531)	1:71:A:CYS:HB3	1:71:A:CYS:H	12	0.47
(1,526)	1:64:A:ARG:H	1:67:A:GLY:H	12	0.47
(1,436)	1:73:A:SER:H	1:72:A:ASP:H	14	0.47
(1,436)	1:73:A:SER:H	1:72:A:ASP:H	18	0.47
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	12	0.47
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	12	0.47
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	12	0.47
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	12	0.47
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB2	12	0.47
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB3	12	0.47
(1,327)	1:22:A:CYS:HB2	1:22:A:CYS:H	13	0.47
(1,327)	1:22:A:CYS:HB3	1:22:A:CYS:H	13	0.47
(1,212)	1:96:A:ARG:H	1:92:A:CYS:HA	7	0.47
(1,212)	1:96:A:ARG:H	1:92:A:CYS:HA	13	0.47
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB2	18	0.47
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB3	18	0.47

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,134)	1:110:A:CYS:H	1:109:A:ASP:HB2	2	0.47
(1,134)	1:110:A:CYS:H	1:109:A:ASP:HB2	2	0.47
(1,134)	1:110:A:CYS:H	1:109:A:ASP:HB3	2	0.47
(1,134)	1:110:A:CYS:H	1:109:A:ASP:HB3	2	0.47
(1,81)	1:28:A:CYS:HA	1:33:A:ASP:H	13	0.47
(1,80)	1:44:A:CYS:HB2	1:45:A:ARG:H	2	0.47
(1,80)	1:44:A:CYS:HB3	1:45:A:ARG:H	2	0.47
(1,73)	1:65:A:CYS:HB2	1:65:A:CYS:H	11	0.47
(1,73)	1:65:A:CYS:HB3	1:65:A:CYS:H	11	0.47
(1,60)	1:56:A:THR:H	1:57:A:GLN:H	2	0.47
(1,58)	1:66:A:ASP:H	1:65:A:CYS:H	2	0.47
(1,27)	1:118:A:ASP:H	1:117:A:LEU:H	18	0.47
(1,2)	1:112:A:ASP:H	1:113:A:GLY:H	9	0.47
(2,337)	1:53:A:ALA:HB3	1:55:A:SER:H	20	0.46
(2,331)	1:101:A:ASN:H	1:99:A:SER:H	5	0.46
(2,298)	1:28:A:CYS:HB3	1:14:A:GLN:HE22	4	0.46
(2,294)	1:61:A:VAL:HG11	1:48:A:GLU:H	19	0.46
(2,257)	1:32:A:SER:HB3	1:38:A:GLN:HE22	8	0.46
(2,253)	1:86:A:SER:HB3	1:89:A:GLU:H	10	0.46
(2,212)	1:88:A:ASP:H	1:86:A:SER:H	6	0.46
(2,212)	1:88:A:ASP:H	1:86:A:SER:H	10	0.46
(2,212)	1:88:A:ASP:H	1:86:A:SER:H	18	0.46
(2,207)	1:79:A:ASN:HB2	1:79:A:ASN:HD22	1	0.46
(2,200)	1:77:A:GLU:HG3	1:76:A:ASP:H	7	0.46
(2,174)	1:117:A:LEU:HB3	1:116:A:GLU:H	2	0.46
(2,114)	1:16:A:VAL:HG11	1:16:A:VAL:H	19	0.46
(2,114)	1:16:A:VAL:HG12	1:16:A:VAL:H	19	0.46
(2,114)	1:16:A:VAL:HG13	1:16:A:VAL:H	19	0.46
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	19	0.46
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	19	0.46
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	19	0.46
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	19	0.46
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	19	0.46
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	19	0.46
(2,66)	1:5:A:GLU:H	1:7:A:ASP:H	18	0.46
(2,12)	1:11:A:ASN:HB2	1:13:A:GLY:H	7	0.46
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB2	1	0.46
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB3	1	0.46
(1,869)	1:14:A:GLN:HE22	1:28:A:CYS:H	7	0.46
(1,859)	1:3:A:CYS:HB2	1:18:A:SER:H	18	0.46
(1,859)	1:3:A:CYS:HB3	1:18:A:SER:H	18	0.46
(1,856)	1:14:A:GLN:H	1:12:A:ASN:HD22	3	0.46

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,833)	1:42:A:ARG:HG2	1:41:A:MET:H	3	0.46
(1,833)	1:42:A:ARG:HG2	1:41:A:MET:H	3	0.46
(1,833)	1:42:A:ARG:HG3	1:41:A:MET:H	3	0.46
(1,833)	1:42:A:ARG:HG3	1:41:A:MET:H	3	0.46
(1,833)	1:42:A:ARG:HG2	1:41:A:MET:H	7	0.46
(1,833)	1:42:A:ARG:HG2	1:41:A:MET:H	7	0.46
(1,833)	1:42:A:ARG:HG3	1:41:A:MET:H	7	0.46
(1,833)	1:42:A:ARG:HG3	1:41:A:MET:H	7	0.46
(1,833)	1:42:A:ARG:HG2	1:41:A:MET:H	17	0.46
(1,833)	1:42:A:ARG:HG2	1:41:A:MET:H	17	0.46
(1,833)	1:42:A:ARG:HG3	1:41:A:MET:H	17	0.46
(1,833)	1:42:A:ARG:HG3	1:41:A:MET:H	17	0.46
(1,831)	1:73:A:SER:H	1:75:A:GLU:H	4	0.46
(1,831)	1:73:A:SER:H	1:75:A:GLU:H	18	0.46
(1,807)	1:98:A:ILE:HG12	1:103:A:VAL:H	13	0.46
(1,807)	1:98:A:ILE:HG13	1:103:A:VAL:H	13	0.46
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	3	0.46
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	3	0.46
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	3	0.46
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	3	0.46
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	5	0.46
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	5	0.46
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	5	0.46
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	5	0.46
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	10	0.46
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	10	0.46
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	10	0.46
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	10	0.46
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	11	0.46
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	11	0.46
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	11	0.46
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	11	0.46
(1,706)	1:45:A:ARG:HB2	1:45:A:ARG:H	20	0.46
(1,706)	1:45:A:ARG:HB3	1:45:A:ARG:H	20	0.46
(1,704)	1:100:A:ARG:HG2	1:100:A:ARG:H	15	0.46
(1,704)	1:100:A:ARG:HG2	1:100:A:ARG:H	15	0.46
(1,704)	1:100:A:ARG:HG3	1:100:A:ARG:H	15	0.46
(1,704)	1:100:A:ARG:HG3	1:100:A:ARG:H	15	0.46
(1,693)	1:21:A:LYS:HD2	1:21:A:LYS:H	19	0.46
(1,693)	1:21:A:LYS:HD3	1:21:A:LYS:H	19	0.46
(1,657)	1:105:A:ASN:HA	1:105:A:ASN:HD22	7	0.46
(1,634)	1:79:A:ASN:HD22	1:79:A:ASN:HA	17	0.46

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,628)	1:71:A:CYS:HB2	1:57:A:GLN:HE22	20	0.46
(1,628)	1:71:A:CYS:HB3	1:57:A:GLN:HE22	20	0.46
(1,619)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	1	0.46
(1,619)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	2	0.46
(1,619)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	3	0.46
(1,619)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	4	0.46
(1,619)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	5	0.46
(1,619)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	6	0.46
(1,619)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	7	0.46
(1,619)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	8	0.46
(1,619)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	9	0.46
(1,619)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	10	0.46
(1,619)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	11	0.46
(1,619)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	12	0.46
(1,619)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	13	0.46
(1,619)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	14	0.46
(1,619)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	15	0.46
(1,619)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	16	0.46
(1,619)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	17	0.46
(1,619)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	18	0.46
(1,619)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	20	0.46
(1,608)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	6	0.46
(1,608)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	6	0.46
(1,608)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	9	0.46
(1,608)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	9	0.46
(1,608)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	13	0.46
(1,608)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	13	0.46
(1,608)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	18	0.46
(1,608)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	18	0.46
(1,583)	1:40:A:HIS:HA	1:38:A:GLN:H	3	0.46
(1,583)	1:40:A:HIS:HA	1:38:A:GLN:H	16	0.46
(1,543)	1:112:A:ASP:HB2	1:114:A:SER:H	1	0.46
(1,543)	1:112:A:ASP:HB3	1:114:A:SER:H	1	0.46
(1,534)	1:77:A:GLU:HB2	1:77:A:GLU:H	14	0.46
(1,534)	1:77:A:GLU:HB3	1:77:A:GLU:H	14	0.46
(1,526)	1:64:A:ARG:H	1:67:A:GLY:H	3	0.46
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	20	0.46
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	20	0.46
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	20	0.46
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	20	0.46
(1,504)	1:39:A:CYS:HB2	1:39:A:CYS:H	15	0.46
(1,504)	1:39:A:CYS:HB3	1:39:A:CYS:H	15	0.46

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,480)	1:10:A:CYS:HB2	1:10:A:CYS:H	7	0.46
(1,480)	1:10:A:CYS:HB3	1:10:A:CYS:H	7	0.46
(1,466)	1:80:A:CYS:HA	1:79:A:ASN:H	8	0.46
(1,466)	1:80:A:CYS:HA	1:79:A:ASN:H	14	0.46
(1,436)	1:73:A:SER:H	1:72:A:ASP:H	15	0.46
(1,436)	1:73:A:SER:H	1:72:A:ASP:H	19	0.46
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB1	10	0.46
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB2	10	0.46
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB3	10	0.46
(1,371)	1:44:A:CYS:HA	1:45:A:ARG:H	3	0.46
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	13	0.46
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	13	0.46
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	13	0.46
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	13	0.46
(1,296)	1:10:A:CYS:HB2	1:10:A:CYS:H	17	0.46
(1,296)	1:10:A:CYS:HB3	1:10:A:CYS:H	17	0.46
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB2	12	0.46
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB3	12	0.46
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB2	17	0.46
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB3	17	0.46
(1,119)	1:112:A:ASP:H	1:115:A:ASP:H	4	0.46
(1,109)	1:119:A:CYS:H	1:117:A:LEU:HG	5	0.46
(1,73)	1:65:A:CYS:HB2	1:65:A:CYS:H	10	0.46
(1,73)	1:65:A:CYS:HB3	1:65:A:CYS:H	10	0.46
(1,58)	1:66:A:ASP:H	1:65:A:CYS:H	13	0.46
(1,56)	1:70:A:ASP:H	1:71:A:CYS:H	18	0.46
(1,27)	1:118:A:ASP:H	1:117:A:LEU:H	11	0.46
(1,2)	1:112:A:ASP:H	1:113:A:GLY:H	16	0.46
(2,381)	1:100:A:ARG:HD3	1:90:A:PHE:H	9	0.45
(2,323)	1:64:A:ARG:HG2	1:68:A:GLU:H	5	0.45
(2,296)	1:113:A:GLY:HA2	1:117:A:LEU:H	14	0.45
(2,244)	1:60:A:PRO:HA	1:47:A:HIS:H	18	0.45
(2,207)	1:79:A:ASN:HB2	1:79:A:ASN:HD22	3	0.45
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	2	0.45
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	2	0.45
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	2	0.45
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	2	0.45
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	2	0.45
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	2	0.45
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	2	0.45
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	2	0.45
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	2	0.45

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	2	0.45
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	2	0.45
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	2	0.45
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	2	0.45
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	2	0.45
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	2	0.45
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	2	0.45
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	2	0.45
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	2	0.45
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	6	0.45
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	6	0.45
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	6	0.45
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	6	0.45
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	6	0.45
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	6	0.45
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	6	0.45
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	6	0.45
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	6	0.45
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	6	0.45
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	6	0.45
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	6	0.45
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	6	0.45
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	6	0.45
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	6	0.45
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	6	0.45
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	6	0.45
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	6	0.45
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	6	0.45
(2,168)	1:38:A:GLN:HG2	1:38:A:GLN:H	17	0.45
(2,154)	1:116:A:GLU:HG3	1:109:A:ASP:H	5	0.45
(2,46)	1:114:A:SER:HG	1:115:A:ASP:H	7	0.45
(2,44)	1:83:A:ILE:HG23	1:97:A:CYS:H	3	0.45
(2,4)	1:46:A:ILE:HG21	1:46:A:ILE:H	19	0.45
(1,923)	1:8:A:PHE:HB2	1:16:A:VAL:HA	4	0.45
(1,916)	1:77:A:GLU:HB2	1:77:A:GLU:H	6	0.45
(1,916)	1:77:A:GLU:HB3	1:77:A:GLU:H	6	0.45
(1,896)	1:64:A:ARG:H	1:66:A:ASP:H	17	0.45
(1,888)	1:49:A:ILE:HA	1:61:A:VAL:H	17	0.45
(1,871)	1:30:A:ASP:HB2	1:32:A:SER:H	3	0.45
(1,871)	1:30:A:ASP:HB3	1:32:A:SER:H	3	0.45
(1,871)	1:30:A:ASP:HB2	1:32:A:SER:H	18	0.45
(1,871)	1:30:A:ASP:HB3	1:32:A:SER:H	18	0.45
(1,856)	1:14:A:GLN:H	1:12:A:ASN:HD22	12	0.45

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,850)	1:12:A:ASN:H	1:11:A:ASN:HD22	20	0.45
(1,833)	1:42:A:ARG:HG2	1:41:A:MET:H	5	0.45
(1,833)	1:42:A:ARG:HG2	1:41:A:MET:H	5	0.45
(1,833)	1:42:A:ARG:HG3	1:41:A:MET:H	5	0.45
(1,833)	1:42:A:ARG:HG3	1:41:A:MET:H	5	0.45
(1,820)	1:110:A:CYS:H	1:115:A:ASP:H	8	0.45
(1,820)	1:110:A:CYS:H	1:115:A:ASP:H	10	0.45
(1,776)	1:77:A:GLU:HG2	1:70:A:ASP:H	2	0.45
(1,776)	1:77:A:GLU:HG3	1:70:A:ASP:H	2	0.45
(1,772)	1:68:A:GLU:H	1:64:A:ARG:H	19	0.45
(1,750)	1:57:A:GLN:HB2	1:52:A:GLY:H	1	0.45
(1,750)	1:57:A:GLN:HB2	1:52:A:GLY:H	1	0.45
(1,750)	1:57:A:GLN:HB3	1:52:A:GLY:H	1	0.45
(1,750)	1:57:A:GLN:HB3	1:52:A:GLY:H	1	0.45
(1,735)	1:28:A:CYS:HB2	1:33:A:ASP:H	18	0.45
(1,735)	1:28:A:CYS:HB3	1:33:A:ASP:H	18	0.45
(1,732)	1:31:A:GLY:HA2	1:32:A:SER:H	11	0.45
(1,732)	1:31:A:GLY:HA3	1:32:A:SER:H	11	0.45
(1,732)	1:31:A:GLY:HA2	1:32:A:SER:H	16	0.45
(1,732)	1:31:A:GLY:HA3	1:32:A:SER:H	16	0.45
(1,721)	1:21:A:LYS:HG2	1:22:A:CYS:H	7	0.45
(1,721)	1:21:A:LYS:HG3	1:22:A:CYS:H	7	0.45
(1,706)	1:45:A:ARG:HB2	1:45:A:ARG:H	18	0.45
(1,706)	1:45:A:ARG:HB3	1:45:A:ARG:H	18	0.45
(1,704)	1:100:A:ARG:HG2	1:100:A:ARG:H	20	0.45
(1,704)	1:100:A:ARG:HG2	1:100:A:ARG:H	20	0.45
(1,704)	1:100:A:ARG:HG3	1:100:A:ARG:H	20	0.45
(1,704)	1:100:A:ARG:HG3	1:100:A:ARG:H	20	0.45
(1,693)	1:21:A:LYS:HD2	1:21:A:LYS:H	7	0.45
(1,693)	1:21:A:LYS:HD3	1:21:A:LYS:H	7	0.45
(1,687)	1:69:A:ASN:HD21	1:74:A:GLY:H	20	0.45
(1,686)	1:74:A:GLY:H	1:69:A:ASN:HD22	19	0.45
(1,685)	1:107:A:GLN:HG2	1:107:A:GLN:HE21	4	0.45
(1,685)	1:107:A:GLN:HG2	1:107:A:GLN:HE21	4	0.45
(1,685)	1:107:A:GLN:HG3	1:107:A:GLN:HE21	4	0.45
(1,685)	1:107:A:GLN:HG3	1:107:A:GLN:HE21	4	0.45
(1,670)	1:107:A:GLN:HB2	1:105:A:ASN:HD22	16	0.45
(1,670)	1:107:A:GLN:HB2	1:105:A:ASN:HD22	16	0.45
(1,670)	1:107:A:GLN:HB3	1:105:A:ASN:HD22	16	0.45
(1,670)	1:107:A:GLN:HB3	1:105:A:ASN:HD22	16	0.45
(1,654)	1:107:A:GLN:HB2	1:107:A:GLN:HE22	5	0.45
(1,654)	1:107:A:GLN:HB2	1:107:A:GLN:HE22	5	0.45

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,654)	1:107:A:GLN:HB3	1:107:A:GLN:HE22	5	0.45
(1,654)	1:107:A:GLN:HB3	1:107:A:GLN:HE22	5	0.45
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	8	0.45
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	8	0.45
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	8	0.45
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	8	0.45
(1,642)	1:82:A:ASN:HA	1:82:A:ASN:HD22	17	0.45
(1,619)	1:12:A:ASN:HD21	1:12:A:ASN:HD22	19	0.45
(1,608)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	10	0.45
(1,608)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	10	0.45
(1,608)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	14	0.45
(1,608)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	14	0.45
(1,587)	1:14:A:GLN:H	1:12:A:ASN:H	11	0.45
(1,587)	1:14:A:GLN:H	1:12:A:ASN:H	16	0.45
(1,587)	1:14:A:GLN:H	1:12:A:ASN:H	19	0.45
(1,587)	1:14:A:GLN:H	1:12:A:ASN:H	20	0.45
(1,583)	1:40:A:HIS:HA	1:38:A:GLN:H	1	0.45
(1,466)	1:80:A:CYS:HA	1:79:A:ASN:H	12	0.45
(1,466)	1:80:A:CYS:HA	1:79:A:ASN:H	18	0.45
(1,454)	1:78:A:GLU:HG2	1:76:A:ASP:H	10	0.45
(1,454)	1:78:A:GLU:HG3	1:76:A:ASP:H	10	0.45
(1,447)	1:71:A:CYS:HA	1:74:A:GLY:H	11	0.45
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	7	0.45
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	7	0.45
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	7	0.45
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	7	0.45
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB2	8	0.45
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB3	8	0.45
(1,346)	1:32:A:SER:H	1:31:A:GLY:H	7	0.45
(1,327)	1:22:A:CYS:HB2	1:22:A:CYS:H	7	0.45
(1,327)	1:22:A:CYS:HB3	1:22:A:CYS:H	7	0.45
(1,327)	1:22:A:CYS:HB2	1:22:A:CYS:H	20	0.45
(1,327)	1:22:A:CYS:HB3	1:22:A:CYS:H	20	0.45
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB2	11	0.45
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB3	11	0.45
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB2	16	0.45
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB3	16	0.45
(1,298)	1:14:A:GLN:H	1:11:A:ASN:H	5	0.45
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	10	0.45
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	10	0.45
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	10	0.45
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	10	0.45

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB2	20	0.45
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB3	20	0.45
(1,119)	1:112:A:ASP:H	1:115:A:ASP:H	7	0.45
(1,118)	1:115:A:ASP:H	1:113:A:GLY:H	13	0.45
(1,118)	1:115:A:ASP:H	1:113:A:GLY:H	18	0.45
(1,97)	1:98:A:ILE:HD11	1:99:A:SER:H	6	0.45
(1,97)	1:98:A:ILE:HD12	1:99:A:SER:H	6	0.45
(1,97)	1:98:A:ILE:HD13	1:99:A:SER:H	6	0.45
(1,97)	1:98:A:ILE:HD11	1:99:A:SER:H	7	0.45
(1,97)	1:98:A:ILE:HD12	1:99:A:SER:H	7	0.45
(1,97)	1:98:A:ILE:HD13	1:99:A:SER:H	7	0.45
(1,97)	1:98:A:ILE:HD11	1:99:A:SER:H	17	0.45
(1,97)	1:98:A:ILE:HD12	1:99:A:SER:H	17	0.45
(1,97)	1:98:A:ILE:HD13	1:99:A:SER:H	17	0.45
(1,93)	1:8:A:PHE:H	1:7:A:ASP:HA	6	0.45
(1,85)	1:21:A:LYS:HG2	1:22:A:CYS:H	1	0.45
(1,85)	1:21:A:LYS:HG3	1:22:A:CYS:H	1	0.45
(1,81)	1:28:A:CYS:HA	1:33:A:ASP:H	20	0.45
(1,73)	1:65:A:CYS:HB2	1:65:A:CYS:H	8	0.45
(1,73)	1:65:A:CYS:HB3	1:65:A:CYS:H	8	0.45
(1,60)	1:56:A:THR:H	1:57:A:GLN:H	17	0.45
(1,58)	1:66:A:ASP:H	1:65:A:CYS:H	6	0.45
(1,56)	1:70:A:ASP:H	1:71:A:CYS:H	14	0.45
(1,27)	1:118:A:ASP:H	1:117:A:LEU:H	12	0.45
(2,278)	1:42:A:ARG:HA	1:42:A:ARG:H	2	0.44
(2,278)	1:42:A:ARG:HA	1:42:A:ARG:H	15	0.44
(2,212)	1:88:A:ASP:H	1:86:A:SER:H	8	0.44
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	8	0.44
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	8	0.44
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	8	0.44
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	8	0.44
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	8	0.44
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	8	0.44
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	8	0.44
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	8	0.44
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	8	0.44
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	8	0.44
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	8	0.44
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	8	0.44
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	8	0.44
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	8	0.44
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	8	0.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	8	0.44
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	8	0.44
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	8	0.44
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	10	0.44
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	10	0.44
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	10	0.44
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	10	0.44
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	10	0.44
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	10	0.44
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	10	0.44
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	10	0.44
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	10	0.44
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	10	0.44
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	10	0.44
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	10	0.44
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	10	0.44
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	10	0.44
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	10	0.44
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	10	0.44
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	10	0.44
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	10	0.44
(2,154)	1:116:A:GLU:HG3	1:109:A:ASP:H	17	0.44
(2,114)	1:16:A:VAL:HG11	1:16:A:VAL:H	2	0.44
(2,114)	1:16:A:VAL:HG12	1:16:A:VAL:H	2	0.44
(2,114)	1:16:A:VAL:HG13	1:16:A:VAL:H	2	0.44
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	2	0.44
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	2	0.44
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	2	0.44
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	2	0.44
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	2	0.44
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	2	0.44
(2,114)	1:16:A:VAL:HG11	1:16:A:VAL:H	7	0.44
(2,114)	1:16:A:VAL:HG12	1:16:A:VAL:H	7	0.44
(2,114)	1:16:A:VAL:HG13	1:16:A:VAL:H	7	0.44
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	7	0.44
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	7	0.44
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	7	0.44
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	7	0.44
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	7	0.44
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	7	0.44
(2,25)	1:79:A:ASN:HD22	1:80:A:CYS:HA	10	0.44
(2,25)	1:79:A:ASN:HD22	1:80:A:CYS:HA	17	0.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,898)	1:57:A:GLN:HE22	1:71:A:CYS:H	10	0.44
(1,896)	1:64:A:ARG:H	1:66:A:ASP:H	4	0.44
(1,896)	1:64:A:ARG:H	1:66:A:ASP:H	14	0.44
(1,831)	1:73:A:SER:H	1:75:A:GLU:H	12	0.44
(1,831)	1:73:A:SER:H	1:75:A:GLU:H	14	0.44
(1,831)	1:73:A:SER:H	1:75:A:GLU:H	15	0.44
(1,819)	1:112:A:ASP:HB2	1:115:A:ASP:H	20	0.44
(1,819)	1:112:A:ASP:HB3	1:115:A:ASP:H	20	0.44
(1,807)	1:98:A:ILE:HG12	1:103:A:VAL:H	14	0.44
(1,807)	1:98:A:ILE:HG13	1:103:A:VAL:H	14	0.44
(1,807)	1:98:A:ILE:HG12	1:103:A:VAL:H	15	0.44
(1,807)	1:98:A:ILE:HG13	1:103:A:VAL:H	15	0.44
(1,789)	1:85:A:CYS:H	1:84:A:THR:HB	1	0.44
(1,789)	1:85:A:CYS:H	1:84:A:THR:HB	6	0.44
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	1	0.44
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	1	0.44
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	1	0.44
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	1	0.44
(1,747)	1:57:A:GLN:HB2	1:51:A:CYS:H	20	0.44
(1,747)	1:57:A:GLN:HB2	1:51:A:CYS:H	20	0.44
(1,747)	1:57:A:GLN:HB3	1:51:A:CYS:H	20	0.44
(1,747)	1:57:A:GLN:HB3	1:51:A:CYS:H	20	0.44
(1,733)	1:32:A:SER:H	1:28:A:CYS:H	6	0.44
(1,732)	1:31:A:GLY:HA2	1:32:A:SER:H	13	0.44
(1,732)	1:31:A:GLY:HA3	1:32:A:SER:H	13	0.44
(1,732)	1:31:A:GLY:HA2	1:32:A:SER:H	20	0.44
(1,732)	1:31:A:GLY:HA3	1:32:A:SER:H	20	0.44
(1,729)	1:32:A:SER:H	1:28:A:CYS:H	6	0.44
(1,721)	1:21:A:LYS:HG2	1:22:A:CYS:H	17	0.44
(1,721)	1:21:A:LYS:HG3	1:22:A:CYS:H	17	0.44
(1,721)	1:21:A:LYS:HG2	1:22:A:CYS:H	19	0.44
(1,721)	1:21:A:LYS:HG3	1:22:A:CYS:H	19	0.44
(1,708)	1:44:A:CYS:HB2	1:45:A:ARG:H	19	0.44
(1,708)	1:44:A:CYS:HB3	1:45:A:ARG:H	19	0.44
(1,706)	1:45:A:ARG:HB2	1:45:A:ARG:H	9	0.44
(1,706)	1:45:A:ARG:HB3	1:45:A:ARG:H	9	0.44
(1,706)	1:45:A:ARG:HB2	1:45:A:ARG:H	12	0.44
(1,706)	1:45:A:ARG:HB3	1:45:A:ARG:H	12	0.44
(1,696)	1:44:A:CYS:HB2	1:34:A:GLU:H	11	0.44
(1,696)	1:44:A:CYS:HB3	1:34:A:GLU:H	11	0.44
(1,693)	1:21:A:LYS:HD2	1:21:A:LYS:H	13	0.44
(1,693)	1:21:A:LYS:HD3	1:21:A:LYS:H	13	0.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,687)	1:69:A:ASN:HD21	1:74:A:GLY:H	17	0.44
(1,657)	1:105:A:ASN:HA	1:105:A:ASN:HD22	1	0.44
(1,657)	1:105:A:ASN:HA	1:105:A:ASN:HD22	8	0.44
(1,657)	1:105:A:ASN:HA	1:105:A:ASN:HD22	10	0.44
(1,657)	1:105:A:ASN:HA	1:105:A:ASN:HD22	16	0.44
(1,654)	1:107:A:GLN:HB2	1:107:A:GLN:HE22	19	0.44
(1,654)	1:107:A:GLN:HB2	1:107:A:GLN:HE22	19	0.44
(1,654)	1:107:A:GLN:HB3	1:107:A:GLN:HE22	19	0.44
(1,654)	1:107:A:GLN:HB3	1:107:A:GLN:HE22	19	0.44
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	12	0.44
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	12	0.44
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	12	0.44
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	12	0.44
(1,634)	1:79:A:ASN:HD22	1:79:A:ASN:HA	12	0.44
(1,634)	1:79:A:ASN:HD22	1:79:A:ASN:HA	15	0.44
(1,587)	1:14:A:GLN:H	1:12:A:ASN:H	17	0.44
(1,553)	1:115:A:ASP:HB2	1:104:A:CYS:H	20	0.44
(1,553)	1:115:A:ASP:HB3	1:104:A:CYS:H	20	0.44
(1,504)	1:39:A:CYS:HB2	1:39:A:CYS:H	14	0.44
(1,504)	1:39:A:CYS:HB3	1:39:A:CYS:H	14	0.44
(1,486)	1:7:A:ASP:HA	1:19:A:ARG:H	14	0.44
(1,446)	1:73:A:SER:H	1:74:A:GLY:H	10	0.44
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	19	0.44
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	19	0.44
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	19	0.44
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	19	0.44
(1,327)	1:22:A:CYS:HB2	1:22:A:CYS:H	11	0.44
(1,327)	1:22:A:CYS:HB3	1:22:A:CYS:H	11	0.44
(1,327)	1:22:A:CYS:HB2	1:22:A:CYS:H	12	0.44
(1,327)	1:22:A:CYS:HB3	1:22:A:CYS:H	12	0.44
(1,320)	1:7:A:ASP:HA	1:18:A:SER:H	20	0.44
(1,298)	1:14:A:GLN:H	1:11:A:ASN:H	16	0.44
(1,174)	1:103:A:VAL:H	1:101:A:ASN:HB2	6	0.44
(1,174)	1:103:A:VAL:H	1:101:A:ASN:HB3	6	0.44
(1,158)	1:104:A:CYS:HA	1:105:A:ASN:H	9	0.44
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB2	11	0.44
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB3	11	0.44
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB2	14	0.44
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB3	14	0.44
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB2	15	0.44
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB3	15	0.44
(1,118)	1:115:A:ASP:H	1:113:A:GLY:H	12	0.44

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,99)	1:98:A:ILE:HG12	1:99:A:SER:H	12	0.44
(1,99)	1:98:A:ILE:HG13	1:99:A:SER:H	12	0.44
(1,93)	1:8:A:PHE:H	1:7:A:ASP:HA	12	0.44
(1,60)	1:56:A:THR:H	1:57:A:GLN:H	5	0.44
(1,60)	1:56:A:THR:H	1:57:A:GLN:H	13	0.44
(1,27)	1:118:A:ASP:H	1:117:A:LEU:H	15	0.44
(4,8)	1:8:A:PHE:O	1:16:A:VAL:H	18	0.43
(2,381)	1:100:A:ARG:HD3	1:90:A:PHE:H	11	0.43
(2,368)	1:87:A:PRO:HD2	1:88:A:ASP:H	11	0.43
(2,302)	1:119:A:CYS:HA	1:120:A:ALA:H	5	0.43
(2,298)	1:28:A:CYS:HB2	1:14:A:GLN:HE22	17	0.43
(2,278)	1:42:A:ARG:HA	1:42:A:ARG:H	10	0.43
(2,207)	1:79:A:ASN:HB2	1:79:A:ASN:HD22	7	0.43
(2,190)	1:56:A:THR:HA	1:57:A:GLN:H	18	0.43
(2,154)	1:116:A:GLU:HG3	1:109:A:ASP:H	10	0.43
(2,114)	1:16:A:VAL:HG11	1:16:A:VAL:H	18	0.43
(2,114)	1:16:A:VAL:HG12	1:16:A:VAL:H	18	0.43
(2,114)	1:16:A:VAL:HG13	1:16:A:VAL:H	18	0.43
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	18	0.43
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	18	0.43
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	18	0.43
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	18	0.43
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	18	0.43
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	18	0.43
(2,90)	1:60:A:PRO:HB2	1:63:A:TRP:HE1	17	0.43
(2,66)	1:4:A:ALA:H	1:7:A:ASP:H	15	0.43
(2,11)	1:110:A:CYS:HA	1:113:A:GLY:H	16	0.43
(1,888)	1:49:A:ILE:HA	1:61:A:VAL:H	1	0.43
(1,862)	1:21:A:LYS:HE2	1:19:A:ARG:H	15	0.43
(1,862)	1:21:A:LYS:HE3	1:19:A:ARG:H	15	0.43
(1,862)	1:21:A:LYS:HE2	1:19:A:ARG:H	20	0.43
(1,862)	1:21:A:LYS:HE3	1:19:A:ARG:H	20	0.43
(1,859)	1:3:A:CYS:HB2	1:18:A:SER:H	3	0.43
(1,859)	1:3:A:CYS:HB3	1:18:A:SER:H	3	0.43
(1,859)	1:3:A:CYS:HB2	1:18:A:SER:H	4	0.43
(1,859)	1:3:A:CYS:HB3	1:18:A:SER:H	4	0.43
(1,853)	1:10:A:CYS:HB2	1:12:A:ASN:H	20	0.43
(1,853)	1:10:A:CYS:HB3	1:12:A:ASN:H	20	0.43
(1,850)	1:12:A:ASN:H	1:11:A:ASN:HD22	16	0.43
(1,794)	1:82:A:ASN:HD22	1:94:A:SER:H	13	0.43
(1,772)	1:68:A:GLU:H	1:64:A:ARG:H	11	0.43
(1,750)	1:57:A:GLN:HB2	1:52:A:GLY:H	18	0.43

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,750)	1:57:A:GLN:HB2	1:52:A:GLY:H	18	0.43
(1,750)	1:57:A:GLN:HB3	1:52:A:GLY:H	18	0.43
(1,750)	1:57:A:GLN:HB3	1:52:A:GLY:H	18	0.43
(1,744)	1:48:A:GLU:H	1:47:A:HIS:H	14	0.43
(1,735)	1:28:A:CYS:HB2	1:33:A:ASP:H	14	0.43
(1,735)	1:28:A:CYS:HB3	1:33:A:ASP:H	14	0.43
(1,732)	1:31:A:GLY:HA2	1:32:A:SER:H	7	0.43
(1,732)	1:31:A:GLY:HA3	1:32:A:SER:H	7	0.43
(1,724)	1:34:A:GLU:HB2	1:25:A:ASP:H	14	0.43
(1,724)	1:34:A:GLU:HB3	1:25:A:ASP:H	14	0.43
(1,706)	1:45:A:ARG:HB2	1:45:A:ARG:H	10	0.43
(1,706)	1:45:A:ARG:HB3	1:45:A:ARG:H	10	0.43
(1,704)	1:100:A:ARG:HG2	1:100:A:ARG:H	19	0.43
(1,704)	1:100:A:ARG:HG2	1:100:A:ARG:H	19	0.43
(1,704)	1:100:A:ARG:HG3	1:100:A:ARG:H	19	0.43
(1,704)	1:100:A:ARG:HG3	1:100:A:ARG:H	19	0.43
(1,696)	1:44:A:CYS:HB2	1:34:A:GLU:H	6	0.43
(1,696)	1:44:A:CYS:HB3	1:34:A:GLU:H	6	0.43
(1,688)	1:69:A:ASN:H	1:69:A:ASN:HD22	12	0.43
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD2	3	0.43
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD3	3	0.43
(1,679)	1:78:A:GLU:HG2	1:79:A:ASN:HD22	4	0.43
(1,679)	1:78:A:GLU:HG3	1:79:A:ASN:HD22	4	0.43
(1,670)	1:107:A:GLN:HB2	1:105:A:ASN:HD22	4	0.43
(1,670)	1:107:A:GLN:HB2	1:105:A:ASN:HD22	4	0.43
(1,670)	1:107:A:GLN:HB3	1:105:A:ASN:HD22	4	0.43
(1,670)	1:107:A:GLN:HB3	1:105:A:ASN:HD22	4	0.43
(1,667)	1:107:A:GLN:HG2	1:105:A:ASN:HD22	1	0.43
(1,667)	1:107:A:GLN:HG2	1:105:A:ASN:HD22	1	0.43
(1,667)	1:107:A:GLN:HG3	1:105:A:ASN:HD22	1	0.43
(1,667)	1:107:A:GLN:HG3	1:105:A:ASN:HD22	1	0.43
(1,667)	1:107:A:GLN:HG2	1:105:A:ASN:HD22	5	0.43
(1,667)	1:107:A:GLN:HG2	1:105:A:ASN:HD22	5	0.43
(1,667)	1:107:A:GLN:HG3	1:105:A:ASN:HD22	5	0.43
(1,667)	1:107:A:GLN:HG3	1:105:A:ASN:HD22	5	0.43
(1,667)	1:107:A:GLN:HG2	1:105:A:ASN:HD22	7	0.43
(1,667)	1:107:A:GLN:HG2	1:105:A:ASN:HD22	7	0.43
(1,667)	1:107:A:GLN:HG3	1:105:A:ASN:HD22	7	0.43
(1,667)	1:107:A:GLN:HG3	1:105:A:ASN:HD22	7	0.43
(1,667)	1:107:A:GLN:HG2	1:105:A:ASN:HD22	19	0.43
(1,667)	1:107:A:GLN:HG2	1:105:A:ASN:HD22	19	0.43
(1,667)	1:107:A:GLN:HG3	1:105:A:ASN:HD22	19	0.43

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,667)	1:107:A:GLN:HG3	1:105:A:ASN:HD22	19	0.43
(1,657)	1:105:A:ASN:HA	1:105:A:ASN:HD22	5	0.43
(1,657)	1:105:A:ASN:HA	1:105:A:ASN:HD22	11	0.43
(1,654)	1:107:A:GLN:HB2	1:107:A:GLN:HE22	1	0.43
(1,654)	1:107:A:GLN:HB2	1:107:A:GLN:HE22	1	0.43
(1,654)	1:107:A:GLN:HB3	1:107:A:GLN:HE22	1	0.43
(1,654)	1:107:A:GLN:HB3	1:107:A:GLN:HE22	1	0.43
(1,654)	1:107:A:GLN:HB2	1:107:A:GLN:HE22	8	0.43
(1,654)	1:107:A:GLN:HB2	1:107:A:GLN:HE22	8	0.43
(1,654)	1:107:A:GLN:HB3	1:107:A:GLN:HE22	8	0.43
(1,654)	1:107:A:GLN:HB3	1:107:A:GLN:HE22	8	0.43
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	4	0.43
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	4	0.43
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	4	0.43
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	4	0.43
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	19	0.43
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	19	0.43
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	19	0.43
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	19	0.43
(1,608)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	20	0.43
(1,608)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	20	0.43
(1,587)	1:14:A:GLN:H	1:12:A:ASN:H	2	0.43
(1,587)	1:14:A:GLN:H	1:12:A:ASN:H	7	0.43
(1,587)	1:14:A:GLN:H	1:12:A:ASN:H	13	0.43
(1,531)	1:71:A:CYS:HB2	1:71:A:CYS:H	2	0.43
(1,531)	1:71:A:CYS:HB3	1:71:A:CYS:H	2	0.43
(1,529)	1:59:A:ILE:HD11	1:70:A:ASP:H	4	0.43
(1,529)	1:59:A:ILE:HD12	1:70:A:ASP:H	4	0.43
(1,529)	1:59:A:ILE:HD13	1:70:A:ASP:H	4	0.43
(1,504)	1:39:A:CYS:HB2	1:39:A:CYS:H	18	0.43
(1,504)	1:39:A:CYS:HB3	1:39:A:CYS:H	18	0.43
(1,466)	1:80:A:CYS:HA	1:79:A:ASN:H	15	0.43
(1,447)	1:71:A:CYS:HA	1:74:A:GLY:H	3	0.43
(1,447)	1:71:A:CYS:HA	1:74:A:GLY:H	16	0.43
(1,390)	1:51:A:CYS:HB2	1:52:A:GLY:H	6	0.43
(1,390)	1:51:A:CYS:HB3	1:52:A:GLY:H	6	0.43
(1,346)	1:32:A:SER:H	1:31:A:GLY:H	11	0.43
(1,327)	1:22:A:CYS:HB2	1:22:A:CYS:H	4	0.43
(1,327)	1:22:A:CYS:HB3	1:22:A:CYS:H	4	0.43
(1,327)	1:22:A:CYS:HB2	1:22:A:CYS:H	16	0.43
(1,327)	1:22:A:CYS:HB3	1:22:A:CYS:H	16	0.43
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB2	9	0.43

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB3	9	0.43
(1,248)	1:83:A:ILE:HB	1:84:A:THR:H	12	0.43
(1,224)	1:92:A:CYS:HA	1:94:A:SER:H	20	0.43
(1,212)	1:96:A:ARG:H	1:92:A:CYS:HA	4	0.43
(1,212)	1:96:A:ARG:H	1:92:A:CYS:HA	14	0.43
(1,212)	1:96:A:ARG:H	1:92:A:CYS:HA	15	0.43
(1,212)	1:96:A:ARG:H	1:92:A:CYS:HA	17	0.43
(1,174)	1:103:A:VAL:H	1:101:A:ASN:HB2	4	0.43
(1,174)	1:103:A:VAL:H	1:101:A:ASN:HB3	4	0.43
(1,158)	1:104:A:CYS:HA	1:105:A:ASN:H	16	0.43
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB2	2	0.43
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB3	2	0.43
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB2	5	0.43
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB3	5	0.43
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB2	9	0.43
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB3	9	0.43
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB2	13	0.43
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB3	13	0.43
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB2	19	0.43
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB3	19	0.43
(1,125)	1:114:A:SER:H	1:113:A:GLY:HA2	9	0.43
(1,125)	1:114:A:SER:H	1:113:A:GLY:HA3	9	0.43
(1,97)	1:98:A:ILE:HD11	1:99:A:SER:H	5	0.43
(1,97)	1:98:A:ILE:HD12	1:99:A:SER:H	5	0.43
(1,97)	1:98:A:ILE:HD13	1:99:A:SER:H	5	0.43
(1,93)	1:8:A:PHE:H	1:7:A:ASP:HA	14	0.43
(1,92)	1:7:A:ASP:HB2	1:8:A:PHE:H	19	0.43
(1,92)	1:7:A:ASP:HB3	1:8:A:PHE:H	19	0.43
(1,81)	1:28:A:CYS:HA	1:33:A:ASP:H	12	0.43
(1,73)	1:65:A:CYS:HB2	1:65:A:CYS:H	3	0.43
(1,73)	1:65:A:CYS:HB3	1:65:A:CYS:H	3	0.43
(1,60)	1:56:A:THR:H	1:57:A:GLN:H	6	0.43
(4,8)	1:8:A:PHE:O	1:16:A:VAL:H	1	0.42
(4,8)	1:8:A:PHE:O	1:16:A:VAL:H	5	0.42
(4,8)	1:8:A:PHE:O	1:16:A:VAL:H	6	0.42
(2,381)	1:100:A:ARG:HD3	1:90:A:PHE:H	1	0.42
(2,331)	1:101:A:ASN:H	1:99:A:SER:H	17	0.42
(2,323)	1:64:A:ARG:HG2	1:68:A:GLU:H	6	0.42
(2,278)	1:42:A:ARG:HA	1:42:A:ARG:H	4	0.42
(2,278)	1:42:A:ARG:HA	1:42:A:ARG:H	5	0.42
(2,278)	1:42:A:ARG:HA	1:42:A:ARG:H	6	0.42
(2,278)	1:42:A:ARG:HA	1:42:A:ARG:H	17	0.42

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,278)	1:42:A:ARG:HA	1:42:A:ARG:H	19	0.42
(2,200)	1:77:A:GLU:HG3	1:76:A:ASP:H	19	0.42
(2,190)	1:56:A:THR:HA	1:57:A:GLN:H	4	0.42
(2,190)	1:56:A:THR:HA	1:57:A:GLN:H	20	0.42
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	3	0.42
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	3	0.42
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	3	0.42
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	3	0.42
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	3	0.42
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	3	0.42
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	3	0.42
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	3	0.42
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	3	0.42
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	3	0.42
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	3	0.42
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	3	0.42
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	3	0.42
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	3	0.42
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	3	0.42
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	3	0.42
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	3	0.42
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	3	0.42
(2,114)	1:16:A:VAL:HG11	1:16:A:VAL:H	3	0.42
(2,114)	1:16:A:VAL:HG12	1:16:A:VAL:H	3	0.42
(2,114)	1:16:A:VAL:HG13	1:16:A:VAL:H	3	0.42
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	3	0.42
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	3	0.42
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	3	0.42
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	3	0.42
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	3	0.42
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	3	0.42
(2,114)	1:16:A:VAL:HG11	1:16:A:VAL:H	16	0.42
(2,114)	1:16:A:VAL:HG12	1:16:A:VAL:H	16	0.42
(2,114)	1:16:A:VAL:HG13	1:16:A:VAL:H	16	0.42
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	16	0.42
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	16	0.42
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	16	0.42
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	16	0.42
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	16	0.42
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	16	0.42
(2,89)	1:107:A:GLN:HB2	1:108:A:ASP:H	17	0.42
(2,89)	1:107:A:GLN:HB3	1:108:A:ASP:H	17	0.42

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,80)	1:41:A:MET:HA	1:56:A:THR:H	18	0.42
(2,8)	1:45:A:ARG:HA	1:46:A:ILE:H	19	0.42
(2,4)	1:46:A:ILE:HG23	1:46:A:ILE:H	10	0.42
(1,911)	1:57:A:GLN:HE21	1:71:A:CYS:H	5	0.42
(1,862)	1:21:A:LYS:HE2	1:19:A:ARG:H	3	0.42
(1,862)	1:21:A:LYS:HE3	1:19:A:ARG:H	3	0.42
(1,853)	1:10:A:CYS:HB2	1:12:A:ASN:H	11	0.42
(1,853)	1:10:A:CYS:HB3	1:12:A:ASN:H	11	0.42
(1,850)	1:12:A:ASN:H	1:11:A:ASN:HD22	11	0.42
(1,849)	1:33:A:ASP:H	1:11:A:ASN:H	12	0.42
(1,849)	1:33:A:ASP:H	1:11:A:ASN:H	14	0.42
(1,819)	1:112:A:ASP:HB2	1:115:A:ASP:H	14	0.42
(1,819)	1:112:A:ASP:HB3	1:115:A:ASP:H	14	0.42
(1,806)	1:101:A:ASN:HD21	1:102:A:PHE:H	19	0.42
(1,803)	1:101:A:ASN:HD21	1:99:A:SER:H	8	0.42
(1,788)	1:80:A:CYS:H	1:78:A:GLU:H	12	0.42
(1,745)	1:48:A:GLU:HB2	1:49:A:ILE:H	14	0.42
(1,745)	1:48:A:GLU:HB3	1:49:A:ILE:H	14	0.42
(1,735)	1:28:A:CYS:HB2	1:33:A:ASP:H	3	0.42
(1,735)	1:28:A:CYS:HB3	1:33:A:ASP:H	3	0.42
(1,735)	1:28:A:CYS:HB2	1:33:A:ASP:H	15	0.42
(1,735)	1:28:A:CYS:HB3	1:33:A:ASP:H	15	0.42
(1,732)	1:31:A:GLY:HA2	1:32:A:SER:H	8	0.42
(1,732)	1:31:A:GLY:HA3	1:32:A:SER:H	8	0.42
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD2	16	0.42
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD3	16	0.42
(1,693)	1:21:A:LYS:HD2	1:21:A:LYS:H	8	0.42
(1,693)	1:21:A:LYS:HD3	1:21:A:LYS:H	8	0.42
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD2	6	0.42
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD3	6	0.42
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD2	9	0.42
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD3	9	0.42
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	15	0.42
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	15	0.42
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	15	0.42
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	15	0.42
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	20	0.42
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	20	0.42
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	20	0.42
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	20	0.42
(1,634)	1:79:A:ASN:HD22	1:79:A:ASN:HA	18	0.42
(1,596)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	14	0.42

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,596)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	14	0.42
(1,587)	1:14:A:GLN:H	1:12:A:ASN:H	1	0.42
(1,555)	1:103:A:VAL:HG11	1:104:A:CYS:H	6	0.42
(1,555)	1:103:A:VAL:HG12	1:104:A:CYS:H	6	0.42
(1,555)	1:103:A:VAL:HG13	1:104:A:CYS:H	6	0.42
(1,555)	1:103:A:VAL:HG21	1:104:A:CYS:H	6	0.42
(1,555)	1:103:A:VAL:HG22	1:104:A:CYS:H	6	0.42
(1,555)	1:103:A:VAL:HG23	1:104:A:CYS:H	6	0.42
(1,531)	1:71:A:CYS:HB2	1:71:A:CYS:H	6	0.42
(1,531)	1:71:A:CYS:HB3	1:71:A:CYS:H	6	0.42
(1,531)	1:71:A:CYS:HB2	1:71:A:CYS:H	7	0.42
(1,531)	1:71:A:CYS:HB3	1:71:A:CYS:H	7	0.42
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	7	0.42
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	7	0.42
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	7	0.42
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	7	0.42
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	9	0.42
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	9	0.42
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	9	0.42
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	9	0.42
(1,466)	1:80:A:CYS:HA	1:79:A:ASN:H	4	0.42
(1,466)	1:80:A:CYS:HA	1:79:A:ASN:H	10	0.42
(1,447)	1:71:A:CYS:HA	1:74:A:GLY:H	17	0.42
(1,437)	1:72:A:ASP:H	1:71:A:CYS:H	6	0.42
(1,436)	1:73:A:SER:H	1:72:A:ASP:H	2	0.42
(1,346)	1:32:A:SER:H	1:31:A:GLY:H	13	0.42
(1,346)	1:32:A:SER:H	1:31:A:GLY:H	16	0.42
(1,346)	1:32:A:SER:H	1:31:A:GLY:H	20	0.42
(1,327)	1:22:A:CYS:HB2	1:22:A:CYS:H	3	0.42
(1,327)	1:22:A:CYS:HB3	1:22:A:CYS:H	3	0.42
(1,327)	1:22:A:CYS:HB2	1:22:A:CYS:H	5	0.42
(1,327)	1:22:A:CYS:HB3	1:22:A:CYS:H	5	0.42
(1,327)	1:22:A:CYS:HB2	1:22:A:CYS:H	6	0.42
(1,327)	1:22:A:CYS:HB3	1:22:A:CYS:H	6	0.42
(1,327)	1:22:A:CYS:HB2	1:22:A:CYS:H	19	0.42
(1,327)	1:22:A:CYS:HB3	1:22:A:CYS:H	19	0.42
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB2	20	0.42
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB3	20	0.42
(1,298)	1:14:A:GLN:H	1:11:A:ASN:H	11	0.42
(1,289)	1:8:A:PHE:HA	1:8:A:PHE:H	17	0.42
(1,224)	1:92:A:CYS:HA	1:94:A:SER:H	15	0.42
(1,212)	1:96:A:ARG:H	1:92:A:CYS:HA	18	0.42

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,125)	1:114:A:SER:H	1:113:A:GLY:HA2	16	0.42
(1,125)	1:114:A:SER:H	1:113:A:GLY:HA3	16	0.42
(1,118)	1:115:A:ASP:H	1:113:A:GLY:H	2	0.42
(1,99)	1:98:A:ILE:HG12	1:99:A:SER:H	18	0.42
(1,99)	1:98:A:ILE:HG13	1:99:A:SER:H	18	0.42
(1,97)	1:98:A:ILE:HD11	1:99:A:SER:H	4	0.42
(1,97)	1:98:A:ILE:HD12	1:99:A:SER:H	4	0.42
(1,97)	1:98:A:ILE:HD13	1:99:A:SER:H	4	0.42
(1,81)	1:28:A:CYS:HA	1:33:A:ASP:H	4	0.42
(1,81)	1:28:A:CYS:HA	1:33:A:ASP:H	6	0.42
(1,81)	1:28:A:CYS:HA	1:33:A:ASP:H	15	0.42
(1,60)	1:56:A:THR:H	1:57:A:GLN:H	7	0.42
(1,60)	1:56:A:THR:H	1:57:A:GLN:H	16	0.42
(1,60)	1:56:A:THR:H	1:57:A:GLN:H	20	0.42
(4,8)	1:8:A:PHE:O	1:16:A:VAL:H	3	0.41
(4,8)	1:8:A:PHE:O	1:16:A:VAL:H	19	0.41
(2,302)	1:119:A:CYS:HA	1:120:A:ALA:H	14	0.41
(2,296)	1:113:A:GLY:HA2	1:117:A:LEU:H	11	0.41
(2,278)	1:42:A:ARG:HA	1:42:A:ARG:H	1	0.41
(2,278)	1:42:A:ARG:HA	1:42:A:ARG:H	3	0.41
(2,278)	1:42:A:ARG:HA	1:42:A:ARG:H	7	0.41
(2,278)	1:42:A:ARG:HA	1:42:A:ARG:H	11	0.41
(2,278)	1:42:A:ARG:HA	1:42:A:ARG:H	12	0.41
(2,278)	1:42:A:ARG:HA	1:42:A:ARG:H	13	0.41
(2,270)	1:113:A:GLY:HA2	1:110:A:CYS:H	1	0.41
(2,114)	1:16:A:VAL:HG11	1:16:A:VAL:H	5	0.41
(2,114)	1:16:A:VAL:HG12	1:16:A:VAL:H	5	0.41
(2,114)	1:16:A:VAL:HG13	1:16:A:VAL:H	5	0.41
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	5	0.41
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	5	0.41
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	5	0.41
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	5	0.41
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	5	0.41
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	5	0.41
(2,83)	1:35:A:SER:HB3	1:38:A:GLN:H	20	0.41
(2,72)	1:112:A:ASP:HB3	1:113:A:GLY:H	5	0.41
(2,46)	1:114:A:SER:HG	1:115:A:ASP:H	8	0.41
(2,38)	1:96:A:ARG:HB3	1:97:A:CYS:H	20	0.41
(2,25)	1:79:A:ASN:HD22	1:80:A:CYS:HA	1	0.41
(2,25)	1:79:A:ASN:HD22	1:80:A:CYS:HA	2	0.41
(2,25)	1:79:A:ASN:HD22	1:80:A:CYS:HA	9	0.41
(1,923)	1:8:A:PHE:HB2	1:16:A:VAL:HA	12	0.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,911)	1:57:A:GLN:HE21	1:71:A:CYS:H	17	0.41
(1,909)	1:43:A:THR:HG23	1:46:A:ILE:H	4	0.41
(1,897)	1:77:A:GLU:HB2	1:69:A:ASN:HD22	13	0.41
(1,897)	1:77:A:GLU:HB3	1:69:A:ASN:HD22	13	0.41
(1,862)	1:21:A:LYS:HE2	1:19:A:ARG:H	7	0.41
(1,862)	1:21:A:LYS:HE3	1:19:A:ARG:H	7	0.41
(1,856)	1:14:A:GLN:H	1:12:A:ASN:HD22	8	0.41
(1,850)	1:12:A:ASN:H	1:11:A:ASN:HD22	17	0.41
(1,833)	1:42:A:ARG:HG2	1:41:A:MET:H	11	0.41
(1,833)	1:42:A:ARG:HG2	1:41:A:MET:H	11	0.41
(1,833)	1:42:A:ARG:HG3	1:41:A:MET:H	11	0.41
(1,833)	1:42:A:ARG:HG3	1:41:A:MET:H	11	0.41
(1,801)	1:102:A:PHE:HB2	1:98:A:ILE:H	18	0.41
(1,801)	1:102:A:PHE:HB3	1:98:A:ILE:H	18	0.41
(1,799)	1:85:A:CYS:HA	1:97:A:CYS:H	1	0.41
(1,799)	1:85:A:CYS:HA	1:97:A:CYS:H	17	0.41
(1,797)	1:91:A:THR:HG23	1:96:A:ARG:H	2	0.41
(1,794)	1:82:A:ASN:HD22	1:94:A:SER:H	15	0.41
(1,783)	1:71:A:CYS:HB2	1:74:A:GLY:H	16	0.41
(1,783)	1:71:A:CYS:HB3	1:74:A:GLY:H	16	0.41
(1,761)	1:72:A:ASP:H	1:57:A:GLN:HE21	2	0.41
(1,750)	1:57:A:GLN:HB2	1:52:A:GLY:H	8	0.41
(1,750)	1:57:A:GLN:HB2	1:52:A:GLY:H	8	0.41
(1,750)	1:57:A:GLN:HB3	1:52:A:GLY:H	8	0.41
(1,750)	1:57:A:GLN:HB3	1:52:A:GLY:H	8	0.41
(1,745)	1:48:A:GLU:HB2	1:49:A:ILE:H	2	0.41
(1,745)	1:48:A:GLU:HB3	1:49:A:ILE:H	2	0.41
(1,745)	1:48:A:GLU:HB2	1:49:A:ILE:H	6	0.41
(1,745)	1:48:A:GLU:HB3	1:49:A:ILE:H	6	0.41
(1,735)	1:28:A:CYS:HB2	1:33:A:ASP:H	4	0.41
(1,735)	1:28:A:CYS:HB3	1:33:A:ASP:H	4	0.41
(1,735)	1:28:A:CYS:HB2	1:33:A:ASP:H	5	0.41
(1,735)	1:28:A:CYS:HB3	1:33:A:ASP:H	5	0.41
(1,735)	1:28:A:CYS:HB2	1:33:A:ASP:H	17	0.41
(1,735)	1:28:A:CYS:HB3	1:33:A:ASP:H	17	0.41
(1,732)	1:31:A:GLY:HA2	1:32:A:SER:H	4	0.41
(1,732)	1:31:A:GLY:HA3	1:32:A:SER:H	4	0.41
(1,732)	1:31:A:GLY:HA2	1:32:A:SER:H	5	0.41
(1,732)	1:31:A:GLY:HA3	1:32:A:SER:H	5	0.41
(1,732)	1:31:A:GLY:HA2	1:32:A:SER:H	12	0.41
(1,732)	1:31:A:GLY:HA3	1:32:A:SER:H	12	0.41
(1,706)	1:45:A:ARG:HB2	1:45:A:ARG:H	17	0.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,706)	1:45:A:ARG:HB3	1:45:A:ARG:H	17	0.41
(1,696)	1:44:A:CYS:HB2	1:34:A:GLU:H	7	0.41
(1,696)	1:44:A:CYS:HB3	1:34:A:GLU:H	7	0.41
(1,691)	1:49:A:ILE:HG12	1:49:A:ILE:H	8	0.41
(1,691)	1:49:A:ILE:HG13	1:49:A:ILE:H	8	0.41
(1,686)	1:74:A:GLY:H	1:69:A:ASN:HD22	12	0.41
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD2	5	0.41
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD3	5	0.41
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD2	11	0.41
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD3	11	0.41
(1,670)	1:107:A:GLN:HB2	1:105:A:ASN:HD22	7	0.41
(1,670)	1:107:A:GLN:HB2	1:105:A:ASN:HD22	7	0.41
(1,670)	1:107:A:GLN:HB3	1:105:A:ASN:HD22	7	0.41
(1,670)	1:107:A:GLN:HB3	1:105:A:ASN:HD22	7	0.41
(1,667)	1:107:A:GLN:HG2	1:105:A:ASN:HD22	2	0.41
(1,667)	1:107:A:GLN:HG2	1:105:A:ASN:HD22	2	0.41
(1,667)	1:107:A:GLN:HG3	1:105:A:ASN:HD22	2	0.41
(1,667)	1:107:A:GLN:HG3	1:105:A:ASN:HD22	2	0.41
(1,657)	1:105:A:ASN:HA	1:105:A:ASN:HD22	20	0.41
(1,654)	1:107:A:GLN:HB2	1:107:A:GLN:HE22	15	0.41
(1,654)	1:107:A:GLN:HB2	1:107:A:GLN:HE22	15	0.41
(1,654)	1:107:A:GLN:HB3	1:107:A:GLN:HE22	15	0.41
(1,654)	1:107:A:GLN:HB3	1:107:A:GLN:HE22	15	0.41
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	16	0.41
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	16	0.41
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	16	0.41
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	16	0.41
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	17	0.41
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	17	0.41
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	17	0.41
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	17	0.41
(1,642)	1:82:A:ASN:HA	1:82:A:ASN:HD22	7	0.41
(1,642)	1:82:A:ASN:HA	1:82:A:ASN:HD22	13	0.41
(1,642)	1:82:A:ASN:HA	1:82:A:ASN:HD22	16	0.41
(1,642)	1:82:A:ASN:HA	1:82:A:ASN:HD22	19	0.41
(1,636)	1:78:A:GLU:HB2	1:79:A:ASN:HD22	15	0.41
(1,636)	1:78:A:GLU:HB2	1:79:A:ASN:HD22	15	0.41
(1,636)	1:78:A:GLU:HB3	1:79:A:ASN:HD22	15	0.41
(1,636)	1:78:A:GLU:HB3	1:79:A:ASN:HD22	15	0.41
(1,636)	1:78:A:GLU:HB2	1:79:A:ASN:HD22	17	0.41
(1,636)	1:78:A:GLU:HB2	1:79:A:ASN:HD22	17	0.41
(1,636)	1:78:A:GLU:HB3	1:79:A:ASN:HD22	17	0.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,636)	1:78:A:GLU:HB3	1:79:A:ASN:HD22	17	0.41
(1,596)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	13	0.41
(1,596)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	13	0.41
(1,565)	1:91:A:THR:HG22	1:91:A:THR:H	20	0.41
(1,555)	1:103:A:VAL:HG11	1:104:A:CYS:H	3	0.41
(1,555)	1:103:A:VAL:HG12	1:104:A:CYS:H	3	0.41
(1,555)	1:103:A:VAL:HG13	1:104:A:CYS:H	3	0.41
(1,555)	1:103:A:VAL:HG21	1:104:A:CYS:H	3	0.41
(1,555)	1:103:A:VAL:HG22	1:104:A:CYS:H	3	0.41
(1,555)	1:103:A:VAL:HG23	1:104:A:CYS:H	3	0.41
(1,553)	1:115:A:ASP:HB2	1:104:A:CYS:H	15	0.41
(1,553)	1:115:A:ASP:HB3	1:104:A:CYS:H	15	0.41
(1,534)	1:77:A:GLU:HB2	1:77:A:GLU:H	17	0.41
(1,534)	1:77:A:GLU:HB3	1:77:A:GLU:H	17	0.41
(1,529)	1:59:A:ILE:HD11	1:70:A:ASP:H	14	0.41
(1,529)	1:59:A:ILE:HD12	1:70:A:ASP:H	14	0.41
(1,529)	1:59:A:ILE:HD13	1:70:A:ASP:H	14	0.41
(1,526)	1:64:A:ARG:H	1:67:A:GLY:H	19	0.41
(1,504)	1:39:A:CYS:HB2	1:39:A:CYS:H	2	0.41
(1,504)	1:39:A:CYS:HB3	1:39:A:CYS:H	2	0.41
(1,486)	1:7:A:ASP:HA	1:19:A:ARG:H	2	0.41
(1,483)	1:10:A:CYS:HB2	1:14:A:GLN:H	1	0.41
(1,483)	1:10:A:CYS:HB3	1:14:A:GLN:H	1	0.41
(1,483)	1:10:A:CYS:HB2	1:14:A:GLN:H	2	0.41
(1,483)	1:10:A:CYS:HB3	1:14:A:GLN:H	2	0.41
(1,457)	1:74:A:GLY:HA2	1:76:A:ASP:H	6	0.41
(1,457)	1:74:A:GLY:HA3	1:76:A:ASP:H	6	0.41
(1,436)	1:73:A:SER:H	1:72:A:ASP:H	13	0.41
(1,375)	1:48:A:GLU:HA	1:49:A:ILE:H	17	0.41
(1,371)	1:44:A:CYS:HA	1:45:A:ARG:H	8	0.41
(1,371)	1:44:A:CYS:HA	1:45:A:ARG:H	19	0.41
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	10	0.41
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	10	0.41
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	10	0.41
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	10	0.41
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	15	0.41
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	15	0.41
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	15	0.41
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	15	0.41
(1,365)	1:43:A:THR:HB	1:43:A:THR:H	14	0.41
(1,365)	1:43:A:THR:HB	1:43:A:THR:H	18	0.41
(1,327)	1:22:A:CYS:HB2	1:22:A:CYS:H	1	0.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,327)	1:22:A:CYS:HB3	1:22:A:CYS:H	1	0.41
(1,327)	1:22:A:CYS:HB2	1:22:A:CYS:H	17	0.41
(1,327)	1:22:A:CYS:HB3	1:22:A:CYS:H	17	0.41
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB2	3	0.41
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB3	3	0.41
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB2	5	0.41
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB3	5	0.41
(1,298)	1:14:A:GLN:H	1:11:A:ASN:H	13	0.41
(1,298)	1:14:A:GLN:H	1:11:A:ASN:H	20	0.41
(1,289)	1:8:A:PHE:HA	1:8:A:PHE:H	8	0.41
(1,289)	1:8:A:PHE:HA	1:8:A:PHE:H	13	0.41
(1,224)	1:92:A:CYS:HA	1:94:A:SER:H	18	0.41
(1,158)	1:104:A:CYS:HA	1:105:A:ASN:H	2	0.41
(1,109)	1:119:A:CYS:H	1:117:A:LEU:HG	11	0.41
(1,109)	1:119:A:CYS:H	1:117:A:LEU:HG	13	0.41
(1,99)	1:98:A:ILE:HG12	1:99:A:SER:H	11	0.41
(1,99)	1:98:A:ILE:HG13	1:99:A:SER:H	11	0.41
(1,97)	1:98:A:ILE:HD11	1:99:A:SER:H	19	0.41
(1,97)	1:98:A:ILE:HD12	1:99:A:SER:H	19	0.41
(1,97)	1:98:A:ILE:HD13	1:99:A:SER:H	19	0.41
(1,93)	1:8:A:PHE:H	1:7:A:ASP:HA	4	0.41
(1,93)	1:8:A:PHE:H	1:7:A:ASP:HA	11	0.41
(1,92)	1:7:A:ASP:HB2	1:8:A:PHE:H	8	0.41
(1,92)	1:7:A:ASP:HB3	1:8:A:PHE:H	8	0.41
(1,85)	1:21:A:LYS:HG2	1:22:A:CYS:H	8	0.41
(1,85)	1:21:A:LYS:HG3	1:22:A:CYS:H	8	0.41
(1,81)	1:28:A:CYS:HA	1:33:A:ASP:H	1	0.41
(1,73)	1:65:A:CYS:HB2	1:65:A:CYS:H	19	0.41
(1,73)	1:65:A:CYS:HB3	1:65:A:CYS:H	19	0.41
(1,66)	1:23:A:ASP:H	1:24:A:GLY:H	15	0.41
(1,60)	1:56:A:THR:H	1:57:A:GLN:H	8	0.41
(1,60)	1:56:A:THR:H	1:57:A:GLN:H	9	0.41
(2,298)	1:28:A:CYS:HB3	1:14:A:GLN:HE22	8	0.4
(2,278)	1:42:A:ARG:HA	1:42:A:ARG:H	8	0.4
(2,278)	1:42:A:ARG:HA	1:42:A:ARG:H	9	0.4
(2,278)	1:42:A:ARG:HA	1:42:A:ARG:H	14	0.4
(2,278)	1:42:A:ARG:HA	1:42:A:ARG:H	20	0.4
(2,212)	1:88:A:ASP:H	1:86:A:SER:H	16	0.4
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	13	0.4
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	13	0.4
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	13	0.4
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	13	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	13	0.4
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	13	0.4
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	13	0.4
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	13	0.4
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	13	0.4
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	13	0.4
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	13	0.4
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	13	0.4
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	13	0.4
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	13	0.4
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	13	0.4
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	13	0.4
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	13	0.4
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	13	0.4
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	18	0.4
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	18	0.4
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	18	0.4
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	18	0.4
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	18	0.4
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	18	0.4
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	18	0.4
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	18	0.4
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	18	0.4
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	18	0.4
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	18	0.4
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	18	0.4
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	18	0.4
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	18	0.4
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	18	0.4
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	18	0.4
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	18	0.4
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	18	0.4
(2,178)	1:59:A:ILE:HG22	1:57:A:GLN:HE22	2	0.4
(2,38)	1:96:A:ARG:HB3	1:97:A:CYS:H	10	0.4
(2,20)	1:82:A:ASN:H	1:83:A:ILE:H	8	0.4
(2,8)	1:45:A:ARG:HA	1:46:A:ILE:H	20	0.4
(1,911)	1:57:A:GLN:HE21	1:71:A:CYS:H	9	0.4
(1,911)	1:57:A:GLN:HE21	1:71:A:CYS:H	11	0.4
(1,896)	1:64:A:ARG:H	1:66:A:ASP:H	12	0.4
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB2	12	0.4
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB3	12	0.4
(1,888)	1:49:A:ILE:HA	1:61:A:VAL:H	5	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,862)	1:21:A:LYS:HE2	1:19:A:ARG:H	4	0.4
(1,862)	1:21:A:LYS:HE3	1:19:A:ARG:H	4	0.4
(1,862)	1:21:A:LYS:HE2	1:19:A:ARG:H	12	0.4
(1,862)	1:21:A:LYS:HE3	1:19:A:ARG:H	12	0.4
(1,859)	1:3:A:CYS:HB2	1:18:A:SER:H	10	0.4
(1,859)	1:3:A:CYS:HB3	1:18:A:SER:H	10	0.4
(1,837)	1:50:A:SER:H	1:45:A:ARG:HD2	13	0.4
(1,837)	1:50:A:SER:H	1:45:A:ARG:HD3	13	0.4
(1,833)	1:42:A:ARG:HG2	1:41:A:MET:H	6	0.4
(1,833)	1:42:A:ARG:HG2	1:41:A:MET:H	6	0.4
(1,833)	1:42:A:ARG:HG3	1:41:A:MET:H	6	0.4
(1,833)	1:42:A:ARG:HG3	1:41:A:MET:H	6	0.4
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG21	12	0.4
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG22	12	0.4
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG23	12	0.4
(1,783)	1:71:A:CYS:HB2	1:74:A:GLY:H	1	0.4
(1,783)	1:71:A:CYS:HB3	1:74:A:GLY:H	1	0.4
(1,772)	1:68:A:GLU:H	1:64:A:ARG:H	20	0.4
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG12	12	0.4
(1,746)	1:50:A:SER:H	1:49:A:ILE:HG13	12	0.4
(1,745)	1:48:A:GLU:HB2	1:49:A:ILE:H	3	0.4
(1,745)	1:48:A:GLU:HB3	1:49:A:ILE:H	3	0.4
(1,735)	1:28:A:CYS:HB2	1:33:A:ASP:H	8	0.4
(1,735)	1:28:A:CYS:HB3	1:33:A:ASP:H	8	0.4
(1,735)	1:28:A:CYS:HB2	1:33:A:ASP:H	11	0.4
(1,735)	1:28:A:CYS:HB3	1:33:A:ASP:H	11	0.4
(1,733)	1:32:A:SER:H	1:28:A:CYS:H	3	0.4
(1,733)	1:32:A:SER:H	1:28:A:CYS:H	18	0.4
(1,732)	1:31:A:GLY:HA2	1:32:A:SER:H	2	0.4
(1,732)	1:31:A:GLY:HA3	1:32:A:SER:H	2	0.4
(1,732)	1:31:A:GLY:HA2	1:32:A:SER:H	6	0.4
(1,732)	1:31:A:GLY:HA3	1:32:A:SER:H	6	0.4
(1,732)	1:31:A:GLY:HA2	1:32:A:SER:H	9	0.4
(1,732)	1:31:A:GLY:HA3	1:32:A:SER:H	9	0.4
(1,732)	1:31:A:GLY:HA2	1:32:A:SER:H	15	0.4
(1,732)	1:31:A:GLY:HA3	1:32:A:SER:H	15	0.4
(1,729)	1:32:A:SER:H	1:28:A:CYS:H	3	0.4
(1,729)	1:32:A:SER:H	1:28:A:CYS:H	18	0.4
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD2	7	0.4
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD3	7	0.4
(1,705)	1:100:A:ARG:H	1:100:A:ARG:HD2	19	0.4
(1,705)	1:100:A:ARG:H	1:100:A:ARG:HD3	19	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,704)	1:100:A:ARG:HG2	1:100:A:ARG:H	9	0.4
(1,704)	1:100:A:ARG:HG2	1:100:A:ARG:H	9	0.4
(1,704)	1:100:A:ARG:HG3	1:100:A:ARG:H	9	0.4
(1,704)	1:100:A:ARG:HG3	1:100:A:ARG:H	9	0.4
(1,688)	1:69:A:ASN:H	1:69:A:ASN:HD22	19	0.4
(1,685)	1:107:A:GLN:HG2	1:107:A:GLN:HE21	12	0.4
(1,685)	1:107:A:GLN:HG2	1:107:A:GLN:HE21	12	0.4
(1,685)	1:107:A:GLN:HG3	1:107:A:GLN:HE21	12	0.4
(1,685)	1:107:A:GLN:HG3	1:107:A:GLN:HE21	12	0.4
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD2	13	0.4
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD3	13	0.4
(1,667)	1:107:A:GLN:HG2	1:105:A:ASN:HD22	6	0.4
(1,667)	1:107:A:GLN:HG2	1:105:A:ASN:HD22	6	0.4
(1,667)	1:107:A:GLN:HG3	1:105:A:ASN:HD22	6	0.4
(1,667)	1:107:A:GLN:HG3	1:105:A:ASN:HD22	6	0.4
(1,657)	1:105:A:ASN:HA	1:105:A:ASN:HD22	12	0.4
(1,657)	1:105:A:ASN:HA	1:105:A:ASN:HD22	13	0.4
(1,657)	1:105:A:ASN:HA	1:105:A:ASN:HD22	15	0.4
(1,657)	1:105:A:ASN:HA	1:105:A:ASN:HD22	18	0.4
(1,654)	1:107:A:GLN:HB2	1:107:A:GLN:HE22	14	0.4
(1,654)	1:107:A:GLN:HB2	1:107:A:GLN:HE22	14	0.4
(1,654)	1:107:A:GLN:HB3	1:107:A:GLN:HE22	14	0.4
(1,654)	1:107:A:GLN:HB3	1:107:A:GLN:HE22	14	0.4
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	1	0.4
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	1	0.4
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	1	0.4
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	1	0.4
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	2	0.4
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	2	0.4
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	2	0.4
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	2	0.4
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	13	0.4
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	13	0.4
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	13	0.4
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	13	0.4
(1,596)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	18	0.4
(1,596)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	18	0.4
(1,543)	1:112:A:ASP:HB2	1:114:A:SER:H	19	0.4
(1,543)	1:112:A:ASP:HB3	1:114:A:SER:H	19	0.4
(1,534)	1:77:A:GLU:HB2	1:77:A:GLU:H	15	0.4
(1,534)	1:77:A:GLU:HB3	1:77:A:GLU:H	15	0.4
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	16	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	16	0.4
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	16	0.4
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	16	0.4
(1,447)	1:71:A:CYS:HA	1:74:A:GLY:H	5	0.4
(1,436)	1:73:A:SER:H	1:72:A:ASP:H	3	0.4
(1,398)	1:54:A:HIS:HB2	1:54:A:HIS:H	6	0.4
(1,398)	1:54:A:HIS:HB3	1:54:A:HIS:H	6	0.4
(1,398)	1:54:A:HIS:HB2	1:54:A:HIS:H	17	0.4
(1,398)	1:54:A:HIS:HB3	1:54:A:HIS:H	17	0.4
(1,398)	1:54:A:HIS:HB2	1:54:A:HIS:H	19	0.4
(1,398)	1:54:A:HIS:HB3	1:54:A:HIS:H	19	0.4
(1,398)	1:54:A:HIS:HB2	1:54:A:HIS:H	20	0.4
(1,398)	1:54:A:HIS:HB3	1:54:A:HIS:H	20	0.4
(1,390)	1:51:A:CYS:HB2	1:52:A:GLY:H	2	0.4
(1,390)	1:51:A:CYS:HB3	1:52:A:GLY:H	2	0.4
(1,376)	1:49:A:ILE:HA	1:49:A:ILE:H	3	0.4
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB2	12	0.4
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB3	12	0.4
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB2	19	0.4
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB3	19	0.4
(1,320)	1:7:A:ASP:HA	1:18:A:SER:H	1	0.4
(1,320)	1:7:A:ASP:HA	1:18:A:SER:H	5	0.4
(1,320)	1:7:A:ASP:HA	1:18:A:SER:H	8	0.4
(1,289)	1:8:A:PHE:HA	1:8:A:PHE:H	1	0.4
(1,289)	1:8:A:PHE:HA	1:8:A:PHE:H	3	0.4
(1,289)	1:8:A:PHE:HA	1:8:A:PHE:H	5	0.4
(1,289)	1:8:A:PHE:HA	1:8:A:PHE:H	15	0.4
(1,289)	1:8:A:PHE:HA	1:8:A:PHE:H	18	0.4
(1,289)	1:8:A:PHE:HA	1:8:A:PHE:H	20	0.4
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	4	0.4
(1,252)	1:82:A:ASN:HB2	1:83:A:ILE:H	4	0.4
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	4	0.4
(1,252)	1:82:A:ASN:HB3	1:83:A:ILE:H	4	0.4
(1,224)	1:92:A:CYS:HA	1:94:A:SER:H	13	0.4
(1,174)	1:103:A:VAL:H	1:101:A:ASN:HB2	3	0.4
(1,174)	1:103:A:VAL:H	1:101:A:ASN:HB3	3	0.4
(1,158)	1:104:A:CYS:HA	1:105:A:ASN:H	19	0.4
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB2	16	0.4
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB3	16	0.4
(1,118)	1:115:A:ASP:H	1:113:A:GLY:H	11	0.4
(1,109)	1:119:A:CYS:H	1:117:A:LEU:HG	18	0.4
(1,93)	1:8:A:PHE:H	1:7:A:ASP:HA	10	0.4

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	1:28:A:CYS:HA	1:33:A:ASP:H	18	0.4
(1,73)	1:65:A:CYS:HB2	1:65:A:CYS:H	6	0.4
(1,73)	1:65:A:CYS:HB3	1:65:A:CYS:H	6	0.4
(1,73)	1:65:A:CYS:HB2	1:65:A:CYS:H	7	0.4
(1,73)	1:65:A:CYS:HB3	1:65:A:CYS:H	7	0.4
(1,73)	1:65:A:CYS:HB2	1:65:A:CYS:H	12	0.4
(1,73)	1:65:A:CYS:HB3	1:65:A:CYS:H	12	0.4
(1,73)	1:65:A:CYS:HB2	1:65:A:CYS:H	14	0.4
(1,73)	1:65:A:CYS:HB3	1:65:A:CYS:H	14	0.4
(1,73)	1:65:A:CYS:HB2	1:65:A:CYS:H	18	0.4
(1,73)	1:65:A:CYS:HB3	1:65:A:CYS:H	18	0.4
(1,66)	1:23:A:ASP:H	1:24:A:GLY:H	12	0.4
(1,60)	1:56:A:THR:H	1:57:A:GLN:H	4	0.4
(1,14)	1:110:A:CYS:H	1:109:A:ASP:H	13	0.4
(2,313)	1:17:A:PRO:HB2	1:20:A:TRP:H	12	0.39
(2,313)	1:17:A:PRO:HB2	1:20:A:TRP:H	14	0.39
(2,278)	1:42:A:ARG:HA	1:42:A:ARG:H	16	0.39
(2,278)	1:42:A:ARG:HA	1:42:A:ARG:H	18	0.39
(2,270)	1:113:A:GLY:HA2	1:110:A:CYS:H	10	0.39
(2,200)	1:77:A:GLU:HG2	1:76:A:ASP:H	5	0.39
(2,196)	1:56:A:THR:HA	1:42:A:ARG:H	10	0.39
(2,190)	1:56:A:THR:HA	1:57:A:GLN:H	6	0.39
(2,190)	1:56:A:THR:HA	1:57:A:GLN:H	8	0.39
(2,168)	1:37:A:GLU:HG3	1:38:A:GLN:H	11	0.39
(2,31)	1:59:A:ILE:HD11	1:71:A:CYS:H	14	0.39
(2,22)	1:75:A:GLU:HA	1:78:A:GLU:H	8	0.39
(2,12)	1:10:A:CYS:HB2	1:13:A:GLY:H	6	0.39
(2,8)	1:45:A:ARG:HA	1:46:A:ILE:H	11	0.39
(1,896)	1:64:A:ARG:H	1:66:A:ASP:H	13	0.39
(1,895)	1:77:A:GLU:HG2	1:66:A:ASP:H	15	0.39
(1,895)	1:77:A:GLU:HG3	1:66:A:ASP:H	15	0.39
(1,894)	1:66:A:ASP:H	1:77:A:GLU:HG2	15	0.39
(1,894)	1:66:A:ASP:H	1:77:A:GLU:HG3	15	0.39
(1,881)	1:48:A:GLU:H	1:45:A:ARG:H	15	0.39
(1,879)	1:48:A:GLU:H	1:45:A:ARG:H	15	0.39
(1,862)	1:21:A:LYS:HE2	1:19:A:ARG:H	2	0.39
(1,862)	1:21:A:LYS:HE3	1:19:A:ARG:H	2	0.39
(1,860)	1:16:A:VAL:HB	1:19:A:ARG:H	9	0.39
(1,859)	1:3:A:CYS:HB2	1:18:A:SER:H	2	0.39
(1,859)	1:3:A:CYS:HB3	1:18:A:SER:H	2	0.39
(1,853)	1:10:A:CYS:HB2	1:12:A:ASN:H	16	0.39
(1,853)	1:10:A:CYS:HB3	1:12:A:ASN:H	16	0.39

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,831)	1:73:A:SER:H	1:75:A:GLU:H	10	0.39
(1,807)	1:98:A:ILE:HG12	1:103:A:VAL:H	20	0.39
(1,807)	1:98:A:ILE:HG13	1:103:A:VAL:H	20	0.39
(1,795)	1:91:A:THR:HG23	1:95:A:GLY:H	9	0.39
(1,791)	1:85:A:CYS:HB2	1:89:A:GLU:H	7	0.39
(1,791)	1:85:A:CYS:HB3	1:89:A:GLU:H	7	0.39
(1,791)	1:85:A:CYS:HB2	1:89:A:GLU:H	9	0.39
(1,791)	1:85:A:CYS:HB3	1:89:A:GLU:H	9	0.39
(1,788)	1:80:A:CYS:H	1:78:A:GLU:H	14	0.39
(1,783)	1:71:A:CYS:HB2	1:74:A:GLY:H	3	0.39
(1,783)	1:71:A:CYS:HB3	1:74:A:GLY:H	3	0.39
(1,783)	1:71:A:CYS:HB2	1:74:A:GLY:H	9	0.39
(1,783)	1:71:A:CYS:HB3	1:74:A:GLY:H	9	0.39
(1,783)	1:71:A:CYS:HB2	1:74:A:GLY:H	10	0.39
(1,783)	1:71:A:CYS:HB3	1:74:A:GLY:H	10	0.39
(1,733)	1:32:A:SER:H	1:28:A:CYS:H	14	0.39
(1,733)	1:32:A:SER:H	1:28:A:CYS:H	15	0.39
(1,732)	1:31:A:GLY:HA2	1:32:A:SER:H	1	0.39
(1,732)	1:31:A:GLY:HA3	1:32:A:SER:H	1	0.39
(1,732)	1:31:A:GLY:HA2	1:32:A:SER:H	3	0.39
(1,732)	1:31:A:GLY:HA3	1:32:A:SER:H	3	0.39
(1,732)	1:31:A:GLY:HA2	1:32:A:SER:H	10	0.39
(1,732)	1:31:A:GLY:HA3	1:32:A:SER:H	10	0.39
(1,732)	1:31:A:GLY:HA2	1:32:A:SER:H	17	0.39
(1,732)	1:31:A:GLY:HA3	1:32:A:SER:H	17	0.39
(1,732)	1:31:A:GLY:HA2	1:32:A:SER:H	18	0.39
(1,732)	1:31:A:GLY:HA3	1:32:A:SER:H	18	0.39
(1,729)	1:32:A:SER:H	1:28:A:CYS:H	14	0.39
(1,729)	1:32:A:SER:H	1:28:A:CYS:H	15	0.39
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD2	4	0.39
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD3	4	0.39
(1,706)	1:45:A:ARG:HB2	1:45:A:ARG:H	2	0.39
(1,706)	1:45:A:ARG:HB3	1:45:A:ARG:H	2	0.39
(1,696)	1:44:A:CYS:HB2	1:34:A:GLU:H	13	0.39
(1,696)	1:44:A:CYS:HB3	1:34:A:GLU:H	13	0.39
(1,696)	1:44:A:CYS:HB2	1:34:A:GLU:H	18	0.39
(1,696)	1:44:A:CYS:HB3	1:34:A:GLU:H	18	0.39
(1,686)	1:74:A:GLY:H	1:69:A:ASN:HD22	2	0.39
(1,686)	1:74:A:GLY:H	1:69:A:ASN:HD22	8	0.39
(1,685)	1:107:A:GLN:HG2	1:107:A:GLN:HE21	16	0.39
(1,685)	1:107:A:GLN:HG2	1:107:A:GLN:HE21	16	0.39
(1,685)	1:107:A:GLN:HG3	1:107:A:GLN:HE21	16	0.39

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,685)	1:107:A:GLN:HG3	1:107:A:GLN:HE21	16	0.39
(1,685)	1:107:A:GLN:HG2	1:107:A:GLN:HE21	18	0.39
(1,685)	1:107:A:GLN:HG2	1:107:A:GLN:HE21	18	0.39
(1,685)	1:107:A:GLN:HG3	1:107:A:GLN:HE21	18	0.39
(1,685)	1:107:A:GLN:HG3	1:107:A:GLN:HE21	18	0.39
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	5	0.39
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	5	0.39
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	5	0.39
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	5	0.39
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	6	0.39
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	6	0.39
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	6	0.39
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	6	0.39
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	10	0.39
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	10	0.39
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	10	0.39
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	10	0.39
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	14	0.39
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	14	0.39
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	14	0.39
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	14	0.39
(1,642)	1:82:A:ASN:HA	1:82:A:ASN:HD22	1	0.39
(1,642)	1:82:A:ASN:HA	1:82:A:ASN:HD22	11	0.39
(1,608)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	1	0.39
(1,608)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	1	0.39
(1,596)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	4	0.39
(1,596)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	4	0.39
(1,596)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	9	0.39
(1,596)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	9	0.39
(1,534)	1:77:A:GLU:HB2	1:77:A:GLU:H	12	0.39
(1,534)	1:77:A:GLU:HB3	1:77:A:GLU:H	12	0.39
(1,526)	1:64:A:ARG:H	1:67:A:GLY:H	8	0.39
(1,526)	1:64:A:ARG:H	1:67:A:GLY:H	20	0.39
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	5	0.39
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	5	0.39
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	5	0.39
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	5	0.39
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	14	0.39
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	14	0.39
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	14	0.39
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	14	0.39
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	19	0.39

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	19	0.39
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	19	0.39
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	19	0.39
(1,486)	1:7:A:ASP:HA	1:19:A:ARG:H	12	0.39
(1,463)	1:71:A:CYS:HB2	1:78:A:GLU:H	4	0.39
(1,463)	1:71:A:CYS:HB3	1:78:A:GLU:H	4	0.39
(1,431)	1:72:A:ASP:H	1:70:A:ASP:H	8	0.39
(1,398)	1:54:A:HIS:HB2	1:54:A:HIS:H	3	0.39
(1,398)	1:54:A:HIS:HB3	1:54:A:HIS:H	3	0.39
(1,398)	1:54:A:HIS:HB2	1:54:A:HIS:H	4	0.39
(1,398)	1:54:A:HIS:HB3	1:54:A:HIS:H	4	0.39
(1,398)	1:54:A:HIS:HB2	1:54:A:HIS:H	7	0.39
(1,398)	1:54:A:HIS:HB3	1:54:A:HIS:H	7	0.39
(1,398)	1:54:A:HIS:HB2	1:54:A:HIS:H	9	0.39
(1,398)	1:54:A:HIS:HB3	1:54:A:HIS:H	9	0.39
(1,398)	1:54:A:HIS:HB2	1:54:A:HIS:H	12	0.39
(1,398)	1:54:A:HIS:HB3	1:54:A:HIS:H	12	0.39
(1,398)	1:54:A:HIS:HB2	1:54:A:HIS:H	13	0.39
(1,398)	1:54:A:HIS:HB3	1:54:A:HIS:H	13	0.39
(1,398)	1:54:A:HIS:HB2	1:54:A:HIS:H	16	0.39
(1,398)	1:54:A:HIS:HB3	1:54:A:HIS:H	16	0.39
(1,376)	1:49:A:ILE:HA	1:49:A:ILE:H	19	0.39
(1,376)	1:49:A:ILE:HA	1:49:A:ILE:H	20	0.39
(1,375)	1:48:A:GLU:HA	1:49:A:ILE:H	1	0.39
(1,304)	1:14:A:GLN:HB2	1:12:A:ASN:H	17	0.39
(1,304)	1:14:A:GLN:HB2	1:12:A:ASN:H	17	0.39
(1,304)	1:14:A:GLN:HB3	1:12:A:ASN:H	17	0.39
(1,304)	1:14:A:GLN:HB3	1:12:A:ASN:H	17	0.39
(1,298)	1:14:A:GLN:H	1:11:A:ASN:H	4	0.39
(1,224)	1:92:A:CYS:HA	1:94:A:SER:H	12	0.39
(1,224)	1:92:A:CYS:HA	1:94:A:SER:H	14	0.39
(1,174)	1:103:A:VAL:H	1:101:A:ASN:HB2	17	0.39
(1,174)	1:103:A:VAL:H	1:101:A:ASN:HB3	17	0.39
(1,174)	1:103:A:VAL:H	1:101:A:ASN:HB2	19	0.39
(1,174)	1:103:A:VAL:H	1:101:A:ASN:HB3	19	0.39
(1,158)	1:104:A:CYS:HA	1:105:A:ASN:H	3	0.39
(1,158)	1:104:A:CYS:HA	1:105:A:ASN:H	4	0.39
(1,158)	1:104:A:CYS:HA	1:105:A:ASN:H	7	0.39
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB2	3	0.39
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB3	3	0.39
(1,139)	1:109:A:ASP:H	1:109:A:ASP:HB2	1	0.39
(1,139)	1:109:A:ASP:H	1:109:A:ASP:HB3	1	0.39

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,93)	1:8:A:PHE:H	1:7:A:ASP:HA	9	0.39
(1,81)	1:28:A:CYS:HA	1:33:A:ASP:H	10	0.39
(1,73)	1:65:A:CYS:HB2	1:65:A:CYS:H	2	0.39
(1,73)	1:65:A:CYS:HB3	1:65:A:CYS:H	2	0.39
(1,73)	1:65:A:CYS:HB2	1:65:A:CYS:H	4	0.39
(1,73)	1:65:A:CYS:HB3	1:65:A:CYS:H	4	0.39
(1,73)	1:65:A:CYS:HB2	1:65:A:CYS:H	9	0.39
(1,73)	1:65:A:CYS:HB3	1:65:A:CYS:H	9	0.39
(4,2)	1:90:A:PHE:O	1:98:A:ILE:H	7	0.38
(2,376)	1:87:A:PRO:HB2	1:88:A:ASP:H	10	0.38
(2,361)	1:61:A:VAL:HG13	1:64:A:ARG:H	16	0.38
(2,327)	1:68:A:GLU:HG2	1:71:A:CYS:H	14	0.38
(2,302)	1:119:A:CYS:HA	1:120:A:ALA:H	18	0.38
(2,276)	1:43:A:THR:HA	1:57:A:GLN:H	16	0.38
(2,212)	1:88:A:ASP:H	1:86:A:SER:H	20	0.38
(2,190)	1:56:A:THR:HA	1:57:A:GLN:H	1	0.38
(2,190)	1:56:A:THR:HA	1:57:A:GLN:H	2	0.38
(2,190)	1:56:A:THR:HA	1:57:A:GLN:H	15	0.38
(2,190)	1:56:A:THR:HA	1:57:A:GLN:H	17	0.38
(2,178)	1:59:A:ILE:HG22	1:57:A:GLN:HE22	14	0.38
(2,89)	1:107:A:GLN:HB2	1:108:A:ASP:H	2	0.38
(2,89)	1:107:A:GLN:HB3	1:108:A:ASP:H	2	0.38
(2,72)	1:110:A:CYS:HB3	1:113:A:GLY:H	19	0.38
(2,39)	1:117:A:LEU:HD12	1:115:A:ASP:H	14	0.38
(2,22)	1:75:A:GLU:HA	1:78:A:GLU:H	18	0.38
(2,8)	1:45:A:ARG:HA	1:46:A:ILE:H	9	0.38
(1,911)	1:57:A:GLN:HE21	1:71:A:CYS:H	7	0.38
(1,896)	1:64:A:ARG:H	1:66:A:ASP:H	1	0.38
(1,881)	1:48:A:GLU:H	1:45:A:ARG:H	14	0.38
(1,879)	1:48:A:GLU:H	1:45:A:ARG:H	14	0.38
(1,856)	1:14:A:GLN:H	1:12:A:ASN:HD22	13	0.38
(1,853)	1:10:A:CYS:HB2	1:12:A:ASN:H	12	0.38
(1,853)	1:10:A:CYS:HB3	1:12:A:ASN:H	12	0.38
(1,853)	1:10:A:CYS:HB2	1:12:A:ASN:H	13	0.38
(1,853)	1:10:A:CYS:HB3	1:12:A:ASN:H	13	0.38
(1,849)	1:33:A:ASP:H	1:11:A:ASN:H	18	0.38
(1,831)	1:73:A:SER:H	1:75:A:GLU:H	9	0.38
(1,831)	1:73:A:SER:H	1:75:A:GLU:H	20	0.38
(1,806)	1:101:A:ASN:HD21	1:102:A:PHE:H	5	0.38
(1,806)	1:101:A:ASN:HD21	1:102:A:PHE:H	17	0.38
(1,803)	1:101:A:ASN:HD21	1:99:A:SER:H	3	0.38
(1,794)	1:82:A:ASN:HD22	1:94:A:SER:H	1	0.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,794)	1:82:A:ASN:HD22	1:94:A:SER:H	12	0.38
(1,789)	1:85:A:CYS:H	1:84:A:THR:HB	7	0.38
(1,784)	1:71:A:CYS:HB2	1:76:A:ASP:H	10	0.38
(1,784)	1:71:A:CYS:HB3	1:76:A:ASP:H	10	0.38
(1,777)	1:77:A:GLU:HB2	1:70:A:ASP:H	4	0.38
(1,777)	1:77:A:GLU:HB3	1:70:A:ASP:H	4	0.38
(1,772)	1:68:A:GLU:H	1:64:A:ARG:H	16	0.38
(1,770)	1:63:A:TRP:H	1:77:A:GLU:HG2	1	0.38
(1,770)	1:63:A:TRP:H	1:77:A:GLU:HG3	1	0.38
(1,766)	1:48:A:GLU:HB2	1:58:A:CYS:H	17	0.38
(1,766)	1:48:A:GLU:HB3	1:58:A:CYS:H	17	0.38
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	16	0.38
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	16	0.38
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	16	0.38
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	16	0.38
(1,745)	1:48:A:GLU:HB2	1:49:A:ILE:H	8	0.38
(1,745)	1:48:A:GLU:HB3	1:49:A:ILE:H	8	0.38
(1,735)	1:28:A:CYS:HB2	1:33:A:ASP:H	10	0.38
(1,735)	1:28:A:CYS:HB3	1:33:A:ASP:H	10	0.38
(1,735)	1:28:A:CYS:HB2	1:33:A:ASP:H	16	0.38
(1,735)	1:28:A:CYS:HB3	1:33:A:ASP:H	16	0.38
(1,733)	1:32:A:SER:H	1:28:A:CYS:H	4	0.38
(1,732)	1:31:A:GLY:HA2	1:32:A:SER:H	14	0.38
(1,732)	1:31:A:GLY:HA3	1:32:A:SER:H	14	0.38
(1,732)	1:31:A:GLY:HA2	1:32:A:SER:H	19	0.38
(1,732)	1:31:A:GLY:HA3	1:32:A:SER:H	19	0.38
(1,729)	1:32:A:SER:H	1:28:A:CYS:H	4	0.38
(1,706)	1:45:A:ARG:HB2	1:45:A:ARG:H	1	0.38
(1,706)	1:45:A:ARG:HB3	1:45:A:ARG:H	1	0.38
(1,706)	1:45:A:ARG:HB2	1:45:A:ARG:H	4	0.38
(1,706)	1:45:A:ARG:HB3	1:45:A:ARG:H	4	0.38
(1,706)	1:45:A:ARG:HB2	1:45:A:ARG:H	7	0.38
(1,706)	1:45:A:ARG:HB3	1:45:A:ARG:H	7	0.38
(1,706)	1:45:A:ARG:HB2	1:45:A:ARG:H	13	0.38
(1,706)	1:45:A:ARG:HB3	1:45:A:ARG:H	13	0.38
(1,706)	1:45:A:ARG:HB2	1:45:A:ARG:H	14	0.38
(1,706)	1:45:A:ARG:HB3	1:45:A:ARG:H	14	0.38
(1,688)	1:69:A:ASN:H	1:69:A:ASN:HD22	2	0.38
(1,685)	1:107:A:GLN:HG2	1:107:A:GLN:HE21	3	0.38
(1,685)	1:107:A:GLN:HG2	1:107:A:GLN:HE21	3	0.38
(1,685)	1:107:A:GLN:HG3	1:107:A:GLN:HE21	3	0.38
(1,685)	1:107:A:GLN:HG3	1:107:A:GLN:HE21	3	0.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,685)	1:107:A:GLN:HG2	1:107:A:GLN:HE21	6	0.38
(1,685)	1:107:A:GLN:HG2	1:107:A:GLN:HE21	6	0.38
(1,685)	1:107:A:GLN:HG3	1:107:A:GLN:HE21	6	0.38
(1,685)	1:107:A:GLN:HG3	1:107:A:GLN:HE21	6	0.38
(1,685)	1:107:A:GLN:HG2	1:107:A:GLN:HE21	7	0.38
(1,685)	1:107:A:GLN:HG2	1:107:A:GLN:HE21	7	0.38
(1,685)	1:107:A:GLN:HG3	1:107:A:GLN:HE21	7	0.38
(1,685)	1:107:A:GLN:HG3	1:107:A:GLN:HE21	7	0.38
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD2	1	0.38
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD3	1	0.38
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	3	0.38
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	3	0.38
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	3	0.38
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	3	0.38
(1,642)	1:82:A:ASN:HA	1:82:A:ASN:HD22	2	0.38
(1,642)	1:82:A:ASN:HA	1:82:A:ASN:HD22	3	0.38
(1,642)	1:82:A:ASN:HA	1:82:A:ASN:HD22	5	0.38
(1,642)	1:82:A:ASN:HA	1:82:A:ASN:HD22	12	0.38
(1,626)	1:71:A:CYS:HA	1:57:A:GLN:HE22	8	0.38
(1,608)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	2	0.38
(1,608)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	2	0.38
(1,598)	1:74:A:GLY:HA2	1:69:A:ASN:HD22	2	0.38
(1,598)	1:74:A:GLY:HA3	1:69:A:ASN:HD22	2	0.38
(1,597)	1:74:A:GLY:HA2	1:69:A:ASN:HD22	2	0.38
(1,597)	1:74:A:GLY:HA3	1:69:A:ASN:HD22	2	0.38
(1,592)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	10	0.38
(1,592)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	10	0.38
(1,582)	1:46:A:ILE:H	1:45:A:ARG:H	15	0.38
(1,526)	1:64:A:ARG:H	1:67:A:GLY:H	11	0.38
(1,509)	1:46:A:ILE:HA	1:46:A:ILE:H	10	0.38
(1,486)	1:7:A:ASP:HA	1:19:A:ARG:H	7	0.38
(1,486)	1:7:A:ASP:HA	1:19:A:ARG:H	18	0.38
(1,459)	1:70:A:ASP:HA	1:76:A:ASP:H	14	0.38
(1,436)	1:73:A:SER:H	1:72:A:ASP:H	6	0.38
(1,398)	1:54:A:HIS:HB2	1:54:A:HIS:H	2	0.38
(1,398)	1:54:A:HIS:HB3	1:54:A:HIS:H	2	0.38
(1,398)	1:54:A:HIS:HB2	1:54:A:HIS:H	11	0.38
(1,398)	1:54:A:HIS:HB3	1:54:A:HIS:H	11	0.38
(1,398)	1:54:A:HIS:HB2	1:54:A:HIS:H	14	0.38
(1,398)	1:54:A:HIS:HB3	1:54:A:HIS:H	14	0.38
(1,398)	1:54:A:HIS:HB2	1:54:A:HIS:H	15	0.38
(1,398)	1:54:A:HIS:HB3	1:54:A:HIS:H	15	0.38

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,376)	1:49:A:ILE:HA	1:49:A:ILE:H	9	0.38
(1,376)	1:49:A:ILE:HA	1:49:A:ILE:H	13	0.38
(1,376)	1:49:A:ILE:HA	1:49:A:ILE:H	16	0.38
(1,351)	1:32:A:SER:H	1:33:A:ASP:H	15	0.38
(1,349)	1:32:A:SER:H	1:33:A:ASP:H	15	0.38
(1,327)	1:22:A:CYS:HB2	1:22:A:CYS:H	8	0.38
(1,327)	1:22:A:CYS:HB3	1:22:A:CYS:H	8	0.38
(1,327)	1:22:A:CYS:HB2	1:22:A:CYS:H	9	0.38
(1,327)	1:22:A:CYS:HB3	1:22:A:CYS:H	9	0.38
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB2	7	0.38
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB3	7	0.38
(1,298)	1:14:A:GLN:H	1:11:A:ASN:H	10	0.38
(1,224)	1:92:A:CYS:HA	1:94:A:SER:H	7	0.38
(1,158)	1:104:A:CYS:HA	1:105:A:ASN:H	5	0.38
(1,158)	1:104:A:CYS:HA	1:105:A:ASN:H	17	0.38
(1,118)	1:115:A:ASP:H	1:113:A:GLY:H	19	0.38
(1,99)	1:98:A:ILE:HG12	1:99:A:SER:H	13	0.38
(1,99)	1:98:A:ILE:HG13	1:99:A:SER:H	13	0.38
(1,93)	1:8:A:PHE:H	1:7:A:ASP:HA	8	0.38
(1,93)	1:8:A:PHE:H	1:7:A:ASP:HA	18	0.38
(1,85)	1:21:A:LYS:HG2	1:22:A:CYS:H	5	0.38
(1,85)	1:21:A:LYS:HG3	1:22:A:CYS:H	5	0.38
(1,81)	1:28:A:CYS:HA	1:33:A:ASP:H	2	0.38
(1,81)	1:28:A:CYS:HA	1:33:A:ASP:H	16	0.38
(1,66)	1:23:A:ASP:H	1:24:A:GLY:H	3	0.38
(1,66)	1:23:A:ASP:H	1:24:A:GLY:H	4	0.38
(4,8)	1:8:A:PHE:O	1:16:A:VAL:H	17	0.37
(4,2)	1:90:A:PHE:O	1:98:A:ILE:H	20	0.37
(2,298)	1:28:A:CYS:HB3	1:14:A:GLN:HE22	6	0.37
(2,281)	1:10:A:CYS:HA	1:11:A:ASN:HD22	2	0.37
(2,276)	1:43:A:THR:HA	1:57:A:GLN:H	14	0.37
(2,244)	1:45:A:ARG:HA	1:47:A:HIS:H	3	0.37
(2,212)	1:88:A:ASP:H	1:86:A:SER:H	14	0.37
(2,83)	1:35:A:SER:HB3	1:38:A:GLN:H	17	0.37
(2,39)	1:117:A:LEU:HD11	1:115:A:ASP:H	11	0.37
(2,25)	1:79:A:ASN:HD22	1:80:A:CYS:HA	13	0.37
(2,22)	1:75:A:GLU:HA	1:78:A:GLU:H	4	0.37
(2,8)	1:45:A:ARG:HA	1:46:A:ILE:H	13	0.37
(2,8)	1:45:A:ARG:HA	1:46:A:ILE:H	16	0.37
(1,916)	1:77:A:GLU:HB2	1:77:A:GLU:H	4	0.37
(1,916)	1:77:A:GLU:HB3	1:77:A:GLU:H	4	0.37
(1,916)	1:77:A:GLU:HB2	1:77:A:GLU:H	10	0.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,916)	1:77:A:GLU:HB3	1:77:A:GLU:H	10	0.37
(1,916)	1:77:A:GLU:HB2	1:77:A:GLU:H	18	0.37
(1,916)	1:77:A:GLU:HB3	1:77:A:GLU:H	18	0.37
(1,898)	1:57:A:GLN:HE22	1:71:A:CYS:H	20	0.37
(1,871)	1:30:A:ASP:HB2	1:32:A:SER:H	15	0.37
(1,871)	1:30:A:ASP:HB3	1:32:A:SER:H	15	0.37
(1,862)	1:21:A:LYS:HE2	1:19:A:ARG:H	19	0.37
(1,862)	1:21:A:LYS:HE3	1:19:A:ARG:H	19	0.37
(1,859)	1:3:A:CYS:HB2	1:18:A:SER:H	9	0.37
(1,859)	1:3:A:CYS:HB3	1:18:A:SER:H	9	0.37
(1,856)	1:14:A:GLN:H	1:12:A:ASN:HD22	10	0.37
(1,856)	1:14:A:GLN:H	1:12:A:ASN:HD22	20	0.37
(1,849)	1:33:A:ASP:H	1:11:A:ASN:H	7	0.37
(1,831)	1:73:A:SER:H	1:75:A:GLU:H	1	0.37
(1,808)	1:116:A:GLU:HB2	1:104:A:CYS:H	20	0.37
(1,808)	1:116:A:GLU:HB3	1:104:A:CYS:H	20	0.37
(1,801)	1:102:A:PHE:HB2	1:98:A:ILE:H	19	0.37
(1,801)	1:102:A:PHE:HB3	1:98:A:ILE:H	19	0.37
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG21	5	0.37
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG22	5	0.37
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG23	5	0.37
(1,794)	1:82:A:ASN:HD22	1:94:A:SER:H	19	0.37
(1,791)	1:85:A:CYS:HB2	1:89:A:GLU:H	5	0.37
(1,791)	1:85:A:CYS:HB3	1:89:A:GLU:H	5	0.37
(1,789)	1:85:A:CYS:H	1:84:A:THR:HB	19	0.37
(1,783)	1:71:A:CYS:HB2	1:74:A:GLY:H	18	0.37
(1,783)	1:71:A:CYS:HB3	1:74:A:GLY:H	18	0.37
(1,772)	1:68:A:GLU:H	1:64:A:ARG:H	3	0.37
(1,766)	1:48:A:GLU:HB2	1:58:A:CYS:H	7	0.37
(1,766)	1:48:A:GLU:HB3	1:58:A:CYS:H	7	0.37
(1,759)	1:57:A:GLN:HE21	1:71:A:CYS:HA	4	0.37
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	9	0.37
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	9	0.37
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	9	0.37
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	9	0.37
(1,745)	1:48:A:GLU:HB2	1:49:A:ILE:H	5	0.37
(1,745)	1:48:A:GLU:HB3	1:49:A:ILE:H	5	0.37
(1,744)	1:48:A:GLU:H	1:47:A:HIS:H	1	0.37
(1,733)	1:32:A:SER:H	1:28:A:CYS:H	10	0.37
(1,729)	1:32:A:SER:H	1:28:A:CYS:H	10	0.37
(1,711)	1:10:A:CYS:HB2	1:11:A:ASN:H	6	0.37
(1,711)	1:10:A:CYS:HB3	1:11:A:ASN:H	6	0.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,708)	1:44:A:CYS:HB2	1:45:A:ARG:H	3	0.37
(1,708)	1:44:A:CYS:HB3	1:45:A:ARG:H	3	0.37
(1,706)	1:45:A:ARG:HB2	1:45:A:ARG:H	8	0.37
(1,706)	1:45:A:ARG:HB3	1:45:A:ARG:H	8	0.37
(1,693)	1:21:A:LYS:HD2	1:21:A:LYS:H	4	0.37
(1,693)	1:21:A:LYS:HD3	1:21:A:LYS:H	4	0.37
(1,690)	1:61:A:VAL:HG11	1:49:A:ILE:H	9	0.37
(1,690)	1:61:A:VAL:HG12	1:49:A:ILE:H	9	0.37
(1,690)	1:61:A:VAL:HG13	1:49:A:ILE:H	9	0.37
(1,690)	1:61:A:VAL:HG21	1:49:A:ILE:H	9	0.37
(1,690)	1:61:A:VAL:HG22	1:49:A:ILE:H	9	0.37
(1,690)	1:61:A:VAL:HG23	1:49:A:ILE:H	9	0.37
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD2	12	0.37
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD3	12	0.37
(1,657)	1:105:A:ASN:HA	1:105:A:ASN:HD22	14	0.37
(1,654)	1:107:A:GLN:HB2	1:107:A:GLN:HE22	9	0.37
(1,654)	1:107:A:GLN:HB2	1:107:A:GLN:HE22	9	0.37
(1,654)	1:107:A:GLN:HB3	1:107:A:GLN:HE22	9	0.37
(1,654)	1:107:A:GLN:HB3	1:107:A:GLN:HE22	9	0.37
(1,642)	1:82:A:ASN:HA	1:82:A:ASN:HD22	15	0.37
(1,636)	1:78:A:GLU:HB2	1:79:A:ASN:HD22	8	0.37
(1,636)	1:78:A:GLU:HB2	1:79:A:ASN:HD22	8	0.37
(1,636)	1:78:A:GLU:HB3	1:79:A:ASN:HD22	8	0.37
(1,636)	1:78:A:GLU:HB3	1:79:A:ASN:HD22	8	0.37
(1,627)	1:72:A:ASP:HA	1:57:A:GLN:HE22	8	0.37
(1,608)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	5	0.37
(1,608)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	5	0.37
(1,608)	1:14:A:GLN:HG2	1:14:A:GLN:HE21	17	0.37
(1,608)	1:14:A:GLN:HG3	1:14:A:GLN:HE21	17	0.37
(1,592)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	6	0.37
(1,592)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	6	0.37
(1,585)	1:28:A:CYS:H	1:27:A:ASP:H	11	0.37
(1,585)	1:28:A:CYS:H	1:27:A:ASP:H	19	0.37
(1,569)	1:85:A:CYS:H	1:84:A:THR:H	17	0.37
(1,555)	1:103:A:VAL:HG11	1:104:A:CYS:H	10	0.37
(1,555)	1:103:A:VAL:HG12	1:104:A:CYS:H	10	0.37
(1,555)	1:103:A:VAL:HG13	1:104:A:CYS:H	10	0.37
(1,555)	1:103:A:VAL:HG21	1:104:A:CYS:H	10	0.37
(1,555)	1:103:A:VAL:HG22	1:104:A:CYS:H	10	0.37
(1,555)	1:103:A:VAL:HG23	1:104:A:CYS:H	10	0.37
(1,555)	1:103:A:VAL:HG11	1:104:A:CYS:H	19	0.37
(1,555)	1:103:A:VAL:HG12	1:104:A:CYS:H	19	0.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,555)	1:103:A:VAL:HG13	1:104:A:CYS:H	19	0.37
(1,555)	1:103:A:VAL:HG21	1:104:A:CYS:H	19	0.37
(1,555)	1:103:A:VAL:HG22	1:104:A:CYS:H	19	0.37
(1,555)	1:103:A:VAL:HG23	1:104:A:CYS:H	19	0.37
(1,486)	1:7:A:ASP:HA	1:19:A:ARG:H	3	0.37
(1,486)	1:7:A:ASP:HA	1:19:A:ARG:H	4	0.37
(1,398)	1:54:A:HIS:HB2	1:54:A:HIS:H	5	0.37
(1,398)	1:54:A:HIS:HB3	1:54:A:HIS:H	5	0.37
(1,398)	1:54:A:HIS:HB2	1:54:A:HIS:H	8	0.37
(1,398)	1:54:A:HIS:HB3	1:54:A:HIS:H	8	0.37
(1,398)	1:54:A:HIS:HB2	1:54:A:HIS:H	10	0.37
(1,398)	1:54:A:HIS:HB3	1:54:A:HIS:H	10	0.37
(1,376)	1:49:A:ILE:HA	1:49:A:ILE:H	2	0.37
(1,376)	1:49:A:ILE:HA	1:49:A:ILE:H	5	0.37
(1,376)	1:49:A:ILE:HA	1:49:A:ILE:H	6	0.37
(1,376)	1:49:A:ILE:HA	1:49:A:ILE:H	7	0.37
(1,376)	1:49:A:ILE:HA	1:49:A:ILE:H	17	0.37
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	18	0.37
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	18	0.37
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	18	0.37
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	18	0.37
(1,365)	1:43:A:THR:HB	1:43:A:THR:H	10	0.37
(1,348)	1:30:A:ASP:HB2	1:31:A:GLY:H	19	0.37
(1,348)	1:30:A:ASP:HB3	1:31:A:GLY:H	19	0.37
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB2	15	0.37
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB3	15	0.37
(1,320)	1:7:A:ASP:HA	1:18:A:SER:H	10	0.37
(1,298)	1:14:A:GLN:H	1:11:A:ASN:H	17	0.37
(1,281)	1:5:A:GLU:HB2	1:6:A:SER:H	18	0.37
(1,281)	1:5:A:GLU:HB2	1:6:A:SER:H	18	0.37
(1,281)	1:5:A:GLU:HB3	1:6:A:SER:H	18	0.37
(1,281)	1:5:A:GLU:HB3	1:6:A:SER:H	18	0.37
(1,224)	1:92:A:CYS:HA	1:94:A:SER:H	4	0.37
(1,224)	1:92:A:CYS:HA	1:94:A:SER:H	9	0.37
(1,158)	1:104:A:CYS:HA	1:105:A:ASN:H	6	0.37
(1,139)	1:109:A:ASP:H	1:109:A:ASP:HB2	10	0.37
(1,139)	1:109:A:ASP:H	1:109:A:ASP:HB3	10	0.37
(1,109)	1:119:A:CYS:H	1:117:A:LEU:HG	6	0.37
(1,109)	1:119:A:CYS:H	1:117:A:LEU:HG	14	0.37
(1,97)	1:98:A:ILE:HD11	1:99:A:SER:H	8	0.37
(1,97)	1:98:A:ILE:HD12	1:99:A:SER:H	8	0.37
(1,97)	1:98:A:ILE:HD13	1:99:A:SER:H	8	0.37

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,93)	1:8:A:PHE:H	1:7:A:ASP:HA	3	0.37
(1,93)	1:8:A:PHE:H	1:7:A:ASP:HA	7	0.37
(1,81)	1:28:A:CYS:HA	1:33:A:ASP:H	3	0.37
(1,66)	1:23:A:ASP:H	1:24:A:GLY:H	14	0.37
(1,49)	1:94:A:SER:H	1:93:A:SER:H	16	0.37
(4,2)	1:90:A:PHE:O	1:98:A:ILE:H	15	0.36
(2,381)	1:100:A:ARG:HD3	1:90:A:PHE:H	19	0.36
(2,327)	1:68:A:GLU:HG2	1:71:A:CYS:H	4	0.36
(2,296)	1:113:A:GLY:HA2	1:117:A:LEU:H	20	0.36
(2,190)	1:56:A:THR:HA	1:57:A:GLN:H	5	0.36
(2,190)	1:56:A:THR:HA	1:57:A:GLN:H	7	0.36
(2,190)	1:56:A:THR:HA	1:57:A:GLN:H	9	0.36
(2,190)	1:56:A:THR:HA	1:57:A:GLN:H	13	0.36
(2,190)	1:56:A:THR:HA	1:57:A:GLN:H	16	0.36
(2,188)	1:16:A:VAL:HG11	1:19:A:ARG:H	7	0.36
(2,188)	1:16:A:VAL:HG12	1:19:A:ARG:H	7	0.36
(2,188)	1:16:A:VAL:HG13	1:19:A:ARG:H	7	0.36
(2,188)	1:16:A:VAL:HG21	1:19:A:ARG:H	7	0.36
(2,188)	1:16:A:VAL:HG22	1:19:A:ARG:H	7	0.36
(2,188)	1:16:A:VAL:HG23	1:19:A:ARG:H	7	0.36
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	7	0.36
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	7	0.36
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	7	0.36
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	7	0.36
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	7	0.36
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	7	0.36
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	7	0.36
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	7	0.36
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	7	0.36
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	7	0.36
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	7	0.36
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	7	0.36
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	7	0.36
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	7	0.36
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	7	0.36
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	7	0.36
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	7	0.36
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	7	0.36
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	7	0.36
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	7	0.36
(2,174)	1:117:A:LEU:HB3	1:116:A:GLU:H	1	0.36
(2,114)	1:16:A:VAL:HG11	1:16:A:VAL:H	13	0.36
(2,114)	1:16:A:VAL:HG12	1:16:A:VAL:H	13	0.36
(2,114)	1:16:A:VAL:HG13	1:16:A:VAL:H	13	0.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	13	0.36
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	13	0.36
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	13	0.36
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	13	0.36
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	13	0.36
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	13	0.36
(2,49)	1:35:A:SER:HB3	1:39:A:CYS:H	4	0.36
(2,38)	1:96:A:ARG:HB3	1:97:A:CYS:H	8	0.36
(2,8)	1:45:A:ARG:HA	1:46:A:ILE:H	7	0.36
(2,8)	1:45:A:ARG:HA	1:46:A:ILE:H	17	0.36
(2,4)	1:46:A:ILE:HG23	1:46:A:ILE:H	2	0.36
(1,916)	1:77:A:GLU:HB2	1:77:A:GLU:H	14	0.36
(1,916)	1:77:A:GLU:HB3	1:77:A:GLU:H	14	0.36
(1,911)	1:57:A:GLN:HE21	1:71:A:CYS:H	16	0.36
(1,896)	1:64:A:ARG:H	1:66:A:ASP:H	2	0.36
(1,888)	1:49:A:ILE:HA	1:61:A:VAL:H	15	0.36
(1,888)	1:49:A:ILE:HA	1:61:A:VAL:H	16	0.36
(1,863)	1:17:A:PRO:HD2	1:20:A:TRP:HE1	15	0.36
(1,863)	1:17:A:PRO:HD3	1:20:A:TRP:HE1	15	0.36
(1,862)	1:21:A:LYS:HE2	1:19:A:ARG:H	18	0.36
(1,862)	1:21:A:LYS:HE3	1:19:A:ARG:H	18	0.36
(1,860)	1:16:A:VAL:HB	1:19:A:ARG:H	2	0.36
(1,859)	1:3:A:CYS:HB2	1:18:A:SER:H	11	0.36
(1,859)	1:3:A:CYS:HB3	1:18:A:SER:H	11	0.36
(1,853)	1:10:A:CYS:HB2	1:12:A:ASN:H	9	0.36
(1,853)	1:10:A:CYS:HB3	1:12:A:ASN:H	9	0.36
(1,819)	1:112:A:ASP:HB2	1:115:A:ASP:H	13	0.36
(1,819)	1:112:A:ASP:HB3	1:115:A:ASP:H	13	0.36
(1,813)	1:107:A:GLN:HE21	1:108:A:ASP:HA	4	0.36
(1,807)	1:98:A:ILE:HG12	1:103:A:VAL:H	9	0.36
(1,807)	1:98:A:ILE:HG13	1:103:A:VAL:H	9	0.36
(1,799)	1:85:A:CYS:HA	1:97:A:CYS:H	2	0.36
(1,789)	1:85:A:CYS:H	1:84:A:THR:HB	5	0.36
(1,789)	1:85:A:CYS:H	1:84:A:THR:HB	12	0.36
(1,783)	1:71:A:CYS:HB2	1:74:A:GLY:H	4	0.36
(1,783)	1:71:A:CYS:HB3	1:74:A:GLY:H	4	0.36
(1,777)	1:77:A:GLU:HB2	1:70:A:ASP:H	18	0.36
(1,777)	1:77:A:GLU:HB3	1:70:A:ASP:H	18	0.36
(1,766)	1:48:A:GLU:HB2	1:58:A:CYS:H	1	0.36
(1,766)	1:48:A:GLU:HB3	1:58:A:CYS:H	1	0.36
(1,766)	1:48:A:GLU:HB2	1:58:A:CYS:H	3	0.36
(1,766)	1:48:A:GLU:HB3	1:58:A:CYS:H	3	0.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,766)	1:48:A:GLU:HB2	1:58:A:CYS:H	11	0.36
(1,766)	1:48:A:GLU:HB3	1:58:A:CYS:H	11	0.36
(1,766)	1:48:A:GLU:HB2	1:58:A:CYS:H	13	0.36
(1,766)	1:48:A:GLU:HB3	1:58:A:CYS:H	13	0.36
(1,733)	1:32:A:SER:H	1:28:A:CYS:H	5	0.36
(1,729)	1:32:A:SER:H	1:28:A:CYS:H	5	0.36
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD2	2	0.36
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD3	2	0.36
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD2	8	0.36
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD3	8	0.36
(1,667)	1:107:A:GLN:HG2	1:105:A:ASN:HD22	3	0.36
(1,667)	1:107:A:GLN:HG2	1:105:A:ASN:HD22	3	0.36
(1,667)	1:107:A:GLN:HG3	1:105:A:ASN:HD22	3	0.36
(1,667)	1:107:A:GLN:HG3	1:105:A:ASN:HD22	3	0.36
(1,658)	1:102:A:PHE:HA	1:105:A:ASN:HD22	17	0.36
(1,642)	1:82:A:ASN:HA	1:82:A:ASN:HD22	6	0.36
(1,582)	1:46:A:ILE:H	1:45:A:ARG:H	12	0.36
(1,569)	1:85:A:CYS:H	1:84:A:THR:H	15	0.36
(1,555)	1:103:A:VAL:HG11	1:104:A:CYS:H	1	0.36
(1,555)	1:103:A:VAL:HG12	1:104:A:CYS:H	1	0.36
(1,555)	1:103:A:VAL:HG13	1:104:A:CYS:H	1	0.36
(1,555)	1:103:A:VAL:HG21	1:104:A:CYS:H	1	0.36
(1,555)	1:103:A:VAL:HG22	1:104:A:CYS:H	1	0.36
(1,555)	1:103:A:VAL:HG23	1:104:A:CYS:H	1	0.36
(1,555)	1:103:A:VAL:HG11	1:104:A:CYS:H	2	0.36
(1,555)	1:103:A:VAL:HG12	1:104:A:CYS:H	2	0.36
(1,555)	1:103:A:VAL:HG13	1:104:A:CYS:H	2	0.36
(1,555)	1:103:A:VAL:HG21	1:104:A:CYS:H	2	0.36
(1,555)	1:103:A:VAL:HG22	1:104:A:CYS:H	2	0.36
(1,555)	1:103:A:VAL:HG23	1:104:A:CYS:H	2	0.36
(1,555)	1:103:A:VAL:HG11	1:104:A:CYS:H	8	0.36
(1,555)	1:103:A:VAL:HG12	1:104:A:CYS:H	8	0.36
(1,555)	1:103:A:VAL:HG13	1:104:A:CYS:H	8	0.36
(1,555)	1:103:A:VAL:HG21	1:104:A:CYS:H	8	0.36
(1,555)	1:103:A:VAL:HG22	1:104:A:CYS:H	8	0.36
(1,555)	1:103:A:VAL:HG23	1:104:A:CYS:H	8	0.36
(1,534)	1:77:A:GLU:HB2	1:77:A:GLU:H	8	0.36
(1,534)	1:77:A:GLU:HB3	1:77:A:GLU:H	8	0.36
(1,526)	1:64:A:ARG:H	1:67:A:GLY:H	16	0.36
(1,486)	1:7:A:ASP:HA	1:19:A:ARG:H	1	0.36
(1,486)	1:7:A:ASP:HA	1:19:A:ARG:H	16	0.36
(1,483)	1:10:A:CYS:HB2	1:14:A:GLN:H	17	0.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,483)	1:10:A:CYS:HB3	1:14:A:GLN:H	17	0.36
(1,445)	1:75:A:GLU:H	1:74:A:GLY:H	8	0.36
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB2	2	0.36
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB3	2	0.36
(1,436)	1:73:A:SER:H	1:72:A:ASP:H	1	0.36
(1,436)	1:73:A:SER:H	1:72:A:ASP:H	17	0.36
(1,398)	1:54:A:HIS:HB2	1:54:A:HIS:H	1	0.36
(1,398)	1:54:A:HIS:HB3	1:54:A:HIS:H	1	0.36
(1,398)	1:54:A:HIS:HB2	1:54:A:HIS:H	18	0.36
(1,398)	1:54:A:HIS:HB3	1:54:A:HIS:H	18	0.36
(1,376)	1:49:A:ILE:HA	1:49:A:ILE:H	1	0.36
(1,376)	1:49:A:ILE:HA	1:49:A:ILE:H	8	0.36
(1,376)	1:49:A:ILE:HA	1:49:A:ILE:H	11	0.36
(1,376)	1:49:A:ILE:HA	1:49:A:ILE:H	14	0.36
(1,371)	1:44:A:CYS:HA	1:45:A:ARG:H	10	0.36
(1,365)	1:43:A:THR:HB	1:43:A:THR:H	17	0.36
(1,327)	1:22:A:CYS:HB2	1:22:A:CYS:H	10	0.36
(1,327)	1:22:A:CYS:HB3	1:22:A:CYS:H	10	0.36
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB2	13	0.36
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB3	13	0.36
(1,320)	1:7:A:ASP:HA	1:18:A:SER:H	9	0.36
(1,286)	1:7:A:ASP:HB2	1:7:A:ASP:H	20	0.36
(1,286)	1:7:A:ASP:HB3	1:7:A:ASP:H	20	0.36
(1,224)	1:92:A:CYS:HA	1:94:A:SER:H	3	0.36
(1,224)	1:92:A:CYS:HA	1:94:A:SER:H	5	0.36
(1,224)	1:92:A:CYS:HA	1:94:A:SER:H	6	0.36
(1,224)	1:92:A:CYS:HA	1:94:A:SER:H	11	0.36
(1,224)	1:92:A:CYS:HA	1:94:A:SER:H	17	0.36
(1,205)	1:98:A:ILE:HG12	1:98:A:ILE:H	10	0.36
(1,205)	1:98:A:ILE:HG13	1:98:A:ILE:H	10	0.36
(1,189)	1:101:A:ASN:HB2	1:101:A:ASN:H	6	0.36
(1,189)	1:101:A:ASN:HB3	1:101:A:ASN:H	6	0.36
(1,189)	1:101:A:ASN:HB2	1:101:A:ASN:H	18	0.36
(1,189)	1:101:A:ASN:HB3	1:101:A:ASN:H	18	0.36
(1,158)	1:104:A:CYS:HA	1:105:A:ASN:H	12	0.36
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB2	6	0.36
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB3	6	0.36
(1,99)	1:98:A:ILE:HG12	1:99:A:SER:H	14	0.36
(1,99)	1:98:A:ILE:HG13	1:99:A:SER:H	14	0.36
(1,93)	1:8:A:PHE:H	1:7:A:ASP:HA	2	0.36
(1,93)	1:8:A:PHE:H	1:7:A:ASP:HA	5	0.36
(1,93)	1:8:A:PHE:H	1:7:A:ASP:HA	16	0.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,81)	1:28:A:CYS:HA	1:33:A:ASP:H	14	0.36
(1,81)	1:28:A:CYS:HA	1:33:A:ASP:H	17	0.36
(1,56)	1:70:A:ASP:H	1:71:A:CYS:H	4	0.36
(1,55)	1:71:A:CYS:H	1:70:A:ASP:H	2	0.36
(1,49)	1:94:A:SER:H	1:93:A:SER:H	20	0.36
(1,33)	1:115:A:ASP:H	1:114:A:SER:H	3	0.36
(1,33)	1:115:A:ASP:H	1:114:A:SER:H	4	0.36
(1,33)	1:115:A:ASP:H	1:114:A:SER:H	7	0.36
(1,24)	1:104:A:CYS:H	1:105:A:ASN:H	14	0.36
(1,24)	1:104:A:CYS:H	1:105:A:ASN:H	18	0.36
(1,23)	1:104:A:CYS:H	1:105:A:ASN:H	14	0.36
(1,23)	1:104:A:CYS:H	1:105:A:ASN:H	18	0.36
(2,381)	1:100:A:ARG:HD3	1:90:A:PHE:H	20	0.35
(2,376)	1:87:A:PRO:HB2	1:88:A:ASP:H	16	0.35
(2,366)	1:107:A:GLN:HA	1:106:A:GLY:H	1	0.35
(2,330)	1:114:A:SER:HG	1:93:A:SER:H	2	0.35
(2,329)	1:90:A:PHE:HA	1:98:A:ILE:H	1	0.35
(2,281)	1:10:A:CYS:HA	1:11:A:ASN:HD22	1	0.35
(2,190)	1:56:A:THR:HA	1:57:A:GLN:H	19	0.35
(2,188)	1:16:A:VAL:HG11	1:19:A:ARG:H	19	0.35
(2,188)	1:16:A:VAL:HG12	1:19:A:ARG:H	19	0.35
(2,188)	1:16:A:VAL:HG13	1:19:A:ARG:H	19	0.35
(2,188)	1:16:A:VAL:HG21	1:19:A:ARG:H	19	0.35
(2,188)	1:16:A:VAL:HG22	1:19:A:ARG:H	19	0.35
(2,188)	1:16:A:VAL:HG23	1:19:A:ARG:H	19	0.35
(2,168)	1:38:A:GLN:HG3	1:38:A:GLN:H	7	0.35
(2,164)	1:14:A:GLN:HB2	1:14:A:GLN:H	5	0.35
(2,164)	1:14:A:GLN:HB3	1:14:A:GLN:H	5	0.35
(2,164)	1:14:A:GLN:HB2	1:14:A:GLN:H	7	0.35
(2,164)	1:14:A:GLN:HB3	1:14:A:GLN:H	7	0.35
(2,114)	1:16:A:VAL:HG11	1:16:A:VAL:H	1	0.35
(2,114)	1:16:A:VAL:HG12	1:16:A:VAL:H	1	0.35
(2,114)	1:16:A:VAL:HG13	1:16:A:VAL:H	1	0.35
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	1	0.35
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	1	0.35
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	1	0.35
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	1	0.35
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	1	0.35
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	1	0.35
(2,114)	1:16:A:VAL:HG11	1:16:A:VAL:H	10	0.35
(2,114)	1:16:A:VAL:HG12	1:16:A:VAL:H	10	0.35
(2,114)	1:16:A:VAL:HG13	1:16:A:VAL:H	10	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	10	0.35
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	10	0.35
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	10	0.35
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	10	0.35
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	10	0.35
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	10	0.35
(2,114)	1:16:A:VAL:HG11	1:16:A:VAL:H	17	0.35
(2,114)	1:16:A:VAL:HG12	1:16:A:VAL:H	17	0.35
(2,114)	1:16:A:VAL:HG13	1:16:A:VAL:H	17	0.35
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	17	0.35
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	17	0.35
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	17	0.35
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	17	0.35
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	17	0.35
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	17	0.35
(2,80)	1:41:A:MET:HA	1:56:A:THR:H	12	0.35
(2,72)	1:112:A:ASP:HB2	1:113:A:GLY:H	17	0.35
(2,66)	1:4:A:ALA:H	1:7:A:ASP:H	4	0.35
(2,8)	1:45:A:ARG:HA	1:46:A:ILE:H	1	0.35
(2,8)	1:45:A:ARG:HA	1:46:A:ILE:H	2	0.35
(2,8)	1:45:A:ARG:HA	1:46:A:ILE:H	5	0.35
(1,907)	1:39:A:CYS:H	1:41:A:MET:H	2	0.35
(1,907)	1:39:A:CYS:H	1:41:A:MET:H	19	0.35
(1,897)	1:77:A:GLU:HB2	1:69:A:ASN:HD22	2	0.35
(1,897)	1:77:A:GLU:HB3	1:69:A:ASN:HD22	2	0.35
(1,897)	1:77:A:GLU:HB2	1:69:A:ASN:HD22	19	0.35
(1,897)	1:77:A:GLU:HB3	1:69:A:ASN:HD22	19	0.35
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB2	11	0.35
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB3	11	0.35
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB2	16	0.35
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB3	16	0.35
(1,888)	1:49:A:ILE:HA	1:61:A:VAL:H	13	0.35
(1,860)	1:16:A:VAL:HB	1:19:A:ARG:H	5	0.35
(1,859)	1:3:A:CYS:HB2	1:18:A:SER:H	7	0.35
(1,859)	1:3:A:CYS:HB3	1:18:A:SER:H	7	0.35
(1,856)	1:14:A:GLN:H	1:12:A:ASN:HD22	7	0.35
(1,856)	1:14:A:GLN:H	1:12:A:ASN:HD22	11	0.35
(1,856)	1:14:A:GLN:H	1:12:A:ASN:HD22	16	0.35
(1,849)	1:33:A:ASP:H	1:11:A:ASN:H	4	0.35
(1,840)	1:71:A:CYS:HB2	1:77:A:GLU:H	17	0.35
(1,840)	1:71:A:CYS:HB3	1:77:A:GLU:H	17	0.35
(1,833)	1:42:A:ARG:HG2	1:41:A:MET:H	20	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,833)	1:42:A:ARG:HG2	1:41:A:MET:H	20	0.35
(1,833)	1:42:A:ARG:HG3	1:41:A:MET:H	20	0.35
(1,833)	1:42:A:ARG:HG3	1:41:A:MET:H	20	0.35
(1,831)	1:73:A:SER:H	1:75:A:GLU:H	5	0.35
(1,831)	1:73:A:SER:H	1:75:A:GLU:H	7	0.35
(1,806)	1:101:A:ASN:HD21	1:102:A:PHE:H	10	0.35
(1,791)	1:85:A:CYS:HB2	1:89:A:GLU:H	1	0.35
(1,791)	1:85:A:CYS:HB3	1:89:A:GLU:H	1	0.35
(1,789)	1:85:A:CYS:H	1:84:A:THR:HB	13	0.35
(1,789)	1:85:A:CYS:H	1:84:A:THR:HB	20	0.35
(1,784)	1:71:A:CYS:HB2	1:76:A:ASP:H	2	0.35
(1,784)	1:71:A:CYS:HB3	1:76:A:ASP:H	2	0.35
(1,783)	1:71:A:CYS:HB2	1:74:A:GLY:H	13	0.35
(1,783)	1:71:A:CYS:HB3	1:74:A:GLY:H	13	0.35
(1,783)	1:71:A:CYS:HB2	1:74:A:GLY:H	14	0.35
(1,783)	1:71:A:CYS:HB3	1:74:A:GLY:H	14	0.35
(1,772)	1:68:A:GLU:H	1:64:A:ARG:H	5	0.35
(1,747)	1:57:A:GLN:HB2	1:51:A:CYS:H	10	0.35
(1,747)	1:57:A:GLN:HB2	1:51:A:CYS:H	10	0.35
(1,747)	1:57:A:GLN:HB3	1:51:A:CYS:H	10	0.35
(1,747)	1:57:A:GLN:HB3	1:51:A:CYS:H	10	0.35
(1,745)	1:48:A:GLU:HB2	1:49:A:ILE:H	7	0.35
(1,745)	1:48:A:GLU:HB3	1:49:A:ILE:H	7	0.35
(1,745)	1:48:A:GLU:HB2	1:49:A:ILE:H	13	0.35
(1,745)	1:48:A:GLU:HB3	1:49:A:ILE:H	13	0.35
(1,745)	1:48:A:GLU:HB2	1:49:A:ILE:H	19	0.35
(1,745)	1:48:A:GLU:HB3	1:49:A:ILE:H	19	0.35
(1,744)	1:48:A:GLU:H	1:47:A:HIS:H	17	0.35
(1,735)	1:28:A:CYS:HB2	1:33:A:ASP:H	2	0.35
(1,735)	1:28:A:CYS:HB3	1:33:A:ASP:H	2	0.35
(1,735)	1:28:A:CYS:HB2	1:33:A:ASP:H	20	0.35
(1,735)	1:28:A:CYS:HB3	1:33:A:ASP:H	20	0.35
(1,733)	1:32:A:SER:H	1:28:A:CYS:H	2	0.35
(1,729)	1:32:A:SER:H	1:28:A:CYS:H	2	0.35
(1,706)	1:45:A:ARG:HB2	1:45:A:ARG:H	19	0.35
(1,706)	1:45:A:ARG:HB3	1:45:A:ARG:H	19	0.35
(1,696)	1:44:A:CYS:HB2	1:34:A:GLU:H	4	0.35
(1,696)	1:44:A:CYS:HB3	1:34:A:GLU:H	4	0.35
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD2	14	0.35
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD3	14	0.35
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD2	17	0.35
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD3	17	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,585)	1:28:A:CYS:H	1:27:A:ASP:H	16	0.35
(1,583)	1:40:A:HIS:HA	1:38:A:GLN:H	8	0.35
(1,583)	1:40:A:HIS:HA	1:38:A:GLN:H	10	0.35
(1,555)	1:103:A:VAL:HG11	1:104:A:CYS:H	17	0.35
(1,555)	1:103:A:VAL:HG12	1:104:A:CYS:H	17	0.35
(1,555)	1:103:A:VAL:HG13	1:104:A:CYS:H	17	0.35
(1,555)	1:103:A:VAL:HG21	1:104:A:CYS:H	17	0.35
(1,555)	1:103:A:VAL:HG22	1:104:A:CYS:H	17	0.35
(1,555)	1:103:A:VAL:HG23	1:104:A:CYS:H	17	0.35
(1,534)	1:77:A:GLU:HB2	1:77:A:GLU:H	13	0.35
(1,534)	1:77:A:GLU:HB3	1:77:A:GLU:H	13	0.35
(1,526)	1:64:A:ARG:H	1:67:A:GLY:H	5	0.35
(1,499)	1:33:A:ASP:HB2	1:33:A:ASP:H	4	0.35
(1,499)	1:33:A:ASP:HB3	1:33:A:ASP:H	4	0.35
(1,486)	1:7:A:ASP:HA	1:19:A:ARG:H	20	0.35
(1,454)	1:78:A:GLU:HG2	1:76:A:ASP:H	9	0.35
(1,454)	1:78:A:GLU:HG3	1:76:A:ASP:H	9	0.35
(1,454)	1:78:A:GLU:HG2	1:76:A:ASP:H	13	0.35
(1,454)	1:78:A:GLU:HG3	1:76:A:ASP:H	13	0.35
(1,376)	1:49:A:ILE:HA	1:49:A:ILE:H	10	0.35
(1,375)	1:48:A:GLU:HA	1:49:A:ILE:H	9	0.35
(1,375)	1:48:A:GLU:HA	1:49:A:ILE:H	20	0.35
(1,365)	1:43:A:THR:HB	1:43:A:THR:H	1	0.35
(1,365)	1:43:A:THR:HB	1:43:A:THR:H	12	0.35
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB2	2	0.35
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB3	2	0.35
(1,319)	1:16:A:VAL:H	1:9:A:VAL:HA	20	0.35
(1,296)	1:10:A:CYS:HB2	1:10:A:CYS:H	5	0.35
(1,296)	1:10:A:CYS:HB3	1:10:A:CYS:H	5	0.35
(1,296)	1:10:A:CYS:HB2	1:10:A:CYS:H	10	0.35
(1,296)	1:10:A:CYS:HB3	1:10:A:CYS:H	10	0.35
(1,296)	1:10:A:CYS:HB2	1:10:A:CYS:H	14	0.35
(1,296)	1:10:A:CYS:HB3	1:10:A:CYS:H	14	0.35
(1,293)	1:8:A:PHE:HB2	1:9:A:VAL:H	11	0.35
(1,293)	1:8:A:PHE:HB3	1:9:A:VAL:H	11	0.35
(1,281)	1:5:A:GLU:HB2	1:6:A:SER:H	2	0.35
(1,281)	1:5:A:GLU:HB2	1:6:A:SER:H	2	0.35
(1,281)	1:5:A:GLU:HB3	1:6:A:SER:H	2	0.35
(1,281)	1:5:A:GLU:HB3	1:6:A:SER:H	2	0.35
(1,281)	1:5:A:GLU:HB2	1:6:A:SER:H	5	0.35
(1,281)	1:5:A:GLU:HB2	1:6:A:SER:H	5	0.35
(1,281)	1:5:A:GLU:HB3	1:6:A:SER:H	5	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,281)	1:5:A:GLU:HB3	1:6:A:SER:H	5	0.35
(1,280)	1:5:A:GLU:HG2	1:6:A:SER:H	5	0.35
(1,280)	1:5:A:GLU:HG2	1:6:A:SER:H	5	0.35
(1,280)	1:5:A:GLU:HG3	1:6:A:SER:H	5	0.35
(1,280)	1:5:A:GLU:HG3	1:6:A:SER:H	5	0.35
(1,280)	1:5:A:GLU:HG2	1:6:A:SER:H	18	0.35
(1,280)	1:5:A:GLU:HG2	1:6:A:SER:H	18	0.35
(1,280)	1:5:A:GLU:HG3	1:6:A:SER:H	18	0.35
(1,280)	1:5:A:GLU:HG3	1:6:A:SER:H	18	0.35
(1,228)	1:92:A:CYS:HB2	1:93:A:SER:H	15	0.35
(1,228)	1:92:A:CYS:HB3	1:93:A:SER:H	15	0.35
(1,189)	1:101:A:ASN:HB2	1:101:A:ASN:H	8	0.35
(1,189)	1:101:A:ASN:HB3	1:101:A:ASN:H	8	0.35
(1,189)	1:101:A:ASN:HB2	1:101:A:ASN:H	19	0.35
(1,189)	1:101:A:ASN:HB3	1:101:A:ASN:H	19	0.35
(1,174)	1:103:A:VAL:H	1:101:A:ASN:HB2	5	0.35
(1,174)	1:103:A:VAL:H	1:101:A:ASN:HB3	5	0.35
(1,158)	1:104:A:CYS:HA	1:105:A:ASN:H	1	0.35
(1,158)	1:104:A:CYS:HA	1:105:A:ASN:H	20	0.35
(1,134)	1:110:A:CYS:H	1:109:A:ASP:HB2	8	0.35
(1,134)	1:110:A:CYS:H	1:109:A:ASP:HB2	8	0.35
(1,134)	1:110:A:CYS:H	1:109:A:ASP:HB3	8	0.35
(1,134)	1:110:A:CYS:H	1:109:A:ASP:HB3	8	0.35
(1,118)	1:115:A:ASP:H	1:113:A:GLY:H	5	0.35
(1,97)	1:98:A:ILE:HD11	1:99:A:SER:H	2	0.35
(1,97)	1:98:A:ILE:HD12	1:99:A:SER:H	2	0.35
(1,97)	1:98:A:ILE:HD13	1:99:A:SER:H	2	0.35
(1,85)	1:21:A:LYS:HG2	1:22:A:CYS:H	9	0.35
(1,85)	1:21:A:LYS:HG3	1:22:A:CYS:H	9	0.35
(1,85)	1:21:A:LYS:HG2	1:22:A:CYS:H	14	0.35
(1,85)	1:21:A:LYS:HG3	1:22:A:CYS:H	14	0.35
(1,85)	1:21:A:LYS:HG2	1:22:A:CYS:H	20	0.35
(1,85)	1:21:A:LYS:HG3	1:22:A:CYS:H	20	0.35
(1,73)	1:65:A:CYS:HB2	1:65:A:CYS:H	13	0.35
(1,73)	1:65:A:CYS:HB3	1:65:A:CYS:H	13	0.35
(1,73)	1:65:A:CYS:HB2	1:65:A:CYS:H	15	0.35
(1,73)	1:65:A:CYS:HB3	1:65:A:CYS:H	15	0.35
(1,66)	1:23:A:ASP:H	1:24:A:GLY:H	18	0.35
(1,66)	1:23:A:ASP:H	1:24:A:GLY:H	20	0.35
(1,60)	1:56:A:THR:H	1:57:A:GLN:H	11	0.35
(1,53)	1:77:A:GLU:H	1:76:A:ASP:H	4	0.35
(1,52)	1:76:A:ASP:H	1:77:A:GLU:H	4	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,49)	1:94:A:SER:H	1:93:A:SER:H	9	0.35
(1,24)	1:104:A:CYS:H	1:105:A:ASN:H	11	0.35
(1,24)	1:104:A:CYS:H	1:105:A:ASN:H	12	0.35
(1,24)	1:104:A:CYS:H	1:105:A:ASN:H	15	0.35
(1,23)	1:104:A:CYS:H	1:105:A:ASN:H	11	0.35
(1,23)	1:104:A:CYS:H	1:105:A:ASN:H	12	0.35
(1,23)	1:104:A:CYS:H	1:105:A:ASN:H	15	0.35
(1,17)	1:81:A:GLY:H	1:80:A:CYS:H	9	0.35
(1,17)	1:81:A:GLY:H	1:80:A:CYS:H	19	0.35
(1,14)	1:110:A:CYS:H	1:109:A:ASP:H	11	0.35
(1,14)	1:110:A:CYS:H	1:109:A:ASP:H	12	0.35
(4,7)	1:8:A:PHE:H	1:16:A:VAL:O	2	0.34
(2,376)	1:87:A:PRO:HB2	1:88:A:ASP:H	8	0.34
(2,298)	1:28:A:CYS:HB2	1:14:A:GLN:HE22	3	0.34
(2,270)	1:113:A:GLY:HA2	1:110:A:CYS:H	8	0.34
(2,168)	1:39:A:CYS:HB2	1:38:A:GLN:H	15	0.34
(2,164)	1:14:A:GLN:HB2	1:14:A:GLN:H	1	0.34
(2,164)	1:14:A:GLN:HB3	1:14:A:GLN:H	1	0.34
(2,154)	1:116:A:GLU:HG3	1:109:A:ASP:H	8	0.34
(2,46)	1:114:A:SER:HG	1:115:A:ASP:H	1	0.34
(2,41)	1:97:A:CYS:HB2	1:92:A:CYS:H	19	0.34
(2,39)	1:117:A:LEU:HD12	1:115:A:ASP:H	20	0.34
(2,38)	1:96:A:ARG:HB3	1:97:A:CYS:H	4	0.34
(2,38)	1:96:A:ARG:HB3	1:97:A:CYS:H	5	0.34
(2,12)	1:11:A:ASN:HB2	1:13:A:GLY:H	4	0.34
(2,11)	1:109:A:ASP:HA	1:113:A:GLY:H	15	0.34
(2,8)	1:45:A:ARG:HA	1:46:A:ILE:H	8	0.34
(1,907)	1:39:A:CYS:H	1:41:A:MET:H	5	0.34
(1,907)	1:39:A:CYS:H	1:41:A:MET:H	11	0.34
(1,907)	1:39:A:CYS:H	1:41:A:MET:H	13	0.34
(1,907)	1:39:A:CYS:H	1:41:A:MET:H	18	0.34
(1,898)	1:57:A:GLN:HE22	1:71:A:CYS:H	8	0.34
(1,898)	1:57:A:GLN:HE22	1:71:A:CYS:H	18	0.34
(1,888)	1:49:A:ILE:HA	1:61:A:VAL:H	11	0.34
(1,884)	1:50:A:SER:H	1:59:A:ILE:H	1	0.34
(1,881)	1:48:A:GLU:H	1:45:A:ARG:H	16	0.34
(1,880)	1:45:A:ARG:HD2	1:46:A:ILE:H	12	0.34
(1,880)	1:45:A:ARG:HD3	1:46:A:ILE:H	12	0.34
(1,879)	1:48:A:GLU:H	1:45:A:ARG:H	16	0.34
(1,860)	1:16:A:VAL:HB	1:19:A:ARG:H	14	0.34
(1,856)	1:14:A:GLN:H	1:12:A:ASN:HD22	6	0.34
(1,853)	1:10:A:CYS:HB2	1:12:A:ASN:H	8	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,853)	1:10:A:CYS:HB3	1:12:A:ASN:H	8	0.34
(1,833)	1:42:A:ARG:HG2	1:41:A:MET:H	4	0.34
(1,833)	1:42:A:ARG:HG2	1:41:A:MET:H	4	0.34
(1,833)	1:42:A:ARG:HG3	1:41:A:MET:H	4	0.34
(1,833)	1:42:A:ARG:HG3	1:41:A:MET:H	4	0.34
(1,833)	1:42:A:ARG:HG2	1:41:A:MET:H	12	0.34
(1,833)	1:42:A:ARG:HG2	1:41:A:MET:H	12	0.34
(1,833)	1:42:A:ARG:HG3	1:41:A:MET:H	12	0.34
(1,833)	1:42:A:ARG:HG3	1:41:A:MET:H	12	0.34
(1,831)	1:73:A:SER:H	1:75:A:GLU:H	19	0.34
(1,820)	1:110:A:CYS:H	1:115:A:ASP:H	5	0.34
(1,803)	1:101:A:ASN:HD21	1:99:A:SER:H	7	0.34
(1,799)	1:85:A:CYS:HA	1:97:A:CYS:H	18	0.34
(1,789)	1:85:A:CYS:H	1:84:A:THR:HB	8	0.34
(1,789)	1:85:A:CYS:H	1:84:A:THR:HB	14	0.34
(1,788)	1:80:A:CYS:H	1:78:A:GLU:H	4	0.34
(1,772)	1:68:A:GLU:H	1:64:A:ARG:H	7	0.34
(1,766)	1:48:A:GLU:HB2	1:58:A:CYS:H	16	0.34
(1,766)	1:48:A:GLU:HB3	1:58:A:CYS:H	16	0.34
(1,735)	1:28:A:CYS:HB2	1:33:A:ASP:H	12	0.34
(1,735)	1:28:A:CYS:HB3	1:33:A:ASP:H	12	0.34
(1,733)	1:32:A:SER:H	1:28:A:CYS:H	17	0.34
(1,729)	1:32:A:SER:H	1:28:A:CYS:H	17	0.34
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD2	13	0.34
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD3	13	0.34
(1,706)	1:45:A:ARG:HB2	1:45:A:ARG:H	3	0.34
(1,706)	1:45:A:ARG:HB3	1:45:A:ARG:H	3	0.34
(1,693)	1:21:A:LYS:HD2	1:21:A:LYS:H	1	0.34
(1,693)	1:21:A:LYS:HD3	1:21:A:LYS:H	1	0.34
(1,693)	1:21:A:LYS:HD2	1:21:A:LYS:H	2	0.34
(1,693)	1:21:A:LYS:HD3	1:21:A:LYS:H	2	0.34
(1,693)	1:21:A:LYS:HD2	1:21:A:LYS:H	12	0.34
(1,693)	1:21:A:LYS:HD3	1:21:A:LYS:H	12	0.34
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	7	0.34
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	7	0.34
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	7	0.34
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	7	0.34
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	9	0.34
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	9	0.34
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	9	0.34
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	9	0.34
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	11	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	11	0.34
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	11	0.34
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	11	0.34
(1,642)	1:82:A:ASN:HA	1:82:A:ASN:HD22	9	0.34
(1,635)	1:78:A:GLU:HB2	1:79:A:ASN:HD21	19	0.34
(1,635)	1:78:A:GLU:HB2	1:79:A:ASN:HD21	19	0.34
(1,635)	1:78:A:GLU:HB3	1:79:A:ASN:HD21	19	0.34
(1,635)	1:78:A:GLU:HB3	1:79:A:ASN:HD21	19	0.34
(1,596)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	1	0.34
(1,596)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	1	0.34
(1,596)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	5	0.34
(1,596)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	5	0.34
(1,585)	1:28:A:CYS:H	1:27:A:ASP:H	13	0.34
(1,585)	1:28:A:CYS:H	1:27:A:ASP:H	20	0.34
(1,582)	1:46:A:ILE:H	1:45:A:ARG:H	4	0.34
(1,526)	1:64:A:ARG:H	1:67:A:GLY:H	7	0.34
(1,526)	1:64:A:ARG:H	1:67:A:GLY:H	10	0.34
(1,480)	1:10:A:CYS:HB2	1:10:A:CYS:H	4	0.34
(1,480)	1:10:A:CYS:HB3	1:10:A:CYS:H	4	0.34
(1,466)	1:80:A:CYS:HA	1:79:A:ASN:H	17	0.34
(1,454)	1:78:A:GLU:HG2	1:76:A:ASP:H	1	0.34
(1,454)	1:78:A:GLU:HG3	1:76:A:ASP:H	1	0.34
(1,436)	1:73:A:SER:H	1:72:A:ASP:H	16	0.34
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB1	12	0.34
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB2	12	0.34
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB3	12	0.34
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB1	18	0.34
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB2	18	0.34
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB3	18	0.34
(1,376)	1:49:A:ILE:HA	1:49:A:ILE:H	12	0.34
(1,376)	1:49:A:ILE:HA	1:49:A:ILE:H	15	0.34
(1,376)	1:49:A:ILE:HA	1:49:A:ILE:H	18	0.34
(1,375)	1:48:A:GLU:HA	1:49:A:ILE:H	16	0.34
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	20	0.34
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	20	0.34
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	20	0.34
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	20	0.34
(1,365)	1:43:A:THR:HB	1:43:A:THR:H	2	0.34
(1,351)	1:32:A:SER:H	1:33:A:ASP:H	14	0.34
(1,349)	1:32:A:SER:H	1:33:A:ASP:H	14	0.34
(1,320)	1:7:A:ASP:HA	1:18:A:SER:H	2	0.34
(1,298)	1:14:A:GLN:H	1:11:A:ASN:H	15	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,296)	1:10:A:CYS:HB2	1:10:A:CYS:H	1	0.34
(1,296)	1:10:A:CYS:HB3	1:10:A:CYS:H	1	0.34
(1,296)	1:10:A:CYS:HB2	1:10:A:CYS:H	19	0.34
(1,296)	1:10:A:CYS:HB3	1:10:A:CYS:H	19	0.34
(1,295)	1:15:A:CYS:HA	1:10:A:CYS:H	11	0.34
(1,228)	1:92:A:CYS:HB2	1:93:A:SER:H	10	0.34
(1,228)	1:92:A:CYS:HB3	1:93:A:SER:H	10	0.34
(1,224)	1:92:A:CYS:HA	1:94:A:SER:H	16	0.34
(1,224)	1:92:A:CYS:HA	1:94:A:SER:H	19	0.34
(1,205)	1:98:A:ILE:HG12	1:98:A:ILE:H	2	0.34
(1,205)	1:98:A:ILE:HG13	1:98:A:ILE:H	2	0.34
(1,205)	1:98:A:ILE:HG12	1:98:A:ILE:H	3	0.34
(1,205)	1:98:A:ILE:HG13	1:98:A:ILE:H	3	0.34
(1,189)	1:101:A:ASN:HB2	1:101:A:ASN:H	1	0.34
(1,189)	1:101:A:ASN:HB3	1:101:A:ASN:H	1	0.34
(1,189)	1:101:A:ASN:HB2	1:101:A:ASN:H	17	0.34
(1,189)	1:101:A:ASN:HB3	1:101:A:ASN:H	17	0.34
(1,165)	1:104:A:CYS:H	1:116:A:GLU:HA	17	0.34
(1,98)	1:98:A:ILE:HG12	1:99:A:SER:H	12	0.34
(1,98)	1:98:A:ILE:HG13	1:99:A:SER:H	12	0.34
(1,81)	1:28:A:CYS:HA	1:33:A:ASP:H	11	0.34
(1,80)	1:44:A:CYS:HB2	1:45:A:ARG:H	19	0.34
(1,80)	1:44:A:CYS:HB3	1:45:A:ARG:H	19	0.34
(1,73)	1:65:A:CYS:HB2	1:65:A:CYS:H	17	0.34
(1,73)	1:65:A:CYS:HB3	1:65:A:CYS:H	17	0.34
(1,60)	1:56:A:THR:H	1:57:A:GLN:H	15	0.34
(1,54)	1:73:A:SER:H	1:74:A:GLY:H	6	0.34
(1,28)	1:118:A:ASP:H	1:117:A:LEU:H	19	0.34
(1,24)	1:104:A:CYS:H	1:105:A:ASN:H	13	0.34
(1,24)	1:104:A:CYS:H	1:105:A:ASN:H	20	0.34
(1,23)	1:104:A:CYS:H	1:105:A:ASN:H	13	0.34
(1,23)	1:104:A:CYS:H	1:105:A:ASN:H	20	0.34
(1,14)	1:110:A:CYS:H	1:109:A:ASP:H	18	0.34
(1,14)	1:110:A:CYS:H	1:109:A:ASP:H	20	0.34
(4,8)	1:8:A:PHE:O	1:16:A:VAL:H	4	0.33
(4,8)	1:8:A:PHE:O	1:16:A:VAL:H	8	0.33
(4,8)	1:8:A:PHE:O	1:16:A:VAL:H	14	0.33
(2,376)	1:87:A:PRO:HB2	1:88:A:ASP:H	19	0.33
(2,313)	1:17:A:PRO:HB2	1:20:A:TRP:H	15	0.33
(2,298)	1:28:A:CYS:HB3	1:14:A:GLN:HE22	9	0.33
(2,257)	1:33:A:ASP:HA	1:38:A:GLN:HE22	10	0.33
(2,257)	1:33:A:ASP:HA	1:38:A:GLN:HE22	17	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,245)	1:36:A:PRO:HA	1:39:A:CYS:H	2	0.33
(2,188)	1:16:A:VAL:HG11	1:19:A:ARG:H	1	0.33
(2,188)	1:16:A:VAL:HG12	1:19:A:ARG:H	1	0.33
(2,188)	1:16:A:VAL:HG13	1:19:A:ARG:H	1	0.33
(2,188)	1:16:A:VAL:HG21	1:19:A:ARG:H	1	0.33
(2,188)	1:16:A:VAL:HG22	1:19:A:ARG:H	1	0.33
(2,188)	1:16:A:VAL:HG23	1:19:A:ARG:H	1	0.33
(2,188)	1:16:A:VAL:HG11	1:19:A:ARG:H	11	0.33
(2,188)	1:16:A:VAL:HG12	1:19:A:ARG:H	11	0.33
(2,188)	1:16:A:VAL:HG13	1:19:A:ARG:H	11	0.33
(2,188)	1:16:A:VAL:HG21	1:19:A:ARG:H	11	0.33
(2,188)	1:16:A:VAL:HG22	1:19:A:ARG:H	11	0.33
(2,188)	1:16:A:VAL:HG23	1:19:A:ARG:H	11	0.33
(2,114)	1:16:A:VAL:HG11	1:16:A:VAL:H	15	0.33
(2,114)	1:16:A:VAL:HG12	1:16:A:VAL:H	15	0.33
(2,114)	1:16:A:VAL:HG13	1:16:A:VAL:H	15	0.33
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	15	0.33
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	15	0.33
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	15	0.33
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	15	0.33
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	15	0.33
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	15	0.33
(2,39)	1:117:A:LEU:HD11	1:115:A:ASP:H	15	0.33
(2,38)	1:96:A:ARG:HB3	1:97:A:CYS:H	15	0.33
(2,38)	1:96:A:ARG:HB3	1:97:A:CYS:H	17	0.33
(2,25)	1:79:A:ASN:HD22	1:80:A:CYS:HA	15	0.33
(2,20)	1:82:A:ASN:H	1:83:A:ILE:H	16	0.33
(2,12)	1:10:A:CYS:HB2	1:13:A:GLY:H	8	0.33
(2,4)	1:46:A:ILE:HG22	1:46:A:ILE:H	6	0.33
(1,907)	1:39:A:CYS:H	1:41:A:MET:H	6	0.33
(1,907)	1:39:A:CYS:H	1:41:A:MET:H	7	0.33
(1,896)	1:64:A:ARG:H	1:66:A:ASP:H	10	0.33
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB2	9	0.33
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB3	9	0.33
(1,888)	1:49:A:ILE:HA	1:61:A:VAL:H	20	0.33
(1,872)	1:32:A:SER:H	1:33:A:ASP:HB2	8	0.33
(1,872)	1:32:A:SER:H	1:33:A:ASP:HB3	8	0.33
(1,863)	1:17:A:PRO:HD2	1:20:A:TRP:HE1	8	0.33
(1,863)	1:17:A:PRO:HD3	1:20:A:TRP:HE1	8	0.33
(1,837)	1:50:A:SER:H	1:45:A:ARG:HD2	1	0.33
(1,837)	1:50:A:SER:H	1:45:A:ARG:HD3	1	0.33
(1,837)	1:50:A:SER:H	1:45:A:ARG:HD2	7	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,837)	1:50:A:SER:H	1:45:A:ARG:HD3	7	0.33
(1,833)	1:42:A:ARG:HG2	1:41:A:MET:H	8	0.33
(1,833)	1:42:A:ARG:HG2	1:41:A:MET:H	8	0.33
(1,833)	1:42:A:ARG:HG3	1:41:A:MET:H	8	0.33
(1,833)	1:42:A:ARG:HG3	1:41:A:MET:H	8	0.33
(1,821)	1:117:A:LEU:HD11	1:116:A:GLU:H	5	0.33
(1,821)	1:117:A:LEU:HD11	1:116:A:GLU:H	5	0.33
(1,821)	1:117:A:LEU:HD12	1:116:A:GLU:H	5	0.33
(1,821)	1:117:A:LEU:HD12	1:116:A:GLU:H	5	0.33
(1,821)	1:117:A:LEU:HD13	1:116:A:GLU:H	5	0.33
(1,821)	1:117:A:LEU:HD13	1:116:A:GLU:H	5	0.33
(1,821)	1:117:A:LEU:HD21	1:116:A:GLU:H	5	0.33
(1,821)	1:117:A:LEU:HD21	1:116:A:GLU:H	5	0.33
(1,821)	1:117:A:LEU:HD22	1:116:A:GLU:H	5	0.33
(1,821)	1:117:A:LEU:HD22	1:116:A:GLU:H	5	0.33
(1,821)	1:117:A:LEU:HD23	1:116:A:GLU:H	5	0.33
(1,821)	1:117:A:LEU:HD23	1:116:A:GLU:H	5	0.33
(1,807)	1:98:A:ILE:HG12	1:103:A:VAL:H	16	0.33
(1,807)	1:98:A:ILE:HG13	1:103:A:VAL:H	16	0.33
(1,806)	1:101:A:ASN:HD21	1:102:A:PHE:H	1	0.33
(1,801)	1:102:A:PHE:HB2	1:98:A:ILE:H	2	0.33
(1,801)	1:102:A:PHE:HB3	1:98:A:ILE:H	2	0.33
(1,800)	1:85:A:CYS:HB2	1:98:A:ILE:H	5	0.33
(1,800)	1:85:A:CYS:HB3	1:98:A:ILE:H	5	0.33
(1,788)	1:80:A:CYS:H	1:78:A:GLU:H	18	0.33
(1,777)	1:77:A:GLU:HB2	1:70:A:ASP:H	14	0.33
(1,777)	1:77:A:GLU:HB3	1:70:A:ASP:H	14	0.33
(1,772)	1:68:A:GLU:H	1:64:A:ARG:H	1	0.33
(1,768)	1:58:A:CYS:HA	1:59:A:ILE:H	12	0.33
(1,768)	1:58:A:CYS:HA	1:59:A:ILE:H	15	0.33
(1,759)	1:57:A:GLN:HE21	1:71:A:CYS:HA	8	0.33
(1,759)	1:57:A:GLN:HE21	1:71:A:CYS:HA	12	0.33
(1,733)	1:32:A:SER:H	1:28:A:CYS:H	9	0.33
(1,729)	1:32:A:SER:H	1:28:A:CYS:H	9	0.33
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD2	10	0.33
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD3	10	0.33
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD2	11	0.33
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD3	11	0.33
(1,696)	1:44:A:CYS:HB2	1:34:A:GLU:H	16	0.33
(1,696)	1:44:A:CYS:HB3	1:34:A:GLU:H	16	0.33
(1,667)	1:107:A:GLN:HG2	1:105:A:ASN:HD22	8	0.33
(1,667)	1:107:A:GLN:HG2	1:105:A:ASN:HD22	8	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,667)	1:107:A:GLN:HG3	1:105:A:ASN:HD22	8	0.33
(1,667)	1:107:A:GLN:HG3	1:105:A:ASN:HD22	8	0.33
(1,642)	1:82:A:ASN:HA	1:82:A:ASN:HD22	18	0.33
(1,628)	1:71:A:CYS:HB2	1:57:A:GLN:HE22	13	0.33
(1,628)	1:71:A:CYS:HB3	1:57:A:GLN:HE22	13	0.33
(1,534)	1:77:A:GLU:HB2	1:77:A:GLU:H	2	0.33
(1,534)	1:77:A:GLU:HB3	1:77:A:GLU:H	2	0.33
(1,531)	1:71:A:CYS:HB2	1:71:A:CYS:H	15	0.33
(1,531)	1:71:A:CYS:HB3	1:71:A:CYS:H	15	0.33
(1,526)	1:64:A:ARG:H	1:67:A:GLY:H	4	0.33
(1,459)	1:70:A:ASP:HA	1:76:A:ASP:H	4	0.33
(1,436)	1:73:A:SER:H	1:72:A:ASP:H	11	0.33
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB1	14	0.33
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB2	14	0.33
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB3	14	0.33
(1,386)	1:51:A:CYS:HB2	1:51:A:CYS:H	8	0.33
(1,386)	1:51:A:CYS:HB3	1:51:A:CYS:H	8	0.33
(1,376)	1:49:A:ILE:HA	1:49:A:ILE:H	4	0.33
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB2	20	0.33
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB3	20	0.33
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB2	6	0.33
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB3	6	0.33
(1,320)	1:7:A:ASP:HA	1:18:A:SER:H	13	0.33
(1,320)	1:7:A:ASP:HA	1:18:A:SER:H	15	0.33
(1,189)	1:101:A:ASN:HB2	1:101:A:ASN:H	4	0.33
(1,189)	1:101:A:ASN:HB3	1:101:A:ASN:H	4	0.33
(1,174)	1:103:A:VAL:H	1:101:A:ASN:HB2	8	0.33
(1,174)	1:103:A:VAL:H	1:101:A:ASN:HB3	8	0.33
(1,158)	1:104:A:CYS:HA	1:105:A:ASN:H	8	0.33
(1,158)	1:104:A:CYS:HA	1:105:A:ASN:H	10	0.33
(1,158)	1:104:A:CYS:HA	1:105:A:ASN:H	13	0.33
(1,99)	1:98:A:ILE:HG12	1:99:A:SER:H	20	0.33
(1,99)	1:98:A:ILE:HG13	1:99:A:SER:H	20	0.33
(1,85)	1:21:A:LYS:HG2	1:22:A:CYS:H	6	0.33
(1,85)	1:21:A:LYS:HG3	1:22:A:CYS:H	6	0.33
(1,85)	1:21:A:LYS:HG2	1:22:A:CYS:H	12	0.33
(1,85)	1:21:A:LYS:HG3	1:22:A:CYS:H	12	0.33
(1,81)	1:28:A:CYS:HA	1:33:A:ASP:H	5	0.33
(1,69)	1:78:A:GLU:HG2	1:78:A:GLU:H	10	0.33
(1,69)	1:78:A:GLU:HG3	1:78:A:GLU:H	10	0.33
(1,66)	1:23:A:ASP:H	1:24:A:GLY:H	19	0.33
(1,55)	1:71:A:CYS:H	1:70:A:ASP:H	9	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,17)	1:81:A:GLY:H	1:80:A:CYS:H	12	0.33
(4,7)	1:8:A:PHE:H	1:16:A:VAL:O	10	0.32
(4,7)	1:8:A:PHE:H	1:16:A:VAL:O	12	0.32
(4,5)	1:49:A:ILE:O	1:59:A:ILE:H	19	0.32
(4,2)	1:90:A:PHE:O	1:98:A:ILE:H	4	0.32
(2,376)	1:87:A:PRO:HB2	1:88:A:ASP:H	4	0.32
(2,376)	1:87:A:PRO:HB2	1:88:A:ASP:H	9	0.32
(2,366)	1:107:A:GLN:HA	1:106:A:GLY:H	10	0.32
(2,329)	1:90:A:PHE:HA	1:98:A:ILE:H	2	0.32
(2,298)	1:28:A:CYS:HB2	1:14:A:GLN:HE22	5	0.32
(2,210)	1:33:A:ASP:HA	1:38:A:GLN:HE21	2	0.32
(2,190)	1:56:A:THR:HA	1:57:A:GLN:H	11	0.32
(2,188)	1:16:A:VAL:HG11	1:19:A:ARG:H	20	0.32
(2,188)	1:16:A:VAL:HG12	1:19:A:ARG:H	20	0.32
(2,188)	1:16:A:VAL:HG13	1:19:A:ARG:H	20	0.32
(2,188)	1:16:A:VAL:HG21	1:19:A:ARG:H	20	0.32
(2,188)	1:16:A:VAL:HG22	1:19:A:ARG:H	20	0.32
(2,188)	1:16:A:VAL:HG23	1:19:A:ARG:H	20	0.32
(2,154)	1:116:A:GLU:HG3	1:109:A:ASP:H	2	0.32
(2,135)	1:79:A:ASN:HB2	1:79:A:ASN:HD21	19	0.32
(2,135)	1:79:A:ASN:HB2	1:79:A:ASN:HD21	20	0.32
(2,89)	1:107:A:GLN:HB2	1:108:A:ASP:H	4	0.32
(2,89)	1:107:A:GLN:HB3	1:108:A:ASP:H	4	0.32
(2,38)	1:96:A:ARG:HB3	1:97:A:CYS:H	12	0.32
(2,38)	1:96:A:ARG:HB3	1:97:A:CYS:H	18	0.32
(2,31)	1:59:A:ILE:HD13	1:71:A:CYS:H	13	0.32
(2,11)	1:110:A:CYS:HA	1:113:A:GLY:H	9	0.32
(1,907)	1:39:A:CYS:H	1:41:A:MET:H	14	0.32
(1,907)	1:39:A:CYS:H	1:41:A:MET:H	15	0.32
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB2	20	0.32
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB3	20	0.32
(1,888)	1:49:A:ILE:HA	1:61:A:VAL:H	9	0.32
(1,871)	1:30:A:ASP:HB2	1:32:A:SER:H	5	0.32
(1,871)	1:30:A:ASP:HB3	1:32:A:SER:H	5	0.32
(1,863)	1:17:A:PRO:HD2	1:20:A:TRP:HE1	12	0.32
(1,863)	1:17:A:PRO:HD3	1:20:A:TRP:HE1	12	0.32
(1,860)	1:16:A:VAL:HB	1:19:A:ARG:H	1	0.32
(1,808)	1:116:A:GLU:HB2	1:104:A:CYS:H	11	0.32
(1,808)	1:116:A:GLU:HB3	1:104:A:CYS:H	11	0.32
(1,806)	1:101:A:ASN:HD21	1:102:A:PHE:H	8	0.32
(1,801)	1:102:A:PHE:HB2	1:98:A:ILE:H	1	0.32
(1,801)	1:102:A:PHE:HB3	1:98:A:ILE:H	1	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,801)	1:102:A:PHE:HB2	1:98:A:ILE:H	11	0.32
(1,801)	1:102:A:PHE:HB3	1:98:A:ILE:H	11	0.32
(1,799)	1:85:A:CYS:HA	1:97:A:CYS:H	4	0.32
(1,797)	1:91:A:THR:HG22	1:96:A:ARG:H	8	0.32
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG21	7	0.32
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG22	7	0.32
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG23	7	0.32
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG21	19	0.32
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG22	19	0.32
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG23	19	0.32
(1,789)	1:85:A:CYS:H	1:84:A:THR:HB	2	0.32
(1,789)	1:85:A:CYS:H	1:84:A:THR:HB	11	0.32
(1,783)	1:71:A:CYS:HB2	1:74:A:GLY:H	5	0.32
(1,783)	1:71:A:CYS:HB3	1:74:A:GLY:H	5	0.32
(1,783)	1:71:A:CYS:HB2	1:74:A:GLY:H	15	0.32
(1,783)	1:71:A:CYS:HB3	1:74:A:GLY:H	15	0.32
(1,783)	1:71:A:CYS:HB2	1:74:A:GLY:H	19	0.32
(1,783)	1:71:A:CYS:HB3	1:74:A:GLY:H	19	0.32
(1,768)	1:58:A:CYS:HA	1:59:A:ILE:H	4	0.32
(1,759)	1:57:A:GLN:HE21	1:71:A:CYS:HA	15	0.32
(1,744)	1:48:A:GLU:H	1:47:A:HIS:H	15	0.32
(1,735)	1:28:A:CYS:HB2	1:33:A:ASP:H	1	0.32
(1,735)	1:28:A:CYS:HB3	1:33:A:ASP:H	1	0.32
(1,735)	1:28:A:CYS:HB2	1:33:A:ASP:H	6	0.32
(1,735)	1:28:A:CYS:HB3	1:33:A:ASP:H	6	0.32
(1,733)	1:32:A:SER:H	1:28:A:CYS:H	1	0.32
(1,729)	1:32:A:SER:H	1:28:A:CYS:H	1	0.32
(1,724)	1:34:A:GLU:HB2	1:25:A:ASP:H	4	0.32
(1,724)	1:34:A:GLU:HB3	1:25:A:ASP:H	4	0.32
(1,711)	1:10:A:CYS:HB2	1:11:A:ASN:H	9	0.32
(1,711)	1:10:A:CYS:HB3	1:11:A:ASN:H	9	0.32
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD2	1	0.32
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD3	1	0.32
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD2	6	0.32
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD3	6	0.32
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD2	19	0.32
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD3	19	0.32
(1,704)	1:100:A:ARG:HG2	1:100:A:ARG:H	3	0.32
(1,704)	1:100:A:ARG:HG2	1:100:A:ARG:H	3	0.32
(1,704)	1:100:A:ARG:HG3	1:100:A:ARG:H	3	0.32
(1,704)	1:100:A:ARG:HG3	1:100:A:ARG:H	3	0.32
(1,704)	1:100:A:ARG:HG2	1:100:A:ARG:H	7	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,704)	1:100:A:ARG:HG2	1:100:A:ARG:H	7	0.32
(1,704)	1:100:A:ARG:HG3	1:100:A:ARG:H	7	0.32
(1,704)	1:100:A:ARG:HG3	1:100:A:ARG:H	7	0.32
(1,674)	1:17:A:PRO:HG2	1:20:A:TRP:HE1	11	0.32
(1,674)	1:17:A:PRO:HG3	1:20:A:TRP:HE1	11	0.32
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	18	0.32
(1,643)	1:82:A:ASN:HB2	1:82:A:ASN:HD21	18	0.32
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	18	0.32
(1,643)	1:82:A:ASN:HB3	1:82:A:ASN:HD21	18	0.32
(1,596)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	11	0.32
(1,596)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	11	0.32
(1,596)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	16	0.32
(1,596)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	16	0.32
(1,592)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	14	0.32
(1,592)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	14	0.32
(1,585)	1:28:A:CYS:H	1:27:A:ASP:H	12	0.32
(1,562)	1:102:A:PHE:HB2	1:99:A:SER:H	9	0.32
(1,562)	1:102:A:PHE:HB3	1:99:A:SER:H	9	0.32
(1,518)	1:49:A:ILE:H	1:61:A:VAL:H	9	0.32
(1,479)	1:9:A:VAL:HG11	1:9:A:VAL:H	9	0.32
(1,479)	1:9:A:VAL:HG12	1:9:A:VAL:H	9	0.32
(1,479)	1:9:A:VAL:HG13	1:9:A:VAL:H	9	0.32
(1,479)	1:9:A:VAL:HG21	1:9:A:VAL:H	9	0.32
(1,479)	1:9:A:VAL:HG22	1:9:A:VAL:H	9	0.32
(1,479)	1:9:A:VAL:HG23	1:9:A:VAL:H	9	0.32
(1,463)	1:71:A:CYS:HB2	1:78:A:GLU:H	14	0.32
(1,463)	1:71:A:CYS:HB3	1:78:A:GLU:H	14	0.32
(1,454)	1:78:A:GLU:HG2	1:76:A:ASP:H	7	0.32
(1,454)	1:78:A:GLU:HG3	1:76:A:ASP:H	7	0.32
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB2	12	0.32
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB3	12	0.32
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB1	4	0.32
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB2	4	0.32
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB3	4	0.32
(1,386)	1:51:A:CYS:HB2	1:51:A:CYS:H	10	0.32
(1,386)	1:51:A:CYS:HB3	1:51:A:CYS:H	10	0.32
(1,375)	1:48:A:GLU:HA	1:49:A:ILE:H	4	0.32
(1,375)	1:48:A:GLU:HA	1:49:A:ILE:H	10	0.32
(1,365)	1:43:A:THR:HB	1:43:A:THR:H	6	0.32
(1,365)	1:43:A:THR:HB	1:43:A:THR:H	7	0.32
(1,365)	1:43:A:THR:HB	1:43:A:THR:H	20	0.32
(1,347)	1:31:A:GLY:H	1:28:A:CYS:H	7	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB2	14	0.32
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB3	14	0.32
(1,281)	1:5:A:GLU:HB2	1:6:A:SER:H	1	0.32
(1,281)	1:5:A:GLU:HB2	1:6:A:SER:H	1	0.32
(1,281)	1:5:A:GLU:HB3	1:6:A:SER:H	1	0.32
(1,281)	1:5:A:GLU:HB3	1:6:A:SER:H	1	0.32
(1,281)	1:5:A:GLU:HB2	1:6:A:SER:H	8	0.32
(1,281)	1:5:A:GLU:HB2	1:6:A:SER:H	8	0.32
(1,281)	1:5:A:GLU:HB3	1:6:A:SER:H	8	0.32
(1,281)	1:5:A:GLU:HB3	1:6:A:SER:H	8	0.32
(1,248)	1:83:A:ILE:HB	1:84:A:THR:H	9	0.32
(1,224)	1:92:A:CYS:HA	1:94:A:SER:H	10	0.32
(1,203)	1:89:A:GLU:HB2	1:98:A:ILE:H	3	0.32
(1,203)	1:89:A:GLU:HB3	1:98:A:ILE:H	3	0.32
(1,203)	1:89:A:GLU:HB2	1:98:A:ILE:H	11	0.32
(1,203)	1:89:A:GLU:HB3	1:98:A:ILE:H	11	0.32
(1,189)	1:101:A:ASN:HB2	1:101:A:ASN:H	5	0.32
(1,189)	1:101:A:ASN:HB3	1:101:A:ASN:H	5	0.32
(1,187)	1:103:A:VAL:HG11	1:102:A:PHE:H	9	0.32
(1,187)	1:103:A:VAL:HG12	1:102:A:PHE:H	9	0.32
(1,187)	1:103:A:VAL:HG13	1:102:A:PHE:H	9	0.32
(1,187)	1:103:A:VAL:HG21	1:102:A:PHE:H	9	0.32
(1,187)	1:103:A:VAL:HG22	1:102:A:PHE:H	9	0.32
(1,187)	1:103:A:VAL:HG23	1:102:A:PHE:H	9	0.32
(1,174)	1:103:A:VAL:H	1:101:A:ASN:HB2	1	0.32
(1,174)	1:103:A:VAL:H	1:101:A:ASN:HB3	1	0.32
(1,165)	1:104:A:CYS:H	1:116:A:GLU:HA	5	0.32
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB2	7	0.32
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB3	7	0.32
(1,99)	1:98:A:ILE:HG12	1:99:A:SER:H	15	0.32
(1,99)	1:98:A:ILE:HG13	1:99:A:SER:H	15	0.32
(1,98)	1:98:A:ILE:HG12	1:99:A:SER:H	18	0.32
(1,98)	1:98:A:ILE:HG13	1:99:A:SER:H	18	0.32
(1,97)	1:98:A:ILE:HD11	1:99:A:SER:H	10	0.32
(1,97)	1:98:A:ILE:HD12	1:99:A:SER:H	10	0.32
(1,97)	1:98:A:ILE:HD13	1:99:A:SER:H	10	0.32
(1,93)	1:8:A:PHE:H	1:7:A:ASP:HA	1	0.32
(1,93)	1:8:A:PHE:H	1:7:A:ASP:HA	19	0.32
(1,49)	1:94:A:SER:H	1:93:A:SER:H	18	0.32
(1,28)	1:118:A:ASP:H	1:117:A:LEU:H	1	0.32
(1,17)	1:81:A:GLY:H	1:80:A:CYS:H	7	0.32
(1,9)	1:12:A:ASN:H	1:11:A:ASN:H	17	0.32

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,7)	1:8:A:PHE:H	1:16:A:VAL:O	14	0.31
(2,394)	1:86:A:SER:HB2	1:86:A:SER:H	16	0.31
(2,381)	1:100:A:ARG:HD3	1:90:A:PHE:H	12	0.31
(2,376)	1:87:A:PRO:HB2	1:88:A:ASP:H	14	0.31
(2,366)	1:107:A:GLN:HA	1:106:A:GLY:H	8	0.31
(2,366)	1:116:A:GLU:HA	1:106:A:GLY:H	16	0.31
(2,363)	1:49:A:ILE:HB	1:49:A:ILE:H	12	0.31
(2,341)	1:78:A:GLU:HG3	1:78:A:GLU:H	10	0.31
(2,331)	1:101:A:ASN:H	1:99:A:SER:H	1	0.31
(2,264)	1:49:A:ILE:HB	1:50:A:SER:H	8	0.31
(2,245)	1:36:A:PRO:HA	1:39:A:CYS:H	12	0.31
(2,218)	1:36:A:PRO:HD2	1:37:A:GLU:H	10	0.31
(2,190)	1:56:A:THR:HA	1:57:A:GLN:H	3	0.31
(2,190)	1:56:A:THR:HA	1:57:A:GLN:H	12	0.31
(2,190)	1:56:A:THR:HA	1:57:A:GLN:H	14	0.31
(2,188)	1:16:A:VAL:HG11	1:19:A:ARG:H	16	0.31
(2,188)	1:16:A:VAL:HG12	1:19:A:ARG:H	16	0.31
(2,188)	1:16:A:VAL:HG13	1:19:A:ARG:H	16	0.31
(2,188)	1:16:A:VAL:HG21	1:19:A:ARG:H	16	0.31
(2,188)	1:16:A:VAL:HG22	1:19:A:ARG:H	16	0.31
(2,188)	1:16:A:VAL:HG23	1:19:A:ARG:H	16	0.31
(2,164)	1:14:A:GLN:HB2	1:14:A:GLN:H	2	0.31
(2,164)	1:14:A:GLN:HB3	1:14:A:GLN:H	2	0.31
(2,80)	1:41:A:MET:HA	1:56:A:THR:H	14	0.31
(2,46)	1:114:A:SER:HG	1:115:A:ASP:H	18	0.31
(2,38)	1:96:A:ARG:HB3	1:97:A:CYS:H	14	0.31
(2,33)	1:81:A:GLY:HA2	1:80:A:CYS:H	8	0.31
(2,31)	1:59:A:ILE:HD11	1:71:A:CYS:H	18	0.31
(2,29)	1:28:A:CYS:HA	1:29:A:GLU:H	7	0.31
(1,916)	1:77:A:GLU:HB2	1:77:A:GLU:H	17	0.31
(1,916)	1:77:A:GLU:HB3	1:77:A:GLU:H	17	0.31
(1,911)	1:57:A:GLN:HE21	1:71:A:CYS:H	1	0.31
(1,896)	1:64:A:ARG:H	1:66:A:ASP:H	6	0.31
(1,895)	1:77:A:GLU:HG2	1:66:A:ASP:H	17	0.31
(1,895)	1:77:A:GLU:HG3	1:66:A:ASP:H	17	0.31
(1,894)	1:66:A:ASP:H	1:77:A:GLU:HG2	17	0.31
(1,894)	1:66:A:ASP:H	1:77:A:GLU:HG3	17	0.31
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB2	3	0.31
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB3	3	0.31
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB2	5	0.31
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB3	5	0.31
(1,881)	1:48:A:GLU:H	1:45:A:ARG:H	3	0.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,879)	1:48:A:GLU:H	1:45:A:ARG:H	3	0.31
(1,863)	1:17:A:PRO:HD2	1:20:A:TRP:HE1	18	0.31
(1,863)	1:17:A:PRO:HD3	1:20:A:TRP:HE1	18	0.31
(1,862)	1:21:A:LYS:HE2	1:19:A:ARG:H	17	0.31
(1,862)	1:21:A:LYS:HE3	1:19:A:ARG:H	17	0.31
(1,849)	1:33:A:ASP:H	1:11:A:ASN:H	10	0.31
(1,840)	1:71:A:CYS:HB2	1:77:A:GLU:H	20	0.31
(1,840)	1:71:A:CYS:HB3	1:77:A:GLU:H	20	0.31
(1,831)	1:73:A:SER:H	1:75:A:GLU:H	3	0.31
(1,831)	1:73:A:SER:H	1:75:A:GLU:H	8	0.31
(1,803)	1:101:A:ASN:HD21	1:99:A:SER:H	4	0.31
(1,801)	1:102:A:PHE:HB2	1:98:A:ILE:H	15	0.31
(1,801)	1:102:A:PHE:HB3	1:98:A:ILE:H	15	0.31
(1,791)	1:85:A:CYS:HB2	1:89:A:GLU:H	17	0.31
(1,791)	1:85:A:CYS:HB3	1:89:A:GLU:H	17	0.31
(1,768)	1:58:A:CYS:HA	1:59:A:ILE:H	18	0.31
(1,744)	1:48:A:GLU:H	1:47:A:HIS:H	3	0.31
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD2	2	0.31
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD3	2	0.31
(1,704)	1:100:A:ARG:HG2	1:100:A:ARG:H	10	0.31
(1,704)	1:100:A:ARG:HG2	1:100:A:ARG:H	10	0.31
(1,704)	1:100:A:ARG:HG3	1:100:A:ARG:H	10	0.31
(1,704)	1:100:A:ARG:HG3	1:100:A:ARG:H	10	0.31
(1,690)	1:61:A:VAL:HG11	1:49:A:ILE:H	15	0.31
(1,690)	1:61:A:VAL:HG12	1:49:A:ILE:H	15	0.31
(1,690)	1:61:A:VAL:HG13	1:49:A:ILE:H	15	0.31
(1,690)	1:61:A:VAL:HG21	1:49:A:ILE:H	15	0.31
(1,690)	1:61:A:VAL:HG22	1:49:A:ILE:H	15	0.31
(1,690)	1:61:A:VAL:HG23	1:49:A:ILE:H	15	0.31
(1,688)	1:69:A:ASN:H	1:69:A:ASN:HD22	17	0.31
(1,636)	1:78:A:GLU:HB2	1:79:A:ASN:HD22	10	0.31
(1,636)	1:78:A:GLU:HB2	1:79:A:ASN:HD22	10	0.31
(1,636)	1:78:A:GLU:HB3	1:79:A:ASN:HD22	10	0.31
(1,636)	1:78:A:GLU:HB3	1:79:A:ASN:HD22	10	0.31
(1,628)	1:71:A:CYS:HB2	1:57:A:GLN:HE22	7	0.31
(1,628)	1:71:A:CYS:HB3	1:57:A:GLN:HE22	7	0.31
(1,598)	1:74:A:GLY:HA2	1:69:A:ASN:HD22	17	0.31
(1,598)	1:74:A:GLY:HA3	1:69:A:ASN:HD22	17	0.31
(1,597)	1:74:A:GLY:HA2	1:69:A:ASN:HD22	17	0.31
(1,597)	1:74:A:GLY:HA3	1:69:A:ASN:HD22	17	0.31
(1,592)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	13	0.31
(1,592)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	13	0.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,555)	1:103:A:VAL:HG11	1:104:A:CYS:H	4	0.31
(1,555)	1:103:A:VAL:HG12	1:104:A:CYS:H	4	0.31
(1,555)	1:103:A:VAL:HG13	1:104:A:CYS:H	4	0.31
(1,555)	1:103:A:VAL:HG21	1:104:A:CYS:H	4	0.31
(1,555)	1:103:A:VAL:HG22	1:104:A:CYS:H	4	0.31
(1,555)	1:103:A:VAL:HG23	1:104:A:CYS:H	4	0.31
(1,555)	1:103:A:VAL:HG11	1:104:A:CYS:H	7	0.31
(1,555)	1:103:A:VAL:HG12	1:104:A:CYS:H	7	0.31
(1,555)	1:103:A:VAL:HG13	1:104:A:CYS:H	7	0.31
(1,555)	1:103:A:VAL:HG21	1:104:A:CYS:H	7	0.31
(1,555)	1:103:A:VAL:HG22	1:104:A:CYS:H	7	0.31
(1,555)	1:103:A:VAL:HG23	1:104:A:CYS:H	7	0.31
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	4	0.31
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	4	0.31
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	4	0.31
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	4	0.31
(1,486)	1:7:A:ASP:HA	1:19:A:ARG:H	17	0.31
(1,466)	1:80:A:CYS:HA	1:79:A:ASN:H	2	0.31
(1,454)	1:78:A:GLU:HG2	1:76:A:ASP:H	20	0.31
(1,454)	1:78:A:GLU:HG3	1:76:A:ASP:H	20	0.31
(1,436)	1:73:A:SER:H	1:72:A:ASP:H	7	0.31
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB1	15	0.31
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB2	15	0.31
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB3	15	0.31
(1,386)	1:51:A:CYS:HB2	1:51:A:CYS:H	20	0.31
(1,386)	1:51:A:CYS:HB3	1:51:A:CYS:H	20	0.31
(1,375)	1:48:A:GLU:HA	1:49:A:ILE:H	12	0.31
(1,351)	1:32:A:SER:H	1:33:A:ASP:H	4	0.31
(1,350)	1:31:A:GLY:H	1:32:A:SER:H	19	0.31
(1,349)	1:32:A:SER:H	1:33:A:ASP:H	4	0.31
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB2	4	0.31
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB3	4	0.31
(1,335)	1:45:A:ARG:HD2	1:24:A:GLY:H	18	0.31
(1,335)	1:45:A:ARG:HD3	1:24:A:GLY:H	18	0.31
(1,298)	1:14:A:GLN:H	1:11:A:ASN:H	14	0.31
(1,298)	1:14:A:GLN:H	1:11:A:ASN:H	18	0.31
(1,296)	1:10:A:CYS:HB2	1:10:A:CYS:H	2	0.31
(1,296)	1:10:A:CYS:HB3	1:10:A:CYS:H	2	0.31
(1,296)	1:10:A:CYS:HB2	1:10:A:CYS:H	18	0.31
(1,296)	1:10:A:CYS:HB3	1:10:A:CYS:H	18	0.31
(1,286)	1:7:A:ASP:HB2	1:7:A:ASP:H	13	0.31
(1,286)	1:7:A:ASP:HB3	1:7:A:ASP:H	13	0.31

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,281)	1:5:A:GLU:HB2	1:6:A:SER:H	3	0.31
(1,281)	1:5:A:GLU:HB2	1:6:A:SER:H	3	0.31
(1,281)	1:5:A:GLU:HB3	1:6:A:SER:H	3	0.31
(1,281)	1:5:A:GLU:HB3	1:6:A:SER:H	3	0.31
(1,226)	1:92:A:CYS:HB2	1:94:A:SER:H	10	0.31
(1,226)	1:92:A:CYS:HB3	1:94:A:SER:H	10	0.31
(1,205)	1:98:A:ILE:HG12	1:98:A:ILE:H	4	0.31
(1,205)	1:98:A:ILE:HG13	1:98:A:ILE:H	4	0.31
(1,205)	1:98:A:ILE:HG12	1:98:A:ILE:H	7	0.31
(1,205)	1:98:A:ILE:HG13	1:98:A:ILE:H	7	0.31
(1,205)	1:98:A:ILE:HG12	1:98:A:ILE:H	12	0.31
(1,205)	1:98:A:ILE:HG13	1:98:A:ILE:H	12	0.31
(1,174)	1:103:A:VAL:H	1:101:A:ASN:HB2	2	0.31
(1,174)	1:103:A:VAL:H	1:101:A:ASN:HB3	2	0.31
(1,158)	1:104:A:CYS:HA	1:105:A:ASN:H	18	0.31
(1,98)	1:98:A:ILE:HG12	1:99:A:SER:H	11	0.31
(1,98)	1:98:A:ILE:HG13	1:99:A:SER:H	11	0.31
(1,85)	1:21:A:LYS:HG2	1:22:A:CYS:H	18	0.31
(1,85)	1:21:A:LYS:HG3	1:22:A:CYS:H	18	0.31
(1,66)	1:23:A:ASP:H	1:24:A:GLY:H	8	0.31
(1,60)	1:56:A:THR:H	1:57:A:GLN:H	19	0.31
(1,55)	1:71:A:CYS:H	1:70:A:ASP:H	11	0.31
(1,55)	1:71:A:CYS:H	1:70:A:ASP:H	13	0.31
(1,28)	1:118:A:ASP:H	1:117:A:LEU:H	2	0.31
(1,28)	1:118:A:ASP:H	1:117:A:LEU:H	8	0.31
(1,28)	1:118:A:ASP:H	1:117:A:LEU:H	10	0.31
(1,18)	1:81:A:GLY:H	1:82:A:ASN:H	12	0.31
(1,14)	1:110:A:CYS:H	1:109:A:ASP:H	15	0.31
(1,6)	1:23:A:ASP:H	1:24:A:GLY:H	15	0.31
(4,5)	1:49:A:ILE:O	1:59:A:ILE:H	3	0.3
(4,5)	1:49:A:ILE:O	1:59:A:ILE:H	17	0.3
(4,2)	1:90:A:PHE:O	1:98:A:ILE:H	14	0.3
(2,376)	1:87:A:PRO:HB2	1:88:A:ASP:H	18	0.3
(2,363)	1:49:A:ILE:HB	1:49:A:ILE:H	10	0.3
(2,330)	1:114:A:SER:HG	1:93:A:SER:H	17	0.3
(2,322)	1:69:A:ASN:HB3	1:71:A:CYS:H	18	0.3
(2,313)	1:17:A:PRO:HB2	1:20:A:TRP:H	20	0.3
(2,298)	1:28:A:CYS:HB2	1:14:A:GLN:HE22	10	0.3
(2,210)	1:33:A:ASP:HA	1:38:A:GLN:HE21	4	0.3
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	16	0.3
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	16	0.3
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	16	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	16	0.3
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	16	0.3
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	16	0.3
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	16	0.3
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	16	0.3
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	16	0.3
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	16	0.3
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	16	0.3
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	16	0.3
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	16	0.3
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	16	0.3
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	16	0.3
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	16	0.3
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	16	0.3
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	16	0.3
(2,166)	1:86:A:SER:HA	1:79:A:ASN:HD21	8	0.3
(2,135)	1:79:A:ASN:HB2	1:79:A:ASN:HD21	16	0.3
(2,114)	1:16:A:VAL:HG11	1:16:A:VAL:H	6	0.3
(2,114)	1:16:A:VAL:HG12	1:16:A:VAL:H	6	0.3
(2,114)	1:16:A:VAL:HG13	1:16:A:VAL:H	6	0.3
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	6	0.3
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	6	0.3
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	6	0.3
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	6	0.3
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	6	0.3
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	6	0.3
(2,114)	1:16:A:VAL:HG11	1:16:A:VAL:H	8	0.3
(2,114)	1:16:A:VAL:HG12	1:16:A:VAL:H	8	0.3
(2,114)	1:16:A:VAL:HG13	1:16:A:VAL:H	8	0.3
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	8	0.3
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	8	0.3
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	8	0.3
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	8	0.3
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	8	0.3
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	8	0.3
(2,82)	1:94:A:SER:HB2	1:94:A:SER:H	20	0.3
(2,44)	1:83:A:ILE:HG23	1:97:A:CYS:H	4	0.3
(2,39)	1:117:A:LEU:HD22	1:115:A:ASP:H	1	0.3
(2,25)	1:79:A:ASN:HD22	1:80:A:CYS:HA	6	0.3
(2,22)	1:75:A:GLU:HA	1:78:A:GLU:H	14	0.3
(2,2)	1:35:A:SER:HB2	1:35:A:SER:H	20	0.3
(1,916)	1:77:A:GLU:HB2	1:77:A:GLU:H	15	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,916)	1:77:A:GLU:HB3	1:77:A:GLU:H	15	0.3
(1,907)	1:39:A:CYS:H	1:41:A:MET:H	16	0.3
(1,907)	1:39:A:CYS:H	1:41:A:MET:H	20	0.3
(1,904)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	14	0.3
(1,904)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	14	0.3
(1,896)	1:64:A:ARG:H	1:66:A:ASP:H	19	0.3
(1,895)	1:77:A:GLU:HG2	1:66:A:ASP:H	13	0.3
(1,895)	1:77:A:GLU:HG3	1:66:A:ASP:H	13	0.3
(1,894)	1:66:A:ASP:H	1:77:A:GLU:HG2	13	0.3
(1,894)	1:66:A:ASP:H	1:77:A:GLU:HG3	13	0.3
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB2	19	0.3
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB3	19	0.3
(1,863)	1:17:A:PRO:HD2	1:20:A:TRP:HE1	3	0.3
(1,863)	1:17:A:PRO:HD3	1:20:A:TRP:HE1	3	0.3
(1,863)	1:17:A:PRO:HD2	1:20:A:TRP:HE1	16	0.3
(1,863)	1:17:A:PRO:HD3	1:20:A:TRP:HE1	16	0.3
(1,863)	1:17:A:PRO:HD2	1:20:A:TRP:HE1	17	0.3
(1,863)	1:17:A:PRO:HD3	1:20:A:TRP:HE1	17	0.3
(1,856)	1:14:A:GLN:H	1:12:A:ASN:HD22	19	0.3
(1,831)	1:73:A:SER:H	1:75:A:GLU:H	16	0.3
(1,831)	1:73:A:SER:H	1:75:A:GLU:H	17	0.3
(1,794)	1:82:A:ASN:HD22	1:94:A:SER:H	11	0.3
(1,783)	1:71:A:CYS:HB2	1:74:A:GLY:H	12	0.3
(1,783)	1:71:A:CYS:HB3	1:74:A:GLY:H	12	0.3
(1,783)	1:71:A:CYS:HB2	1:74:A:GLY:H	20	0.3
(1,783)	1:71:A:CYS:HB3	1:74:A:GLY:H	20	0.3
(1,772)	1:68:A:GLU:H	1:64:A:ARG:H	9	0.3
(1,766)	1:48:A:GLU:HB2	1:58:A:CYS:H	6	0.3
(1,766)	1:48:A:GLU:HB3	1:58:A:CYS:H	6	0.3
(1,750)	1:57:A:GLN:HB2	1:52:A:GLY:H	5	0.3
(1,750)	1:57:A:GLN:HB2	1:52:A:GLY:H	5	0.3
(1,750)	1:57:A:GLN:HB3	1:52:A:GLY:H	5	0.3
(1,750)	1:57:A:GLN:HB3	1:52:A:GLY:H	5	0.3
(1,745)	1:48:A:GLU:HB2	1:49:A:ILE:H	10	0.3
(1,745)	1:48:A:GLU:HB3	1:49:A:ILE:H	10	0.3
(1,735)	1:28:A:CYS:HB2	1:33:A:ASP:H	13	0.3
(1,735)	1:28:A:CYS:HB3	1:33:A:ASP:H	13	0.3
(1,733)	1:32:A:SER:H	1:28:A:CYS:H	8	0.3
(1,731)	1:28:A:CYS:HB2	1:32:A:SER:H	1	0.3
(1,731)	1:28:A:CYS:HB3	1:32:A:SER:H	1	0.3
(1,729)	1:32:A:SER:H	1:28:A:CYS:H	8	0.3
(1,704)	1:100:A:ARG:HG2	1:100:A:ARG:H	5	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,704)	1:100:A:ARG:HG2	1:100:A:ARG:H	5	0.3
(1,704)	1:100:A:ARG:HG3	1:100:A:ARG:H	5	0.3
(1,704)	1:100:A:ARG:HG3	1:100:A:ARG:H	5	0.3
(1,696)	1:44:A:CYS:HB2	1:34:A:GLU:H	1	0.3
(1,696)	1:44:A:CYS:HB3	1:34:A:GLU:H	1	0.3
(1,693)	1:21:A:LYS:HD2	1:21:A:LYS:H	14	0.3
(1,693)	1:21:A:LYS:HD3	1:21:A:LYS:H	14	0.3
(1,688)	1:69:A:ASN:H	1:69:A:ASN:HD22	15	0.3
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD2	18	0.3
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD3	18	0.3
(1,666)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	14	0.3
(1,666)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	14	0.3
(1,658)	1:102:A:PHE:HA	1:105:A:ASN:HD22	4	0.3
(1,592)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	18	0.3
(1,592)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	18	0.3
(1,555)	1:103:A:VAL:HG11	1:104:A:CYS:H	5	0.3
(1,555)	1:103:A:VAL:HG12	1:104:A:CYS:H	5	0.3
(1,555)	1:103:A:VAL:HG13	1:104:A:CYS:H	5	0.3
(1,555)	1:103:A:VAL:HG21	1:104:A:CYS:H	5	0.3
(1,555)	1:103:A:VAL:HG22	1:104:A:CYS:H	5	0.3
(1,555)	1:103:A:VAL:HG23	1:104:A:CYS:H	5	0.3
(1,549)	1:115:A:ASP:HA	1:104:A:CYS:H	18	0.3
(1,544)	1:110:A:CYS:H	1:108:A:ASP:HB2	9	0.3
(1,544)	1:110:A:CYS:H	1:108:A:ASP:HB2	9	0.3
(1,544)	1:110:A:CYS:H	1:108:A:ASP:HB3	9	0.3
(1,544)	1:110:A:CYS:H	1:108:A:ASP:HB3	9	0.3
(1,544)	1:110:A:CYS:H	1:108:A:ASP:HB2	16	0.3
(1,544)	1:110:A:CYS:H	1:108:A:ASP:HB2	16	0.3
(1,544)	1:110:A:CYS:H	1:108:A:ASP:HB3	16	0.3
(1,544)	1:110:A:CYS:H	1:108:A:ASP:HB3	16	0.3
(1,542)	1:112:A:ASP:H	1:114:A:SER:H	17	0.3
(1,518)	1:49:A:ILE:H	1:61:A:VAL:H	15	0.3
(1,480)	1:10:A:CYS:HB2	1:10:A:CYS:H	9	0.3
(1,480)	1:10:A:CYS:HB3	1:10:A:CYS:H	9	0.3
(1,436)	1:73:A:SER:H	1:72:A:ASP:H	5	0.3
(1,436)	1:73:A:SER:H	1:72:A:ASP:H	9	0.3
(1,418)	1:64:A:ARG:HA	1:66:A:ASP:H	19	0.3
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB1	11	0.3
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB2	11	0.3
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB3	11	0.3
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB2	6	0.3
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB3	6	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB2	17	0.3
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB3	17	0.3
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB2	19	0.3
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB3	19	0.3
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB2	20	0.3
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB3	20	0.3
(1,386)	1:51:A:CYS:HB2	1:51:A:CYS:H	13	0.3
(1,386)	1:51:A:CYS:HB3	1:51:A:CYS:H	13	0.3
(1,365)	1:43:A:THR:HB	1:43:A:THR:H	13	0.3
(1,351)	1:32:A:SER:H	1:33:A:ASP:H	18	0.3
(1,349)	1:32:A:SER:H	1:33:A:ASP:H	18	0.3
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB2	13	0.3
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB3	13	0.3
(1,327)	1:22:A:CYS:HB2	1:22:A:CYS:H	14	0.3
(1,327)	1:22:A:CYS:HB3	1:22:A:CYS:H	14	0.3
(1,327)	1:22:A:CYS:HB2	1:22:A:CYS:H	15	0.3
(1,327)	1:22:A:CYS:HB3	1:22:A:CYS:H	15	0.3
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB2	18	0.3
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB3	18	0.3
(1,320)	1:7:A:ASP:HA	1:18:A:SER:H	11	0.3
(1,320)	1:7:A:ASP:HA	1:18:A:SER:H	17	0.3
(1,312)	1:14:A:GLN:HG2	1:14:A:GLN:H	18	0.3
(1,312)	1:14:A:GLN:HG3	1:14:A:GLN:H	18	0.3
(1,296)	1:10:A:CYS:HB2	1:10:A:CYS:H	3	0.3
(1,296)	1:10:A:CYS:HB3	1:10:A:CYS:H	3	0.3
(1,296)	1:10:A:CYS:HB2	1:10:A:CYS:H	6	0.3
(1,296)	1:10:A:CYS:HB3	1:10:A:CYS:H	6	0.3
(1,296)	1:10:A:CYS:HB2	1:10:A:CYS:H	8	0.3
(1,296)	1:10:A:CYS:HB3	1:10:A:CYS:H	8	0.3
(1,296)	1:10:A:CYS:HB2	1:10:A:CYS:H	15	0.3
(1,296)	1:10:A:CYS:HB3	1:10:A:CYS:H	15	0.3
(1,293)	1:8:A:PHE:HB2	1:9:A:VAL:H	19	0.3
(1,293)	1:8:A:PHE:HB3	1:9:A:VAL:H	19	0.3
(1,281)	1:5:A:GLU:HB2	1:6:A:SER:H	19	0.3
(1,281)	1:5:A:GLU:HB2	1:6:A:SER:H	19	0.3
(1,281)	1:5:A:GLU:HB3	1:6:A:SER:H	19	0.3
(1,281)	1:5:A:GLU:HB3	1:6:A:SER:H	19	0.3
(1,189)	1:101:A:ASN:HB2	1:101:A:ASN:H	9	0.3
(1,189)	1:101:A:ASN:HB3	1:101:A:ASN:H	9	0.3
(1,158)	1:104:A:CYS:HA	1:105:A:ASN:H	14	0.3
(1,158)	1:104:A:CYS:HA	1:105:A:ASN:H	15	0.3
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB2	4	0.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,140)	1:108:A:ASP:H	1:108:A:ASP:HB3	4	0.3
(1,139)	1:109:A:ASP:H	1:109:A:ASP:HB2	19	0.3
(1,139)	1:109:A:ASP:H	1:109:A:ASP:HB3	19	0.3
(1,109)	1:119:A:CYS:H	1:117:A:LEU:HG	8	0.3
(1,93)	1:8:A:PHE:H	1:7:A:ASP:HA	17	0.3
(1,85)	1:21:A:LYS:HG2	1:22:A:CYS:H	3	0.3
(1,85)	1:21:A:LYS:HG3	1:22:A:CYS:H	3	0.3
(1,66)	1:23:A:ASP:H	1:24:A:GLY:H	9	0.3
(1,66)	1:23:A:ASP:H	1:24:A:GLY:H	11	0.3
(1,55)	1:71:A:CYS:H	1:70:A:ASP:H	16	0.3
(1,51)	1:78:A:GLU:H	1:77:A:GLU:H	17	0.3
(1,28)	1:118:A:ASP:H	1:117:A:LEU:H	3	0.3
(1,28)	1:118:A:ASP:H	1:117:A:LEU:H	16	0.3
(1,17)	1:81:A:GLY:H	1:80:A:CYS:H	3	0.3
(1,15)	1:109:A:ASP:H	1:110:A:CYS:H	13	0.3
(1,6)	1:23:A:ASP:H	1:24:A:GLY:H	12	0.3
(4,7)	1:8:A:PHE:H	1:16:A:VAL:O	4	0.29
(4,7)	1:8:A:PHE:H	1:16:A:VAL:O	9	0.29
(4,5)	1:49:A:ILE:O	1:59:A:ILE:H	8	0.29
(2,376)	1:87:A:PRO:HB2	1:88:A:ASP:H	7	0.29
(2,353)	1:99:A:SER:HG	1:101:A:ASN:HD22	13	0.29
(2,353)	1:99:A:SER:HG	1:101:A:ASN:HD22	16	0.29
(2,331)	1:101:A:ASN:H	1:99:A:SER:H	2	0.29
(2,323)	1:64:A:ARG:HG2	1:68:A:GLU:H	12	0.29
(2,298)	1:28:A:CYS:HB2	1:14:A:GLN:HE22	18	0.29
(2,276)	1:43:A:THR:HA	1:57:A:GLN:H	9	0.29
(2,270)	1:111:A:SER:HA	1:110:A:CYS:H	2	0.29
(2,245)	1:36:A:PRO:HA	1:39:A:CYS:H	6	0.29
(2,188)	1:16:A:VAL:HG11	1:19:A:ARG:H	9	0.29
(2,188)	1:16:A:VAL:HG12	1:19:A:ARG:H	9	0.29
(2,188)	1:16:A:VAL:HG13	1:19:A:ARG:H	9	0.29
(2,188)	1:16:A:VAL:HG21	1:19:A:ARG:H	9	0.29
(2,188)	1:16:A:VAL:HG22	1:19:A:ARG:H	9	0.29
(2,188)	1:16:A:VAL:HG23	1:19:A:ARG:H	9	0.29
(2,188)	1:16:A:VAL:HG11	1:19:A:ARG:H	10	0.29
(2,188)	1:16:A:VAL:HG12	1:19:A:ARG:H	10	0.29
(2,188)	1:16:A:VAL:HG13	1:19:A:ARG:H	10	0.29
(2,188)	1:16:A:VAL:HG21	1:19:A:ARG:H	10	0.29
(2,188)	1:16:A:VAL:HG22	1:19:A:ARG:H	10	0.29
(2,188)	1:16:A:VAL:HG23	1:19:A:ARG:H	10	0.29
(2,187)	1:116:A:GLU:HA	1:119:A:CYS:H	15	0.29
(2,178)	1:59:A:ILE:HG23	1:57:A:GLN:HE22	7	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,135)	1:79:A:ASN:HB2	1:79:A:ASN:HD21	8	0.29
(2,114)	1:16:A:VAL:HG11	1:16:A:VAL:H	14	0.29
(2,114)	1:16:A:VAL:HG12	1:16:A:VAL:H	14	0.29
(2,114)	1:16:A:VAL:HG13	1:16:A:VAL:H	14	0.29
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	14	0.29
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	14	0.29
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	14	0.29
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	14	0.29
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	14	0.29
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	14	0.29
(2,90)	1:59:A:ILE:HD12	1:63:A:TRP:HE1	16	0.29
(2,66)	1:4:A:ALA:H	1:7:A:ASP:H	12	0.29
(2,49)	1:35:A:SER:HB3	1:39:A:CYS:H	20	0.29
(2,30)	1:9:A:VAL:H	1:10:A:CYS:H	5	0.29
(2,8)	1:45:A:ARG:HA	1:46:A:ILE:H	3	0.29
(2,4)	1:46:A:ILE:HG23	1:46:A:ILE:H	20	0.29
(1,916)	1:77:A:GLU:HB2	1:77:A:GLU:H	12	0.29
(1,916)	1:77:A:GLU:HB3	1:77:A:GLU:H	12	0.29
(1,907)	1:39:A:CYS:H	1:41:A:MET:H	1	0.29
(1,907)	1:39:A:CYS:H	1:41:A:MET:H	9	0.29
(1,907)	1:39:A:CYS:H	1:41:A:MET:H	17	0.29
(1,904)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	12	0.29
(1,904)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	12	0.29
(1,904)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	15	0.29
(1,904)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	15	0.29
(1,904)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	16	0.29
(1,904)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	16	0.29
(1,904)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	18	0.29
(1,904)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	18	0.29
(1,896)	1:64:A:ARG:H	1:66:A:ASP:H	5	0.29
(1,886)	1:51:A:CYS:H	1:58:A:CYS:H	1	0.29
(1,886)	1:51:A:CYS:H	1:58:A:CYS:H	5	0.29
(1,862)	1:21:A:LYS:HE2	1:19:A:ARG:H	6	0.29
(1,862)	1:21:A:LYS:HE3	1:19:A:ARG:H	6	0.29
(1,860)	1:16:A:VAL:HB	1:19:A:ARG:H	6	0.29
(1,860)	1:16:A:VAL:HB	1:19:A:ARG:H	8	0.29
(1,859)	1:3:A:CYS:HB2	1:18:A:SER:H	6	0.29
(1,859)	1:3:A:CYS:HB3	1:18:A:SER:H	6	0.29
(1,849)	1:33:A:ASP:H	1:11:A:ASN:H	6	0.29
(1,849)	1:33:A:ASP:H	1:11:A:ASN:H	13	0.29
(1,849)	1:33:A:ASP:H	1:11:A:ASN:H	17	0.29
(1,842)	1:80:A:CYS:HA	1:84:A:THR:H	11	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,831)	1:73:A:SER:H	1:75:A:GLU:H	13	0.29
(1,808)	1:116:A:GLU:HB2	1:104:A:CYS:H	16	0.29
(1,808)	1:116:A:GLU:HB3	1:104:A:CYS:H	16	0.29
(1,801)	1:102:A:PHE:HB2	1:98:A:ILE:H	6	0.29
(1,801)	1:102:A:PHE:HB3	1:98:A:ILE:H	6	0.29
(1,801)	1:102:A:PHE:HB2	1:98:A:ILE:H	8	0.29
(1,801)	1:102:A:PHE:HB3	1:98:A:ILE:H	8	0.29
(1,800)	1:85:A:CYS:HB2	1:98:A:ILE:H	7	0.29
(1,800)	1:85:A:CYS:HB3	1:98:A:ILE:H	7	0.29
(1,800)	1:85:A:CYS:HB2	1:98:A:ILE:H	17	0.29
(1,800)	1:85:A:CYS:HB3	1:98:A:ILE:H	17	0.29
(1,799)	1:85:A:CYS:HA	1:97:A:CYS:H	3	0.29
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG21	1	0.29
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG22	1	0.29
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG23	1	0.29
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG21	16	0.29
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG22	16	0.29
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG23	16	0.29
(1,794)	1:82:A:ASN:HD22	1:94:A:SER:H	4	0.29
(1,783)	1:71:A:CYS:HB2	1:74:A:GLY:H	11	0.29
(1,783)	1:71:A:CYS:HB3	1:74:A:GLY:H	11	0.29
(1,768)	1:58:A:CYS:HA	1:59:A:ILE:H	8	0.29
(1,768)	1:58:A:CYS:HA	1:59:A:ILE:H	14	0.29
(1,768)	1:58:A:CYS:HA	1:59:A:ILE:H	20	0.29
(1,766)	1:48:A:GLU:HB2	1:58:A:CYS:H	20	0.29
(1,766)	1:48:A:GLU:HB3	1:58:A:CYS:H	20	0.29
(1,706)	1:45:A:ARG:HB2	1:45:A:ARG:H	15	0.29
(1,706)	1:45:A:ARG:HB3	1:45:A:ARG:H	15	0.29
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG2	7	0.29
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG3	7	0.29
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD2	15	0.29
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD3	15	0.29
(1,670)	1:107:A:GLN:HB2	1:105:A:ASN:HD22	17	0.29
(1,670)	1:107:A:GLN:HB2	1:105:A:ASN:HD22	17	0.29
(1,670)	1:107:A:GLN:HB3	1:105:A:ASN:HD22	17	0.29
(1,670)	1:107:A:GLN:HB3	1:105:A:ASN:HD22	17	0.29
(1,666)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	12	0.29
(1,666)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	12	0.29
(1,666)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	15	0.29
(1,666)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	15	0.29
(1,666)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	16	0.29
(1,666)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	16	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,666)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	18	0.29
(1,666)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	18	0.29
(1,658)	1:102:A:PHE:HA	1:105:A:ASN:HD22	2	0.29
(1,628)	1:71:A:CYS:HB2	1:57:A:GLN:HE22	2	0.29
(1,628)	1:71:A:CYS:HB3	1:57:A:GLN:HE22	2	0.29
(1,592)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	4	0.29
(1,592)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	4	0.29
(1,592)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	9	0.29
(1,592)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	9	0.29
(1,585)	1:28:A:CYS:H	1:27:A:ASP:H	18	0.29
(1,580)	1:48:A:GLU:HG2	1:49:A:ILE:H	6	0.29
(1,580)	1:48:A:GLU:HG3	1:49:A:ILE:H	6	0.29
(1,569)	1:85:A:CYS:H	1:84:A:THR:H	13	0.29
(1,534)	1:77:A:GLU:HB2	1:77:A:GLU:H	20	0.29
(1,534)	1:77:A:GLU:HB3	1:77:A:GLU:H	20	0.29
(1,526)	1:64:A:ARG:H	1:67:A:GLY:H	1	0.29
(1,526)	1:64:A:ARG:H	1:67:A:GLY:H	18	0.29
(1,518)	1:49:A:ILE:H	1:61:A:VAL:H	13	0.29
(1,499)	1:33:A:ASP:HB2	1:33:A:ASP:H	8	0.29
(1,499)	1:33:A:ASP:HB3	1:33:A:ASP:H	8	0.29
(1,499)	1:33:A:ASP:HB2	1:33:A:ASP:H	14	0.29
(1,499)	1:33:A:ASP:HB3	1:33:A:ASP:H	14	0.29
(1,486)	1:7:A:ASP:HA	1:19:A:ARG:H	5	0.29
(1,483)	1:10:A:CYS:HB2	1:14:A:GLN:H	5	0.29
(1,483)	1:10:A:CYS:HB3	1:14:A:GLN:H	5	0.29
(1,483)	1:10:A:CYS:HB2	1:14:A:GLN:H	10	0.29
(1,483)	1:10:A:CYS:HB3	1:14:A:GLN:H	10	0.29
(1,483)	1:10:A:CYS:HB2	1:14:A:GLN:H	14	0.29
(1,483)	1:10:A:CYS:HB3	1:14:A:GLN:H	14	0.29
(1,466)	1:80:A:CYS:HA	1:79:A:ASN:H	6	0.29
(1,459)	1:70:A:ASP:HA	1:76:A:ASP:H	18	0.29
(1,454)	1:78:A:GLU:HG2	1:76:A:ASP:H	2	0.29
(1,454)	1:78:A:GLU:HG3	1:76:A:ASP:H	2	0.29
(1,431)	1:72:A:ASP:H	1:70:A:ASP:H	10	0.29
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB1	3	0.29
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB2	3	0.29
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB3	3	0.29
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB2	3	0.29
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB3	3	0.29
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB2	4	0.29
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB3	4	0.29
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB2	7	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB3	7	0.29
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB2	9	0.29
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB3	9	0.29
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB2	12	0.29
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB3	12	0.29
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB2	13	0.29
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB3	13	0.29
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB2	16	0.29
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB3	16	0.29
(1,390)	1:51:A:CYS:HB2	1:52:A:GLY:H	7	0.29
(1,390)	1:51:A:CYS:HB3	1:52:A:GLY:H	7	0.29
(1,386)	1:51:A:CYS:HB2	1:51:A:CYS:H	9	0.29
(1,386)	1:51:A:CYS:HB3	1:51:A:CYS:H	9	0.29
(1,386)	1:51:A:CYS:HB2	1:51:A:CYS:H	11	0.29
(1,386)	1:51:A:CYS:HB3	1:51:A:CYS:H	11	0.29
(1,386)	1:51:A:CYS:HB2	1:51:A:CYS:H	16	0.29
(1,386)	1:51:A:CYS:HB3	1:51:A:CYS:H	16	0.29
(1,378)	1:48:A:GLU:HG2	1:49:A:ILE:H	6	0.29
(1,378)	1:48:A:GLU:HG3	1:49:A:ILE:H	6	0.29
(1,375)	1:48:A:GLU:HA	1:49:A:ILE:H	18	0.29
(1,365)	1:43:A:THR:HB	1:43:A:THR:H	8	0.29
(1,365)	1:43:A:THR:HB	1:43:A:THR:H	16	0.29
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB2	8	0.29
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB3	8	0.29
(1,327)	1:22:A:CYS:HB2	1:22:A:CYS:H	2	0.29
(1,327)	1:22:A:CYS:HB3	1:22:A:CYS:H	2	0.29
(1,327)	1:22:A:CYS:HB2	1:22:A:CYS:H	18	0.29
(1,327)	1:22:A:CYS:HB3	1:22:A:CYS:H	18	0.29
(1,320)	1:7:A:ASP:HA	1:18:A:SER:H	19	0.29
(1,312)	1:14:A:GLN:HG2	1:14:A:GLN:H	16	0.29
(1,312)	1:14:A:GLN:HG3	1:14:A:GLN:H	16	0.29
(1,298)	1:14:A:GLN:H	1:11:A:ASN:H	3	0.29
(1,293)	1:8:A:PHE:HB2	1:9:A:VAL:H	2	0.29
(1,293)	1:8:A:PHE:HB3	1:9:A:VAL:H	2	0.29
(1,286)	1:7:A:ASP:HB2	1:7:A:ASP:H	15	0.29
(1,286)	1:7:A:ASP:HB3	1:7:A:ASP:H	15	0.29
(1,286)	1:7:A:ASP:HB2	1:7:A:ASP:H	17	0.29
(1,286)	1:7:A:ASP:HB3	1:7:A:ASP:H	17	0.29
(1,281)	1:5:A:GLU:HB2	1:6:A:SER:H	6	0.29
(1,281)	1:5:A:GLU:HB2	1:6:A:SER:H	6	0.29
(1,281)	1:5:A:GLU:HB3	1:6:A:SER:H	6	0.29
(1,281)	1:5:A:GLU:HB3	1:6:A:SER:H	6	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,203)	1:89:A:GLU:HB2	1:98:A:ILE:H	4	0.29
(1,203)	1:89:A:GLU:HB3	1:98:A:ILE:H	4	0.29
(1,187)	1:103:A:VAL:HG11	1:102:A:PHE:H	18	0.29
(1,187)	1:103:A:VAL:HG12	1:102:A:PHE:H	18	0.29
(1,187)	1:103:A:VAL:HG13	1:102:A:PHE:H	18	0.29
(1,187)	1:103:A:VAL:HG21	1:102:A:PHE:H	18	0.29
(1,187)	1:103:A:VAL:HG22	1:102:A:PHE:H	18	0.29
(1,187)	1:103:A:VAL:HG23	1:102:A:PHE:H	18	0.29
(1,118)	1:115:A:ASP:H	1:113:A:GLY:H	17	0.29
(1,92)	1:7:A:ASP:HB2	1:8:A:PHE:H	13	0.29
(1,92)	1:7:A:ASP:HB3	1:8:A:PHE:H	13	0.29
(1,85)	1:21:A:LYS:HG2	1:22:A:CYS:H	4	0.29
(1,85)	1:21:A:LYS:HG3	1:22:A:CYS:H	4	0.29
(1,85)	1:21:A:LYS:HG2	1:22:A:CYS:H	15	0.29
(1,85)	1:21:A:LYS:HG3	1:22:A:CYS:H	15	0.29
(1,79)	1:61:A:VAL:HB	1:61:A:VAL:H	12	0.29
(1,66)	1:23:A:ASP:H	1:24:A:GLY:H	13	0.29
(1,49)	1:94:A:SER:H	1:93:A:SER:H	13	0.29
(1,28)	1:118:A:ASP:H	1:117:A:LEU:H	13	0.29
(1,17)	1:81:A:GLY:H	1:80:A:CYS:H	17	0.29
(4,8)	1:8:A:PHE:O	1:16:A:VAL:H	20	0.28
(2,329)	1:90:A:PHE:HA	1:98:A:ILE:H	19	0.28
(2,246)	1:90:A:PHE:HB2	1:100:A:ARG:H	20	0.28
(2,246)	1:90:A:PHE:HB3	1:100:A:ARG:H	20	0.28
(2,245)	1:36:A:PRO:HA	1:39:A:CYS:H	14	0.28
(2,226)	1:98:A:ILE:H	1:97:A:CYS:H	8	0.28
(2,210)	1:33:A:ASP:HA	1:38:A:GLN:HE21	1	0.28
(2,187)	1:116:A:GLU:HA	1:119:A:CYS:H	12	0.28
(2,178)	1:59:A:ILE:HG22	1:57:A:GLN:HE22	4	0.28
(2,174)	1:117:A:LEU:HB2	1:116:A:GLU:H	19	0.28
(2,164)	1:14:A:GLN:HB2	1:14:A:GLN:H	19	0.28
(2,164)	1:14:A:GLN:HB3	1:14:A:GLN:H	19	0.28
(2,114)	1:16:A:VAL:HG11	1:16:A:VAL:H	4	0.28
(2,114)	1:16:A:VAL:HG12	1:16:A:VAL:H	4	0.28
(2,114)	1:16:A:VAL:HG13	1:16:A:VAL:H	4	0.28
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	4	0.28
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	4	0.28
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	4	0.28
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	4	0.28
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	4	0.28
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	4	0.28
(2,114)	1:16:A:VAL:HG11	1:16:A:VAL:H	9	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,114)	1:16:A:VAL:HG12	1:16:A:VAL:H	9	0.28
(2,114)	1:16:A:VAL:HG13	1:16:A:VAL:H	9	0.28
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	9	0.28
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	9	0.28
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	9	0.28
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	9	0.28
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	9	0.28
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	9	0.28
(2,44)	1:83:A:ILE:HG23	1:97:A:CYS:H	11	0.28
(2,39)	1:117:A:LEU:HD12	1:115:A:ASP:H	12	0.28
(2,39)	1:117:A:LEU:HD13	1:115:A:ASP:H	13	0.28
(2,38)	1:96:A:ARG:HB3	1:97:A:CYS:H	3	0.28
(2,38)	1:96:A:ARG:HB3	1:97:A:CYS:H	6	0.28
(2,29)	1:28:A:CYS:HA	1:29:A:GLU:H	5	0.28
(2,29)	1:28:A:CYS:HA	1:29:A:GLU:H	6	0.28
(2,29)	1:28:A:CYS:HA	1:29:A:GLU:H	8	0.28
(2,29)	1:28:A:CYS:HA	1:29:A:GLU:H	14	0.28
(2,8)	1:45:A:ARG:HA	1:46:A:ILE:H	6	0.28
(2,8)	1:45:A:ARG:HA	1:46:A:ILE:H	18	0.28
(1,904)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	1	0.28
(1,904)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	1	0.28
(1,904)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	5	0.28
(1,904)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	5	0.28
(1,904)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	8	0.28
(1,904)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	8	0.28
(1,904)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	9	0.28
(1,904)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	9	0.28
(1,904)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	10	0.28
(1,904)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	10	0.28
(1,904)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	13	0.28
(1,904)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	13	0.28
(1,904)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	20	0.28
(1,904)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	20	0.28
(1,896)	1:64:A:ARG:H	1:66:A:ASP:H	9	0.28
(1,896)	1:64:A:ARG:H	1:66:A:ASP:H	16	0.28
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB2	7	0.28
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB3	7	0.28
(1,881)	1:48:A:GLU:H	1:45:A:ARG:H	9	0.28
(1,879)	1:48:A:GLU:H	1:45:A:ARG:H	9	0.28
(1,876)	1:39:A:CYS:HB2	1:43:A:THR:H	9	0.28
(1,876)	1:39:A:CYS:HB3	1:43:A:THR:H	9	0.28
(1,860)	1:16:A:VAL:HB	1:19:A:ARG:H	10	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,859)	1:3:A:CYS:HB2	1:18:A:SER:H	19	0.28
(1,859)	1:3:A:CYS:HB3	1:18:A:SER:H	19	0.28
(1,849)	1:33:A:ASP:H	1:11:A:ASN:H	3	0.28
(1,831)	1:73:A:SER:H	1:75:A:GLU:H	11	0.28
(1,803)	1:101:A:ASN:HD21	1:99:A:SER:H	12	0.28
(1,801)	1:102:A:PHE:HB2	1:98:A:ILE:H	12	0.28
(1,801)	1:102:A:PHE:HB3	1:98:A:ILE:H	12	0.28
(1,801)	1:102:A:PHE:HB2	1:98:A:ILE:H	17	0.28
(1,801)	1:102:A:PHE:HB3	1:98:A:ILE:H	17	0.28
(1,800)	1:85:A:CYS:HB2	1:98:A:ILE:H	1	0.28
(1,800)	1:85:A:CYS:HB3	1:98:A:ILE:H	1	0.28
(1,800)	1:85:A:CYS:HB2	1:98:A:ILE:H	3	0.28
(1,800)	1:85:A:CYS:HB3	1:98:A:ILE:H	3	0.28
(1,800)	1:85:A:CYS:HB2	1:98:A:ILE:H	4	0.28
(1,800)	1:85:A:CYS:HB3	1:98:A:ILE:H	4	0.28
(1,794)	1:82:A:ASN:HD22	1:94:A:SER:H	10	0.28
(1,791)	1:85:A:CYS:HB2	1:89:A:GLU:H	18	0.28
(1,791)	1:85:A:CYS:HB3	1:89:A:GLU:H	18	0.28
(1,761)	1:72:A:ASP:H	1:57:A:GLN:HE21	5	0.28
(1,761)	1:72:A:ASP:H	1:57:A:GLN:HE21	13	0.28
(1,759)	1:57:A:GLN:HE21	1:71:A:CYS:HA	18	0.28
(1,750)	1:57:A:GLN:HB2	1:52:A:GLY:H	9	0.28
(1,750)	1:57:A:GLN:HB2	1:52:A:GLY:H	9	0.28
(1,750)	1:57:A:GLN:HB3	1:52:A:GLY:H	9	0.28
(1,750)	1:57:A:GLN:HB3	1:52:A:GLY:H	9	0.28
(1,731)	1:28:A:CYS:HB2	1:32:A:SER:H	2	0.28
(1,731)	1:28:A:CYS:HB3	1:32:A:SER:H	2	0.28
(1,726)	1:34:A:GLU:HG2	1:27:A:ASP:H	2	0.28
(1,726)	1:34:A:GLU:HG3	1:27:A:ASP:H	2	0.28
(1,718)	1:16:A:VAL:HB	1:20:A:TRP:HE1	16	0.28
(1,718)	1:16:A:VAL:HB	1:20:A:TRP:HE1	17	0.28
(1,704)	1:100:A:ARG:HG2	1:100:A:ARG:H	17	0.28
(1,704)	1:100:A:ARG:HG2	1:100:A:ARG:H	17	0.28
(1,704)	1:100:A:ARG:HG3	1:100:A:ARG:H	17	0.28
(1,704)	1:100:A:ARG:HG3	1:100:A:ARG:H	17	0.28
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG2	5	0.28
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG3	5	0.28
(1,679)	1:78:A:GLU:HG2	1:79:A:ASN:HD22	9	0.28
(1,679)	1:78:A:GLU:HG3	1:79:A:ASN:HD22	9	0.28
(1,679)	1:78:A:GLU:HG2	1:79:A:ASN:HD22	14	0.28
(1,679)	1:78:A:GLU:HG3	1:79:A:ASN:HD22	14	0.28
(1,667)	1:107:A:GLN:HG2	1:105:A:ASN:HD22	15	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,667)	1:107:A:GLN:HG2	1:105:A:ASN:HD22	15	0.28
(1,667)	1:107:A:GLN:HG3	1:105:A:ASN:HD22	15	0.28
(1,667)	1:107:A:GLN:HG3	1:105:A:ASN:HD22	15	0.28
(1,666)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	1	0.28
(1,666)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	1	0.28
(1,666)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	5	0.28
(1,666)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	5	0.28
(1,666)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	8	0.28
(1,666)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	8	0.28
(1,666)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	9	0.28
(1,666)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	9	0.28
(1,666)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	10	0.28
(1,666)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	10	0.28
(1,666)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	13	0.28
(1,666)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	13	0.28
(1,666)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	20	0.28
(1,666)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	20	0.28
(1,658)	1:102:A:PHE:HA	1:105:A:ASN:HD22	9	0.28
(1,585)	1:28:A:CYS:H	1:27:A:ASP:H	3	0.28
(1,569)	1:85:A:CYS:H	1:84:A:THR:H	18	0.28
(1,545)	1:103:A:VAL:HA	1:105:A:ASN:H	5	0.28
(1,545)	1:103:A:VAL:HA	1:105:A:ASN:H	14	0.28
(1,545)	1:103:A:VAL:HA	1:105:A:ASN:H	20	0.28
(1,542)	1:112:A:ASP:H	1:114:A:SER:H	9	0.28
(1,526)	1:64:A:ARG:H	1:67:A:GLY:H	9	0.28
(1,526)	1:64:A:ARG:H	1:67:A:GLY:H	14	0.28
(1,499)	1:33:A:ASP:HB2	1:33:A:ASP:H	9	0.28
(1,499)	1:33:A:ASP:HB3	1:33:A:ASP:H	9	0.28
(1,483)	1:10:A:CYS:HB2	1:14:A:GLN:H	19	0.28
(1,483)	1:10:A:CYS:HB3	1:14:A:GLN:H	19	0.28
(1,480)	1:10:A:CYS:HB2	1:10:A:CYS:H	11	0.28
(1,480)	1:10:A:CYS:HB3	1:10:A:CYS:H	11	0.28
(1,445)	1:75:A:GLU:H	1:74:A:GLY:H	10	0.28
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB2	19	0.28
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB3	19	0.28
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB2	2	0.28
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB3	2	0.28
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB2	11	0.28
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB3	11	0.28
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB2	14	0.28
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB3	14	0.28
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB2	15	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB3	15	0.28
(1,390)	1:51:A:CYS:HB2	1:52:A:GLY:H	17	0.28
(1,390)	1:51:A:CYS:HB3	1:52:A:GLY:H	17	0.28
(1,375)	1:48:A:GLU:HA	1:49:A:ILE:H	14	0.28
(1,375)	1:48:A:GLU:HA	1:49:A:ILE:H	15	0.28
(1,365)	1:43:A:THR:HB	1:43:A:THR:H	3	0.28
(1,351)	1:32:A:SER:H	1:33:A:ASP:H	5	0.28
(1,351)	1:32:A:SER:H	1:33:A:ASP:H	6	0.28
(1,349)	1:32:A:SER:H	1:33:A:ASP:H	5	0.28
(1,349)	1:32:A:SER:H	1:33:A:ASP:H	6	0.28
(1,347)	1:31:A:GLY:H	1:28:A:CYS:H	11	0.28
(1,343)	1:28:A:CYS:HB2	1:28:A:CYS:H	2	0.28
(1,343)	1:28:A:CYS:HB3	1:28:A:CYS:H	2	0.28
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB2	4	0.28
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB3	4	0.28
(1,319)	1:16:A:VAL:H	1:9:A:VAL:HA	15	0.28
(1,281)	1:5:A:GLU:HB2	1:6:A:SER:H	11	0.28
(1,281)	1:5:A:GLU:HB2	1:6:A:SER:H	11	0.28
(1,281)	1:5:A:GLU:HB3	1:6:A:SER:H	11	0.28
(1,281)	1:5:A:GLU:HB3	1:6:A:SER:H	11	0.28
(1,248)	1:83:A:ILE:HB	1:84:A:THR:H	5	0.28
(1,224)	1:92:A:CYS:HA	1:94:A:SER:H	2	0.28
(1,205)	1:98:A:ILE:HG12	1:98:A:ILE:H	8	0.28
(1,205)	1:98:A:ILE:HG13	1:98:A:ILE:H	8	0.28
(1,205)	1:98:A:ILE:HG12	1:98:A:ILE:H	14	0.28
(1,205)	1:98:A:ILE:HG13	1:98:A:ILE:H	14	0.28
(1,203)	1:89:A:GLU:HB2	1:98:A:ILE:H	15	0.28
(1,203)	1:89:A:GLU:HB3	1:98:A:ILE:H	15	0.28
(1,180)	1:99:A:SER:HB2	1:102:A:PHE:H	9	0.28
(1,180)	1:99:A:SER:HB3	1:102:A:PHE:H	9	0.28
(1,98)	1:98:A:ILE:HG12	1:99:A:SER:H	13	0.28
(1,98)	1:98:A:ILE:HG13	1:99:A:SER:H	13	0.28
(1,93)	1:8:A:PHE:H	1:7:A:ASP:HA	13	0.28
(1,93)	1:8:A:PHE:H	1:7:A:ASP:HA	15	0.28
(1,92)	1:7:A:ASP:HB2	1:8:A:PHE:H	2	0.28
(1,92)	1:7:A:ASP:HB3	1:8:A:PHE:H	2	0.28
(1,85)	1:21:A:LYS:HG2	1:22:A:CYS:H	2	0.28
(1,85)	1:21:A:LYS:HG3	1:22:A:CYS:H	2	0.28
(1,81)	1:28:A:CYS:HA	1:33:A:ASP:H	8	0.28
(1,66)	1:23:A:ASP:H	1:24:A:GLY:H	6	0.28
(1,66)	1:23:A:ASP:H	1:24:A:GLY:H	7	0.28
(1,60)	1:56:A:THR:H	1:57:A:GLN:H	14	0.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	1:71:A:CYS:H	1:70:A:ASP:H	6	0.28
(1,28)	1:118:A:ASP:H	1:117:A:LEU:H	7	0.28
(1,24)	1:104:A:CYS:H	1:105:A:ASN:H	1	0.28
(1,24)	1:104:A:CYS:H	1:105:A:ASN:H	10	0.28
(1,23)	1:104:A:CYS:H	1:105:A:ASN:H	1	0.28
(1,23)	1:104:A:CYS:H	1:105:A:ASN:H	10	0.28
(1,17)	1:81:A:GLY:H	1:80:A:CYS:H	11	0.28
(1,9)	1:12:A:ASN:H	1:11:A:ASN:H	1	0.28
(1,6)	1:23:A:ASP:H	1:24:A:GLY:H	3	0.28
(1,6)	1:23:A:ASP:H	1:24:A:GLY:H	4	0.28
(4,8)	1:8:A:PHE:O	1:16:A:VAL:H	15	0.27
(4,2)	1:90:A:PHE:O	1:98:A:ILE:H	13	0.27
(2,376)	1:87:A:PRO:HB2	1:88:A:ASP:H	5	0.27
(2,366)	1:116:A:GLU:HA	1:106:A:GLY:H	9	0.27
(2,323)	1:64:A:ARG:HG2	1:68:A:GLU:H	8	0.27
(2,304)	1:11:A:ASN:HD21	1:12:A:ASN:H	19	0.27
(2,298)	1:28:A:CYS:HB3	1:14:A:GLN:HE22	11	0.27
(2,276)	1:43:A:THR:HA	1:57:A:GLN:H	1	0.27
(2,276)	1:43:A:THR:HA	1:57:A:GLN:H	13	0.27
(2,218)	1:36:A:PRO:HD2	1:37:A:GLU:H	6	0.27
(2,168)	1:38:A:GLN:HG3	1:38:A:GLN:H	1	0.27
(2,154)	1:116:A:GLU:HG3	1:109:A:ASP:H	1	0.27
(2,114)	1:16:A:VAL:HG11	1:16:A:VAL:H	20	0.27
(2,114)	1:16:A:VAL:HG12	1:16:A:VAL:H	20	0.27
(2,114)	1:16:A:VAL:HG13	1:16:A:VAL:H	20	0.27
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	20	0.27
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	20	0.27
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	20	0.27
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	20	0.27
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	20	0.27
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	20	0.27
(2,83)	1:35:A:SER:HB3	1:38:A:GLN:H	10	0.27
(2,82)	1:94:A:SER:HB3	1:94:A:SER:H	18	0.27
(2,46)	1:114:A:SER:HG	1:115:A:ASP:H	3	0.27
(2,46)	1:114:A:SER:HG	1:115:A:ASP:H	6	0.27
(2,38)	1:96:A:ARG:HB3	1:97:A:CYS:H	13	0.27
(2,29)	1:28:A:CYS:HA	1:29:A:GLU:H	9	0.27
(2,29)	1:28:A:CYS:HA	1:29:A:GLU:H	15	0.27
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG21	1	0.27
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG22	1	0.27
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG23	1	0.27
(1,904)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	6	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,904)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	6	0.27
(1,904)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	11	0.27
(1,904)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	11	0.27
(1,904)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	19	0.27
(1,904)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	19	0.27
(1,898)	1:57:A:GLN:HE22	1:71:A:CYS:H	14	0.27
(1,896)	1:64:A:ARG:H	1:66:A:ASP:H	7	0.27
(1,888)	1:49:A:ILE:HA	1:61:A:VAL:H	6	0.27
(1,881)	1:48:A:GLU:H	1:45:A:ARG:H	11	0.27
(1,879)	1:48:A:GLU:H	1:45:A:ARG:H	11	0.27
(1,873)	1:34:A:GLU:HB2	1:33:A:ASP:H	8	0.27
(1,873)	1:34:A:GLU:HB3	1:33:A:ASP:H	8	0.27
(1,863)	1:17:A:PRO:HD2	1:20:A:TRP:HE1	6	0.27
(1,863)	1:17:A:PRO:HD3	1:20:A:TRP:HE1	6	0.27
(1,860)	1:16:A:VAL:HB	1:19:A:ARG:H	16	0.27
(1,860)	1:16:A:VAL:HB	1:19:A:ARG:H	19	0.27
(1,859)	1:3:A:CYS:HB2	1:18:A:SER:H	20	0.27
(1,859)	1:3:A:CYS:HB3	1:18:A:SER:H	20	0.27
(1,856)	1:14:A:GLN:H	1:12:A:ASN:HD22	9	0.27
(1,849)	1:33:A:ASP:H	1:11:A:ASN:H	9	0.27
(1,838)	1:58:A:CYS:HA	1:52:A:GLY:H	19	0.27
(1,822)	1:113:A:GLY:HA2	1:116:A:GLU:H	16	0.27
(1,822)	1:113:A:GLY:HA3	1:116:A:GLU:H	16	0.27
(1,809)	1:106:A:GLY:H	1:104:A:CYS:H	3	0.27
(1,803)	1:101:A:ASN:HD21	1:99:A:SER:H	14	0.27
(1,791)	1:85:A:CYS:HB2	1:89:A:GLU:H	2	0.27
(1,791)	1:85:A:CYS:HB3	1:89:A:GLU:H	2	0.27
(1,789)	1:85:A:CYS:H	1:84:A:THR:HB	3	0.27
(1,772)	1:68:A:GLU:H	1:64:A:ARG:H	6	0.27
(1,768)	1:58:A:CYS:HA	1:59:A:ILE:H	3	0.27
(1,759)	1:57:A:GLN:HE21	1:71:A:CYS:HA	14	0.27
(1,745)	1:48:A:GLU:HB2	1:49:A:ILE:H	16	0.27
(1,745)	1:48:A:GLU:HB3	1:49:A:ILE:H	16	0.27
(1,744)	1:48:A:GLU:H	1:47:A:HIS:H	4	0.27
(1,744)	1:48:A:GLU:H	1:47:A:HIS:H	16	0.27
(1,735)	1:28:A:CYS:HB2	1:33:A:ASP:H	19	0.27
(1,735)	1:28:A:CYS:HB3	1:33:A:ASP:H	19	0.27
(1,731)	1:28:A:CYS:HB2	1:32:A:SER:H	3	0.27
(1,731)	1:28:A:CYS:HB3	1:32:A:SER:H	3	0.27
(1,731)	1:28:A:CYS:HB2	1:32:A:SER:H	8	0.27
(1,731)	1:28:A:CYS:HB3	1:32:A:SER:H	8	0.27
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD2	14	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD3	14	0.27
(1,693)	1:21:A:LYS:HD2	1:21:A:LYS:H	3	0.27
(1,693)	1:21:A:LYS:HD3	1:21:A:LYS:H	3	0.27
(1,679)	1:78:A:GLU:HG2	1:79:A:ASN:HD22	7	0.27
(1,679)	1:78:A:GLU:HG3	1:79:A:ASN:HD22	7	0.27
(1,666)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	6	0.27
(1,666)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	6	0.27
(1,666)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	11	0.27
(1,666)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	11	0.27
(1,666)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	19	0.27
(1,666)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	19	0.27
(1,642)	1:82:A:ASN:HA	1:82:A:ASN:HD22	14	0.27
(1,642)	1:82:A:ASN:HA	1:82:A:ASN:HD22	20	0.27
(1,628)	1:71:A:CYS:HB2	1:57:A:GLN:HE22	1	0.27
(1,628)	1:71:A:CYS:HB3	1:57:A:GLN:HE22	1	0.27
(1,596)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	20	0.27
(1,596)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	20	0.27
(1,569)	1:85:A:CYS:H	1:84:A:THR:H	16	0.27
(1,562)	1:102:A:PHE:HB2	1:99:A:SER:H	10	0.27
(1,562)	1:102:A:PHE:HB3	1:99:A:SER:H	10	0.27
(1,557)	1:100:A:ARG:HB2	1:101:A:ASN:H	19	0.27
(1,557)	1:100:A:ARG:HB3	1:101:A:ASN:H	19	0.27
(1,545)	1:103:A:VAL:HA	1:105:A:ASN:H	2	0.27
(1,545)	1:103:A:VAL:HA	1:105:A:ASN:H	15	0.27
(1,543)	1:112:A:ASP:HB2	1:114:A:SER:H	2	0.27
(1,543)	1:112:A:ASP:HB3	1:114:A:SER:H	2	0.27
(1,542)	1:112:A:ASP:H	1:114:A:SER:H	5	0.27
(1,526)	1:64:A:ARG:H	1:67:A:GLY:H	2	0.27
(1,526)	1:64:A:ARG:H	1:67:A:GLY:H	13	0.27
(1,518)	1:49:A:ILE:H	1:61:A:VAL:H	19	0.27
(1,504)	1:39:A:CYS:HB2	1:39:A:CYS:H	19	0.27
(1,504)	1:39:A:CYS:HB3	1:39:A:CYS:H	19	0.27
(1,501)	1:34:A:GLU:HB2	1:34:A:GLU:H	19	0.27
(1,501)	1:34:A:GLU:HB3	1:34:A:GLU:H	19	0.27
(1,499)	1:33:A:ASP:HB2	1:33:A:ASP:H	7	0.27
(1,499)	1:33:A:ASP:HB3	1:33:A:ASP:H	7	0.27
(1,499)	1:33:A:ASP:HB2	1:33:A:ASP:H	19	0.27
(1,499)	1:33:A:ASP:HB3	1:33:A:ASP:H	19	0.27
(1,486)	1:7:A:ASP:HA	1:19:A:ARG:H	19	0.27
(1,483)	1:10:A:CYS:HB2	1:14:A:GLN:H	3	0.27
(1,483)	1:10:A:CYS:HB3	1:14:A:GLN:H	3	0.27
(1,480)	1:10:A:CYS:HB2	1:10:A:CYS:H	13	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,480)	1:10:A:CYS:HB3	1:10:A:CYS:H	13	0.27
(1,480)	1:10:A:CYS:HB2	1:10:A:CYS:H	16	0.27
(1,480)	1:10:A:CYS:HB3	1:10:A:CYS:H	16	0.27
(1,466)	1:80:A:CYS:HA	1:79:A:ASN:H	13	0.27
(1,446)	1:73:A:SER:H	1:74:A:GLY:H	8	0.27
(1,445)	1:75:A:GLU:H	1:74:A:GLY:H	4	0.27
(1,444)	1:76:A:ASP:H	1:74:A:GLY:H	6	0.27
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB2	13	0.27
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB3	13	0.27
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB2	17	0.27
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB3	17	0.27
(1,418)	1:64:A:ARG:HA	1:66:A:ASP:H	3	0.27
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB2	5	0.27
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB3	5	0.27
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB2	8	0.27
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB3	8	0.27
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB2	10	0.27
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB3	10	0.27
(1,390)	1:51:A:CYS:HB2	1:52:A:GLY:H	1	0.27
(1,390)	1:51:A:CYS:HB3	1:52:A:GLY:H	1	0.27
(1,379)	1:50:A:SER:H	1:50:A:SER:HA	4	0.27
(1,379)	1:50:A:SER:H	1:50:A:SER:HA	12	0.27
(1,375)	1:48:A:GLU:HA	1:49:A:ILE:H	8	0.27
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	2	0.27
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	2	0.27
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	2	0.27
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	2	0.27
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	14	0.27
(1,366)	1:42:A:ARG:HB2	1:43:A:THR:H	14	0.27
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	14	0.27
(1,366)	1:42:A:ARG:HB3	1:43:A:THR:H	14	0.27
(1,347)	1:31:A:GLY:H	1:28:A:CYS:H	16	0.27
(1,335)	1:45:A:ARG:HD2	1:24:A:GLY:H	6	0.27
(1,335)	1:45:A:ARG:HD3	1:24:A:GLY:H	6	0.27
(1,328)	1:22:A:CYS:HB2	1:22:A:CYS:H	13	0.27
(1,328)	1:22:A:CYS:HB3	1:22:A:CYS:H	13	0.27
(1,312)	1:14:A:GLN:HG2	1:14:A:GLN:H	3	0.27
(1,312)	1:14:A:GLN:HG3	1:14:A:GLN:H	3	0.27
(1,298)	1:14:A:GLN:H	1:11:A:ASN:H	7	0.27
(1,283)	1:8:A:PHE:H	1:7:A:ASP:H	8	0.27
(1,248)	1:83:A:ILE:HB	1:84:A:THR:H	7	0.27
(1,203)	1:89:A:GLU:HB2	1:98:A:ILE:H	7	0.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,203)	1:89:A:GLU:HB3	1:98:A:ILE:H	7	0.27
(1,203)	1:89:A:GLU:HB2	1:98:A:ILE:H	17	0.27
(1,203)	1:89:A:GLU:HB3	1:98:A:ILE:H	17	0.27
(1,109)	1:119:A:CYS:H	1:117:A:LEU:HG	10	0.27
(1,97)	1:98:A:ILE:HD11	1:99:A:SER:H	1	0.27
(1,97)	1:98:A:ILE:HD12	1:99:A:SER:H	1	0.27
(1,97)	1:98:A:ILE:HD13	1:99:A:SER:H	1	0.27
(1,85)	1:21:A:LYS:HG2	1:22:A:CYS:H	16	0.27
(1,85)	1:21:A:LYS:HG3	1:22:A:CYS:H	16	0.27
(1,80)	1:44:A:CYS:HB2	1:45:A:ARG:H	3	0.27
(1,80)	1:44:A:CYS:HB3	1:45:A:ARG:H	3	0.27
(1,66)	1:23:A:ASP:H	1:24:A:GLY:H	1	0.27
(1,66)	1:23:A:ASP:H	1:24:A:GLY:H	2	0.27
(1,66)	1:23:A:ASP:H	1:24:A:GLY:H	10	0.27
(1,66)	1:23:A:ASP:H	1:24:A:GLY:H	16	0.27
(1,60)	1:56:A:THR:H	1:57:A:GLN:H	12	0.27
(1,55)	1:71:A:CYS:H	1:70:A:ASP:H	1	0.27
(1,53)	1:77:A:GLU:H	1:76:A:ASP:H	14	0.27
(1,53)	1:77:A:GLU:H	1:76:A:ASP:H	18	0.27
(1,52)	1:76:A:ASP:H	1:77:A:GLU:H	14	0.27
(1,52)	1:76:A:ASP:H	1:77:A:GLU:H	18	0.27
(1,33)	1:115:A:ASP:H	1:114:A:SER:H	17	0.27
(1,28)	1:118:A:ASP:H	1:117:A:LEU:H	4	0.27
(1,24)	1:104:A:CYS:H	1:105:A:ASN:H	8	0.27
(1,23)	1:104:A:CYS:H	1:105:A:ASN:H	8	0.27
(1,17)	1:81:A:GLY:H	1:80:A:CYS:H	1	0.27
(1,17)	1:81:A:GLY:H	1:80:A:CYS:H	5	0.27
(1,17)	1:81:A:GLY:H	1:80:A:CYS:H	15	0.27
(1,6)	1:23:A:ASP:H	1:24:A:GLY:H	14	0.27
(2,376)	1:87:A:PRO:HB2	1:88:A:ASP:H	2	0.26
(2,357)	1:70:A:ASP:HA	1:69:A:ASN:HD21	10	0.26
(2,353)	1:99:A:SER:HG	1:101:A:ASN:HD22	10	0.26
(2,353)	1:99:A:SER:HG	1:101:A:ASN:HD22	11	0.26
(2,331)	1:101:A:ASN:H	1:99:A:SER:H	4	0.26
(2,322)	1:69:A:ASN:HB3	1:71:A:CYS:H	14	0.26
(2,311)	1:97:A:CYS:HB3	1:91:A:THR:H	3	0.26
(2,187)	1:118:A:ASP:HA	1:119:A:CYS:H	11	0.26
(2,174)	1:117:A:LEU:HB2	1:116:A:GLU:H	13	0.26
(2,174)	1:117:A:LEU:HB3	1:116:A:GLU:H	16	0.26
(2,164)	1:14:A:GLN:HB2	1:14:A:GLN:H	9	0.26
(2,164)	1:14:A:GLN:HB3	1:14:A:GLN:H	9	0.26
(2,133)	1:89:A:GLU:HB2	1:79:A:ASN:HD22	17	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,123)	1:16:A:VAL:HG11	1:33:A:ASP:H	1	0.26
(2,123)	1:16:A:VAL:HG12	1:33:A:ASP:H	1	0.26
(2,123)	1:16:A:VAL:HG13	1:33:A:ASP:H	1	0.26
(2,123)	1:16:A:VAL:HG21	1:33:A:ASP:H	1	0.26
(2,123)	1:16:A:VAL:HG22	1:33:A:ASP:H	1	0.26
(2,123)	1:16:A:VAL:HG23	1:33:A:ASP:H	1	0.26
(2,89)	1:107:A:GLN:HB2	1:108:A:ASP:H	5	0.26
(2,89)	1:107:A:GLN:HB3	1:108:A:ASP:H	5	0.26
(2,83)	1:35:A:SER:HB3	1:38:A:GLN:H	3	0.26
(2,46)	1:114:A:SER:HG	1:115:A:ASP:H	4	0.26
(2,38)	1:96:A:ARG:HB3	1:97:A:CYS:H	7	0.26
(2,29)	1:28:A:CYS:HA	1:29:A:GLU:H	1	0.26
(2,29)	1:28:A:CYS:HA	1:29:A:GLU:H	2	0.26
(2,29)	1:28:A:CYS:HA	1:29:A:GLU:H	3	0.26
(2,29)	1:28:A:CYS:HA	1:29:A:GLU:H	10	0.26
(2,29)	1:28:A:CYS:HA	1:29:A:GLU:H	17	0.26
(2,20)	1:82:A:ASN:H	1:83:A:ILE:H	12	0.26
(1,926)	1:16:A:VAL:HG11	1:20:A:TRP:HZ3	17	0.26
(1,926)	1:16:A:VAL:HG12	1:20:A:TRP:HZ3	17	0.26
(1,926)	1:16:A:VAL:HG13	1:20:A:TRP:HZ3	17	0.26
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG21	2	0.26
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG22	2	0.26
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG23	2	0.26
(1,916)	1:77:A:GLU:HB2	1:77:A:GLU:H	8	0.26
(1,916)	1:77:A:GLU:HB3	1:77:A:GLU:H	8	0.26
(1,907)	1:39:A:CYS:H	1:41:A:MET:H	3	0.26
(1,907)	1:39:A:CYS:H	1:41:A:MET:H	12	0.26
(1,904)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	2	0.26
(1,904)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	2	0.26
(1,904)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	3	0.26
(1,904)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	3	0.26
(1,904)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	7	0.26
(1,904)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	7	0.26
(1,904)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	17	0.26
(1,904)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	17	0.26
(1,900)	1:83:A:ILE:HG12	1:82:A:ASN:H	1	0.26
(1,900)	1:83:A:ILE:HG13	1:82:A:ASN:H	1	0.26
(1,897)	1:77:A:GLU:HB2	1:69:A:ASN:HD22	18	0.26
(1,897)	1:77:A:GLU:HB3	1:69:A:ASN:HD22	18	0.26
(1,896)	1:64:A:ARG:H	1:66:A:ASP:H	3	0.26
(1,896)	1:64:A:ARG:H	1:66:A:ASP:H	11	0.26
(1,896)	1:64:A:ARG:H	1:66:A:ASP:H	20	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB2	13	0.26
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB3	13	0.26
(1,888)	1:49:A:ILE:HA	1:61:A:VAL:H	7	0.26
(1,876)	1:39:A:CYS:HB2	1:43:A:THR:H	6	0.26
(1,876)	1:39:A:CYS:HB3	1:43:A:THR:H	6	0.26
(1,869)	1:14:A:GLN:HE22	1:28:A:CYS:H	11	0.26
(1,869)	1:14:A:GLN:HE22	1:28:A:CYS:H	12	0.26
(1,869)	1:14:A:GLN:HE22	1:28:A:CYS:H	16	0.26
(1,860)	1:16:A:VAL:HB	1:19:A:ARG:H	11	0.26
(1,853)	1:10:A:CYS:HB2	1:12:A:ASN:H	6	0.26
(1,853)	1:10:A:CYS:HB3	1:12:A:ASN:H	6	0.26
(1,849)	1:33:A:ASP:H	1:11:A:ASN:H	2	0.26
(1,849)	1:33:A:ASP:H	1:11:A:ASN:H	20	0.26
(1,842)	1:80:A:CYS:HA	1:84:A:THR:H	17	0.26
(1,838)	1:58:A:CYS:HA	1:52:A:GLY:H	13	0.26
(1,837)	1:50:A:SER:H	1:45:A:ARG:HD2	8	0.26
(1,837)	1:50:A:SER:H	1:45:A:ARG:HD3	8	0.26
(1,820)	1:110:A:CYS:H	1:115:A:ASP:H	1	0.26
(1,808)	1:116:A:GLU:HB2	1:104:A:CYS:H	12	0.26
(1,808)	1:116:A:GLU:HB3	1:104:A:CYS:H	12	0.26
(1,808)	1:116:A:GLU:HB2	1:104:A:CYS:H	15	0.26
(1,808)	1:116:A:GLU:HB3	1:104:A:CYS:H	15	0.26
(1,806)	1:101:A:ASN:HD21	1:102:A:PHE:H	3	0.26
(1,803)	1:101:A:ASN:HD21	1:99:A:SER:H	6	0.26
(1,801)	1:102:A:PHE:HB2	1:98:A:ILE:H	5	0.26
(1,801)	1:102:A:PHE:HB3	1:98:A:ILE:H	5	0.26
(1,801)	1:102:A:PHE:HB2	1:98:A:ILE:H	13	0.26
(1,801)	1:102:A:PHE:HB3	1:98:A:ILE:H	13	0.26
(1,801)	1:102:A:PHE:HB2	1:98:A:ILE:H	20	0.26
(1,801)	1:102:A:PHE:HB3	1:98:A:ILE:H	20	0.26
(1,800)	1:85:A:CYS:HB2	1:98:A:ILE:H	11	0.26
(1,800)	1:85:A:CYS:HB3	1:98:A:ILE:H	11	0.26
(1,794)	1:82:A:ASN:HD22	1:94:A:SER:H	5	0.26
(1,794)	1:82:A:ASN:HD22	1:94:A:SER:H	16	0.26
(1,789)	1:85:A:CYS:H	1:84:A:THR:HB	9	0.26
(1,789)	1:85:A:CYS:H	1:84:A:THR:HB	10	0.26
(1,781)	1:73:A:SER:H	1:71:A:CYS:HB2	2	0.26
(1,781)	1:73:A:SER:H	1:71:A:CYS:HB3	2	0.26
(1,772)	1:68:A:GLU:H	1:64:A:ARG:H	2	0.26
(1,768)	1:58:A:CYS:HA	1:59:A:ILE:H	11	0.26
(1,768)	1:58:A:CYS:HA	1:59:A:ILE:H	16	0.26
(1,750)	1:57:A:GLN:HB2	1:52:A:GLY:H	16	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,750)	1:57:A:GLN:HB2	1:52:A:GLY:H	16	0.26
(1,750)	1:57:A:GLN:HB3	1:52:A:GLY:H	16	0.26
(1,750)	1:57:A:GLN:HB3	1:52:A:GLY:H	16	0.26
(1,745)	1:48:A:GLU:HB2	1:49:A:ILE:H	20	0.26
(1,745)	1:48:A:GLU:HB3	1:49:A:ILE:H	20	0.26
(1,724)	1:34:A:GLU:HB2	1:25:A:ASP:H	15	0.26
(1,724)	1:34:A:GLU:HB3	1:25:A:ASP:H	15	0.26
(1,724)	1:34:A:GLU:HB2	1:25:A:ASP:H	18	0.26
(1,724)	1:34:A:GLU:HB3	1:25:A:ASP:H	18	0.26
(1,708)	1:44:A:CYS:HB2	1:45:A:ARG:H	8	0.26
(1,708)	1:44:A:CYS:HB3	1:45:A:ARG:H	8	0.26
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG2	19	0.26
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG3	19	0.26
(1,696)	1:44:A:CYS:HB2	1:34:A:GLU:H	5	0.26
(1,696)	1:44:A:CYS:HB3	1:34:A:GLU:H	5	0.26
(1,696)	1:44:A:CYS:HB2	1:34:A:GLU:H	17	0.26
(1,696)	1:44:A:CYS:HB3	1:34:A:GLU:H	17	0.26
(1,693)	1:21:A:LYS:HD2	1:21:A:LYS:H	10	0.26
(1,693)	1:21:A:LYS:HD3	1:21:A:LYS:H	10	0.26
(1,690)	1:61:A:VAL:HG11	1:49:A:ILE:H	19	0.26
(1,690)	1:61:A:VAL:HG12	1:49:A:ILE:H	19	0.26
(1,690)	1:61:A:VAL:HG13	1:49:A:ILE:H	19	0.26
(1,690)	1:61:A:VAL:HG21	1:49:A:ILE:H	19	0.26
(1,690)	1:61:A:VAL:HG22	1:49:A:ILE:H	19	0.26
(1,690)	1:61:A:VAL:HG23	1:49:A:ILE:H	19	0.26
(1,683)	1:78:A:GLU:HG2	1:79:A:ASN:HD21	15	0.26
(1,683)	1:78:A:GLU:HG3	1:79:A:ASN:HD21	15	0.26
(1,683)	1:78:A:GLU:HG2	1:79:A:ASN:HD21	17	0.26
(1,683)	1:78:A:GLU:HG3	1:79:A:ASN:HD21	17	0.26
(1,673)	1:17:A:PRO:HB2	1:20:A:TRP:HE1	14	0.26
(1,673)	1:17:A:PRO:HB3	1:20:A:TRP:HE1	14	0.26
(1,667)	1:107:A:GLN:HG2	1:105:A:ASN:HD22	10	0.26
(1,667)	1:107:A:GLN:HG2	1:105:A:ASN:HD22	10	0.26
(1,667)	1:107:A:GLN:HG3	1:105:A:ASN:HD22	10	0.26
(1,667)	1:107:A:GLN:HG3	1:105:A:ASN:HD22	10	0.26
(1,666)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	2	0.26
(1,666)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	2	0.26
(1,666)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	3	0.26
(1,666)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	3	0.26
(1,666)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	7	0.26
(1,666)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	7	0.26
(1,666)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	17	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,666)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	17	0.26
(1,658)	1:102:A:PHE:HA	1:105:A:ASN:HD22	6	0.26
(1,658)	1:102:A:PHE:HA	1:105:A:ASN:HD22	7	0.26
(1,658)	1:102:A:PHE:HA	1:105:A:ASN:HD22	19	0.26
(1,627)	1:72:A:ASP:HA	1:57:A:GLN:HE22	19	0.26
(1,591)	1:69:A:ASN:HB2	1:69:A:ASN:HD21	12	0.26
(1,591)	1:69:A:ASN:HB3	1:69:A:ASN:HD21	12	0.26
(1,591)	1:69:A:ASN:HB2	1:69:A:ASN:HD21	15	0.26
(1,591)	1:69:A:ASN:HB3	1:69:A:ASN:HD21	15	0.26
(1,569)	1:85:A:CYS:H	1:84:A:THR:H	9	0.26
(1,569)	1:85:A:CYS:H	1:84:A:THR:H	14	0.26
(1,545)	1:103:A:VAL:HA	1:105:A:ASN:H	1	0.26
(1,545)	1:103:A:VAL:HA	1:105:A:ASN:H	8	0.26
(1,545)	1:103:A:VAL:HA	1:105:A:ASN:H	17	0.26
(1,545)	1:103:A:VAL:HA	1:105:A:ASN:H	18	0.26
(1,542)	1:112:A:ASP:H	1:114:A:SER:H	16	0.26
(1,526)	1:64:A:ARG:H	1:67:A:GLY:H	6	0.26
(1,526)	1:64:A:ARG:H	1:67:A:GLY:H	17	0.26
(1,518)	1:49:A:ILE:H	1:61:A:VAL:H	2	0.26
(1,518)	1:49:A:ILE:H	1:61:A:VAL:H	7	0.26
(1,516)	1:49:A:ILE:H	1:59:A:ILE:H	8	0.26
(1,501)	1:34:A:GLU:HB2	1:34:A:GLU:H	10	0.26
(1,501)	1:34:A:GLU:HB3	1:34:A:GLU:H	10	0.26
(1,486)	1:7:A:ASP:HA	1:19:A:ARG:H	8	0.26
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB2	7	0.26
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB3	7	0.26
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB2	1	0.26
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB3	1	0.26
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB2	18	0.26
(1,397)	1:54:A:HIS:H	1:54:A:HIS:HB3	18	0.26
(1,386)	1:51:A:CYS:HB2	1:51:A:CYS:H	1	0.26
(1,386)	1:51:A:CYS:HB3	1:51:A:CYS:H	1	0.26
(1,386)	1:51:A:CYS:HB2	1:51:A:CYS:H	3	0.26
(1,386)	1:51:A:CYS:HB3	1:51:A:CYS:H	3	0.26
(1,386)	1:51:A:CYS:HB2	1:51:A:CYS:H	5	0.26
(1,386)	1:51:A:CYS:HB3	1:51:A:CYS:H	5	0.26
(1,386)	1:51:A:CYS:HB2	1:51:A:CYS:H	19	0.26
(1,386)	1:51:A:CYS:HB3	1:51:A:CYS:H	19	0.26
(1,369)	1:43:A:THR:HB	1:44:A:CYS:H	10	0.26
(1,365)	1:43:A:THR:HB	1:43:A:THR:H	5	0.26
(1,365)	1:43:A:THR:HB	1:43:A:THR:H	9	0.26
(1,351)	1:32:A:SER:H	1:33:A:ASP:H	3	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,351)	1:32:A:SER:H	1:33:A:ASP:H	10	0.26
(1,349)	1:32:A:SER:H	1:33:A:ASP:H	3	0.26
(1,349)	1:32:A:SER:H	1:33:A:ASP:H	10	0.26
(1,343)	1:28:A:CYS:HB2	1:28:A:CYS:H	1	0.26
(1,343)	1:28:A:CYS:HB3	1:28:A:CYS:H	1	0.26
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB2	1	0.26
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB3	1	0.26
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB2	5	0.26
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB3	5	0.26
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB2	17	0.26
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB3	17	0.26
(1,320)	1:7:A:ASP:HA	1:18:A:SER:H	6	0.26
(1,296)	1:10:A:CYS:HB2	1:10:A:CYS:H	7	0.26
(1,296)	1:10:A:CYS:HB3	1:10:A:CYS:H	7	0.26
(1,228)	1:92:A:CYS:HB2	1:93:A:SER:H	13	0.26
(1,228)	1:92:A:CYS:HB3	1:93:A:SER:H	13	0.26
(1,224)	1:92:A:CYS:HA	1:94:A:SER:H	8	0.26
(1,205)	1:98:A:ILE:HG12	1:98:A:ILE:H	6	0.26
(1,205)	1:98:A:ILE:HG13	1:98:A:ILE:H	6	0.26
(1,205)	1:98:A:ILE:HG12	1:98:A:ILE:H	11	0.26
(1,205)	1:98:A:ILE:HG13	1:98:A:ILE:H	11	0.26
(1,205)	1:98:A:ILE:HG12	1:98:A:ILE:H	13	0.26
(1,205)	1:98:A:ILE:HG13	1:98:A:ILE:H	13	0.26
(1,204)	1:98:A:ILE:HG12	1:98:A:ILE:H	10	0.26
(1,204)	1:98:A:ILE:HG13	1:98:A:ILE:H	10	0.26
(1,187)	1:103:A:VAL:HG11	1:102:A:PHE:H	14	0.26
(1,187)	1:103:A:VAL:HG12	1:102:A:PHE:H	14	0.26
(1,187)	1:103:A:VAL:HG13	1:102:A:PHE:H	14	0.26
(1,187)	1:103:A:VAL:HG21	1:102:A:PHE:H	14	0.26
(1,187)	1:103:A:VAL:HG22	1:102:A:PHE:H	14	0.26
(1,187)	1:103:A:VAL:HG23	1:102:A:PHE:H	14	0.26
(1,187)	1:103:A:VAL:HG11	1:102:A:PHE:H	16	0.26
(1,187)	1:103:A:VAL:HG12	1:102:A:PHE:H	16	0.26
(1,187)	1:103:A:VAL:HG13	1:102:A:PHE:H	16	0.26
(1,187)	1:103:A:VAL:HG21	1:102:A:PHE:H	16	0.26
(1,187)	1:103:A:VAL:HG22	1:102:A:PHE:H	16	0.26
(1,187)	1:103:A:VAL:HG23	1:102:A:PHE:H	16	0.26
(1,158)	1:104:A:CYS:HA	1:105:A:ASN:H	11	0.26
(1,128)	1:114:A:SER:HA	1:114:A:SER:H	16	0.26
(1,123)	1:115:A:ASP:HB2	1:115:A:ASP:H	12	0.26
(1,123)	1:115:A:ASP:HB3	1:115:A:ASP:H	12	0.26
(1,98)	1:98:A:ILE:HG12	1:99:A:SER:H	14	0.26

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,98)	1:98:A:ILE:HG13	1:99:A:SER:H	14	0.26
(1,96)	1:100:A:ARG:H	1:89:A:GLU:HA	7	0.26
(1,66)	1:23:A:ASP:H	1:24:A:GLY:H	5	0.26
(1,51)	1:78:A:GLU:H	1:77:A:GLU:H	2	0.26
(1,49)	1:94:A:SER:H	1:93:A:SER:H	11	0.26
(1,17)	1:81:A:GLY:H	1:80:A:CYS:H	13	0.26
(1,9)	1:12:A:ASN:H	1:11:A:ASN:H	2	0.26
(4,8)	1:8:A:PHE:O	1:16:A:VAL:H	12	0.25
(4,2)	1:90:A:PHE:O	1:98:A:ILE:H	3	0.25
(4,2)	1:90:A:PHE:O	1:98:A:ILE:H	12	0.25
(2,391)	1:17:A:PRO:HD2	1:16:A:VAL:H	5	0.25
(2,359)	1:98:A:ILE:HD12	1:98:A:ILE:H	14	0.25
(2,353)	1:99:A:SER:HG	1:101:A:ASN:HD22	14	0.25
(2,298)	1:28:A:CYS:HB3	1:14:A:GLN:HE22	20	0.25
(2,294)	1:61:A:VAL:HG13	1:48:A:GLU:H	11	0.25
(2,245)	1:36:A:PRO:HA	1:39:A:CYS:H	17	0.25
(2,226)	1:98:A:ILE:H	1:97:A:CYS:H	5	0.25
(2,200)	1:77:A:GLU:HG2	1:76:A:ASP:H	16	0.25
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	19	0.25
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	19	0.25
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	19	0.25
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	19	0.25
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	19	0.25
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	19	0.25
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	19	0.25
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	19	0.25
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	19	0.25
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	19	0.25
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	19	0.25
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	19	0.25
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	19	0.25
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	19	0.25
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	19	0.25
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	19	0.25
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	19	0.25
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	19	0.25
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	19	0.25
(2,168)	1:37:A:GLU:HG2	1:38:A:GLN:H	16	0.25
(2,104)	1:80:A:CYS:HB3	1:80:A:CYS:H	4	0.25
(2,29)	1:28:A:CYS:HA	1:29:A:GLU:H	13	0.25
(2,12)	1:10:A:CYS:HB3	1:13:A:GLY:H	15	0.25
(2,2)	1:35:A:SER:HB2	1:35:A:SER:H	12	0.25
(1,916)	1:77:A:GLU:HB2	1:77:A:GLU:H	13	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,916)	1:77:A:GLU:HB3	1:77:A:GLU:H	13	0.25
(1,907)	1:39:A:CYS:H	1:41:A:MET:H	4	0.25
(1,904)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	4	0.25
(1,904)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	4	0.25
(1,900)	1:83:A:ILE:HG12	1:82:A:ASN:H	17	0.25
(1,900)	1:83:A:ILE:HG13	1:82:A:ASN:H	17	0.25
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB2	2	0.25
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB3	2	0.25
(1,886)	1:51:A:CYS:H	1:58:A:CYS:H	16	0.25
(1,886)	1:51:A:CYS:H	1:58:A:CYS:H	18	0.25
(1,869)	1:14:A:GLN:HE22	1:28:A:CYS:H	4	0.25
(1,869)	1:14:A:GLN:HE22	1:28:A:CYS:H	13	0.25
(1,863)	1:17:A:PRO:HD2	1:20:A:TRP:HE1	4	0.25
(1,863)	1:17:A:PRO:HD3	1:20:A:TRP:HE1	4	0.25
(1,863)	1:17:A:PRO:HD2	1:20:A:TRP:HE1	9	0.25
(1,863)	1:17:A:PRO:HD3	1:20:A:TRP:HE1	9	0.25
(1,863)	1:17:A:PRO:HD2	1:20:A:TRP:HE1	14	0.25
(1,863)	1:17:A:PRO:HD3	1:20:A:TRP:HE1	14	0.25
(1,860)	1:16:A:VAL:HB	1:19:A:ARG:H	4	0.25
(1,860)	1:16:A:VAL:HB	1:19:A:ARG:H	15	0.25
(1,847)	1:13:A:GLY:H	1:10:A:CYS:H	9	0.25
(1,844)	1:79:A:ASN:HB2	1:92:A:CYS:H	20	0.25
(1,844)	1:79:A:ASN:HB3	1:92:A:CYS:H	20	0.25
(1,842)	1:80:A:CYS:HA	1:84:A:THR:H	4	0.25
(1,842)	1:80:A:CYS:HA	1:84:A:THR:H	5	0.25
(1,837)	1:50:A:SER:H	1:45:A:ARG:HD2	11	0.25
(1,837)	1:50:A:SER:H	1:45:A:ARG:HD3	11	0.25
(1,822)	1:113:A:GLY:HA2	1:116:A:GLU:H	9	0.25
(1,822)	1:113:A:GLY:HA3	1:116:A:GLU:H	9	0.25
(1,803)	1:101:A:ASN:HD21	1:99:A:SER:H	13	0.25
(1,801)	1:102:A:PHE:HB2	1:98:A:ILE:H	16	0.25
(1,801)	1:102:A:PHE:HB3	1:98:A:ILE:H	16	0.25
(1,800)	1:85:A:CYS:HB2	1:98:A:ILE:H	9	0.25
(1,800)	1:85:A:CYS:HB3	1:98:A:ILE:H	9	0.25
(1,794)	1:82:A:ASN:HD22	1:94:A:SER:H	6	0.25
(1,794)	1:82:A:ASN:HD22	1:94:A:SER:H	8	0.25
(1,794)	1:82:A:ASN:HD22	1:94:A:SER:H	14	0.25
(1,792)	1:97:A:CYS:HB2	1:91:A:THR:H	15	0.25
(1,792)	1:97:A:CYS:HB3	1:91:A:THR:H	15	0.25
(1,791)	1:85:A:CYS:HB2	1:89:A:GLU:H	13	0.25
(1,791)	1:85:A:CYS:HB3	1:89:A:GLU:H	13	0.25
(1,768)	1:58:A:CYS:HA	1:59:A:ILE:H	9	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,761)	1:72:A:ASP:H	1:57:A:GLN:HE21	9	0.25
(1,759)	1:57:A:GLN:HE21	1:71:A:CYS:HA	19	0.25
(1,744)	1:48:A:GLU:H	1:47:A:HIS:H	18	0.25
(1,737)	1:33:A:ASP:HB2	1:34:A:GLU:H	5	0.25
(1,737)	1:33:A:ASP:HB3	1:34:A:GLU:H	5	0.25
(1,731)	1:28:A:CYS:HB2	1:32:A:SER:H	18	0.25
(1,731)	1:28:A:CYS:HB3	1:32:A:SER:H	18	0.25
(1,711)	1:10:A:CYS:HB2	1:11:A:ASN:H	4	0.25
(1,711)	1:10:A:CYS:HB3	1:11:A:ASN:H	4	0.25
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG2	11	0.25
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG3	11	0.25
(1,693)	1:21:A:LYS:HD2	1:21:A:LYS:H	9	0.25
(1,693)	1:21:A:LYS:HD3	1:21:A:LYS:H	9	0.25
(1,693)	1:21:A:LYS:HD2	1:21:A:LYS:H	18	0.25
(1,693)	1:21:A:LYS:HD3	1:21:A:LYS:H	18	0.25
(1,673)	1:17:A:PRO:HB2	1:20:A:TRP:HE1	4	0.25
(1,673)	1:17:A:PRO:HB3	1:20:A:TRP:HE1	4	0.25
(1,666)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	4	0.25
(1,666)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	4	0.25
(1,623)	1:30:A:ASP:HB2	1:12:A:ASN:HD22	4	0.25
(1,623)	1:30:A:ASP:HB3	1:12:A:ASN:HD22	4	0.25
(1,591)	1:69:A:ASN:HB2	1:69:A:ASN:HD21	19	0.25
(1,591)	1:69:A:ASN:HB3	1:69:A:ASN:HD21	19	0.25
(1,585)	1:28:A:CYS:H	1:27:A:ASP:H	15	0.25
(1,569)	1:85:A:CYS:H	1:84:A:THR:H	7	0.25
(1,569)	1:85:A:CYS:H	1:84:A:THR:H	12	0.25
(1,569)	1:85:A:CYS:H	1:84:A:THR:H	19	0.25
(1,553)	1:115:A:ASP:HB2	1:104:A:CYS:H	10	0.25
(1,553)	1:115:A:ASP:HB3	1:104:A:CYS:H	10	0.25
(1,545)	1:103:A:VAL:HA	1:105:A:ASN:H	10	0.25
(1,545)	1:103:A:VAL:HA	1:105:A:ASN:H	12	0.25
(1,545)	1:103:A:VAL:HA	1:105:A:ASN:H	13	0.25
(1,545)	1:103:A:VAL:HA	1:105:A:ASN:H	19	0.25
(1,542)	1:112:A:ASP:H	1:114:A:SER:H	19	0.25
(1,504)	1:39:A:CYS:HB2	1:39:A:CYS:H	10	0.25
(1,504)	1:39:A:CYS:HB3	1:39:A:CYS:H	10	0.25
(1,504)	1:39:A:CYS:HB2	1:39:A:CYS:H	11	0.25
(1,504)	1:39:A:CYS:HB3	1:39:A:CYS:H	11	0.25
(1,504)	1:39:A:CYS:HB2	1:39:A:CYS:H	13	0.25
(1,504)	1:39:A:CYS:HB3	1:39:A:CYS:H	13	0.25
(1,501)	1:34:A:GLU:HB2	1:34:A:GLU:H	5	0.25
(1,501)	1:34:A:GLU:HB3	1:34:A:GLU:H	5	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,501)	1:34:A:GLU:HB2	1:34:A:GLU:H	11	0.25
(1,501)	1:34:A:GLU:HB3	1:34:A:GLU:H	11	0.25
(1,499)	1:33:A:ASP:HB2	1:33:A:ASP:H	10	0.25
(1,499)	1:33:A:ASP:HB3	1:33:A:ASP:H	10	0.25
(1,483)	1:10:A:CYS:HB2	1:14:A:GLN:H	8	0.25
(1,483)	1:10:A:CYS:HB3	1:14:A:GLN:H	8	0.25
(1,483)	1:10:A:CYS:HB2	1:14:A:GLN:H	18	0.25
(1,483)	1:10:A:CYS:HB3	1:14:A:GLN:H	18	0.25
(1,480)	1:10:A:CYS:HB2	1:10:A:CYS:H	20	0.25
(1,480)	1:10:A:CYS:HB3	1:10:A:CYS:H	20	0.25
(1,470)	1:79:A:ASN:HB2	1:79:A:ASN:H	8	0.25
(1,470)	1:79:A:ASN:HB3	1:79:A:ASN:H	8	0.25
(1,444)	1:76:A:ASP:H	1:74:A:GLY:H	17	0.25
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB2	11	0.25
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB3	11	0.25
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB1	16	0.25
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB2	16	0.25
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB3	16	0.25
(1,375)	1:48:A:GLU:HA	1:49:A:ILE:H	5	0.25
(1,365)	1:43:A:THR:HB	1:43:A:THR:H	4	0.25
(1,365)	1:43:A:THR:HB	1:43:A:THR:H	15	0.25
(1,351)	1:32:A:SER:H	1:33:A:ASP:H	9	0.25
(1,349)	1:32:A:SER:H	1:33:A:ASP:H	9	0.25
(1,335)	1:45:A:ARG:HD2	1:24:A:GLY:H	16	0.25
(1,335)	1:45:A:ARG:HD3	1:24:A:GLY:H	16	0.25
(1,328)	1:22:A:CYS:HB2	1:22:A:CYS:H	7	0.25
(1,328)	1:22:A:CYS:HB3	1:22:A:CYS:H	7	0.25
(1,328)	1:22:A:CYS:HB2	1:22:A:CYS:H	20	0.25
(1,328)	1:22:A:CYS:HB3	1:22:A:CYS:H	20	0.25
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB2	17	0.25
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB3	17	0.25
(1,320)	1:7:A:ASP:HA	1:18:A:SER:H	3	0.25
(1,319)	1:16:A:VAL:H	1:9:A:VAL:HA	14	0.25
(1,312)	1:14:A:GLN:HG2	1:14:A:GLN:H	11	0.25
(1,312)	1:14:A:GLN:HG3	1:14:A:GLN:H	11	0.25
(1,298)	1:14:A:GLN:H	1:11:A:ASN:H	19	0.25
(1,283)	1:8:A:PHE:H	1:7:A:ASP:H	5	0.25
(1,283)	1:8:A:PHE:H	1:7:A:ASP:H	13	0.25
(1,283)	1:8:A:PHE:H	1:7:A:ASP:H	17	0.25
(1,283)	1:8:A:PHE:H	1:7:A:ASP:H	20	0.25
(1,281)	1:5:A:GLU:HB2	1:6:A:SER:H	14	0.25
(1,281)	1:5:A:GLU:HB2	1:6:A:SER:H	14	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,281)	1:5:A:GLU:HB3	1:6:A:SER:H	14	0.25
(1,281)	1:5:A:GLU:HB3	1:6:A:SER:H	14	0.25
(1,279)	1:6:A:SER:HB2	1:6:A:SER:H	7	0.25
(1,279)	1:6:A:SER:HB3	1:6:A:SER:H	7	0.25
(1,279)	1:6:A:SER:HB2	1:6:A:SER:H	10	0.25
(1,279)	1:6:A:SER:HB3	1:6:A:SER:H	10	0.25
(1,279)	1:6:A:SER:HB2	1:6:A:SER:H	20	0.25
(1,279)	1:6:A:SER:HB3	1:6:A:SER:H	20	0.25
(1,277)	1:6:A:SER:HB2	1:6:A:SER:H	7	0.25
(1,277)	1:6:A:SER:HB3	1:6:A:SER:H	7	0.25
(1,277)	1:6:A:SER:HB2	1:6:A:SER:H	10	0.25
(1,277)	1:6:A:SER:HB3	1:6:A:SER:H	10	0.25
(1,277)	1:6:A:SER:HB2	1:6:A:SER:H	20	0.25
(1,277)	1:6:A:SER:HB3	1:6:A:SER:H	20	0.25
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD11	5	0.25
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD12	5	0.25
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD13	5	0.25
(1,224)	1:92:A:CYS:HA	1:94:A:SER:H	1	0.25
(1,136)	1:112:A:ASP:H	1:110:A:CYS:H	3	0.25
(1,134)	1:110:A:CYS:H	1:109:A:ASP:HB2	4	0.25
(1,134)	1:110:A:CYS:H	1:109:A:ASP:HB2	4	0.25
(1,134)	1:110:A:CYS:H	1:109:A:ASP:HB3	4	0.25
(1,134)	1:110:A:CYS:H	1:109:A:ASP:HB3	4	0.25
(1,128)	1:114:A:SER:HA	1:114:A:SER:H	9	0.25
(1,109)	1:119:A:CYS:H	1:117:A:LEU:HG	9	0.25
(1,99)	1:98:A:ILE:HG12	1:99:A:SER:H	16	0.25
(1,99)	1:98:A:ILE:HG13	1:99:A:SER:H	16	0.25
(1,92)	1:7:A:ASP:HB2	1:8:A:PHE:H	7	0.25
(1,92)	1:7:A:ASP:HB3	1:8:A:PHE:H	7	0.25
(1,92)	1:7:A:ASP:HB2	1:8:A:PHE:H	12	0.25
(1,92)	1:7:A:ASP:HB3	1:8:A:PHE:H	12	0.25
(1,85)	1:21:A:LYS:HG2	1:22:A:CYS:H	7	0.25
(1,85)	1:21:A:LYS:HG3	1:22:A:CYS:H	7	0.25
(1,84)	1:14:A:GLN:HG2	1:29:A:GLU:H	12	0.25
(1,84)	1:14:A:GLN:HG3	1:29:A:GLU:H	12	0.25
(1,24)	1:104:A:CYS:H	1:105:A:ASN:H	5	0.25
(1,24)	1:104:A:CYS:H	1:105:A:ASN:H	9	0.25
(1,24)	1:104:A:CYS:H	1:105:A:ASN:H	16	0.25
(1,23)	1:104:A:CYS:H	1:105:A:ASN:H	5	0.25
(1,23)	1:104:A:CYS:H	1:105:A:ASN:H	9	0.25
(1,23)	1:104:A:CYS:H	1:105:A:ASN:H	16	0.25
(1,15)	1:109:A:ASP:H	1:110:A:CYS:H	11	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,15)	1:109:A:ASP:H	1:110:A:CYS:H	12	0.25
(1,6)	1:23:A:ASP:H	1:24:A:GLY:H	18	0.25
(1,6)	1:23:A:ASP:H	1:24:A:GLY:H	20	0.25
(4,7)	1:8:A:PHE:H	1:16:A:VAL:O	7	0.24
(4,2)	1:90:A:PHE:O	1:98:A:ILE:H	17	0.24
(3,7)	2:202:A:CA:CA	1:63:A:TRP:O	7	0.24
(2,394)	1:86:A:SER:HB3	1:86:A:SER:H	6	0.24
(2,391)	1:17:A:PRO:HD2	1:16:A:VAL:H	1	0.24
(2,376)	1:87:A:PRO:HB2	1:88:A:ASP:H	3	0.24
(2,359)	1:98:A:ILE:HD13	1:98:A:ILE:H	20	0.24
(2,353)	1:99:A:SER:HG	1:101:A:ASN:HD22	15	0.24
(2,323)	1:64:A:ARG:HG2	1:68:A:GLU:H	4	0.24
(2,307)	1:60:A:PRO:HB2	1:63:A:TRP:H	7	0.24
(2,304)	1:11:A:ASN:HD21	1:12:A:ASN:H	7	0.24
(2,276)	1:43:A:THR:HA	1:57:A:GLN:H	7	0.24
(2,245)	1:36:A:PRO:HA	1:39:A:CYS:H	3	0.24
(2,218)	1:36:A:PRO:HD2	1:37:A:GLU:H	5	0.24
(2,187)	1:118:A:ASP:HA	1:119:A:CYS:H	14	0.24
(2,181)	1:41:A:MET:HG3	1:41:A:MET:H	12	0.24
(2,164)	1:14:A:GLN:HB2	1:14:A:GLN:H	6	0.24
(2,164)	1:14:A:GLN:HB3	1:14:A:GLN:H	6	0.24
(2,164)	1:14:A:GLN:HB2	1:14:A:GLN:H	10	0.24
(2,164)	1:14:A:GLN:HB3	1:14:A:GLN:H	10	0.24
(2,56)	1:114:A:SER:HA	1:117:A:LEU:H	20	0.24
(2,46)	1:114:A:SER:HG	1:115:A:ASP:H	11	0.24
(2,46)	1:114:A:SER:HG	1:115:A:ASP:H	19	0.24
(2,29)	1:28:A:CYS:HA	1:29:A:GLU:H	4	0.24
(2,29)	1:28:A:CYS:HA	1:29:A:GLU:H	18	0.24
(2,29)	1:28:A:CYS:HA	1:29:A:GLU:H	20	0.24
(2,22)	1:75:A:GLU:HA	1:78:A:GLU:H	15	0.24
(2,12)	1:10:A:CYS:HB2	1:13:A:GLY:H	12	0.24
(2,12)	1:10:A:CYS:HB3	1:13:A:GLY:H	14	0.24
(1,915)	1:51:A:CYS:HA	1:71:A:CYS:H	6	0.24
(1,900)	1:83:A:ILE:HG12	1:82:A:ASN:H	13	0.24
(1,900)	1:83:A:ILE:HG13	1:82:A:ASN:H	13	0.24
(1,896)	1:64:A:ARG:H	1:66:A:ASP:H	8	0.24
(1,888)	1:49:A:ILE:HA	1:61:A:VAL:H	2	0.24
(1,886)	1:51:A:CYS:H	1:58:A:CYS:H	12	0.24
(1,886)	1:51:A:CYS:H	1:58:A:CYS:H	13	0.24
(1,886)	1:51:A:CYS:H	1:58:A:CYS:H	19	0.24
(1,884)	1:50:A:SER:H	1:59:A:ILE:H	20	0.24
(1,872)	1:32:A:SER:H	1:33:A:ASP:HB2	9	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,872)	1:32:A:SER:H	1:33:A:ASP:HB3	9	0.24
(1,869)	1:14:A:GLN:HE22	1:28:A:CYS:H	17	0.24
(1,863)	1:17:A:PRO:HD2	1:20:A:TRP:HE1	10	0.24
(1,863)	1:17:A:PRO:HD3	1:20:A:TRP:HE1	10	0.24
(1,862)	1:21:A:LYS:HE2	1:19:A:ARG:H	16	0.24
(1,862)	1:21:A:LYS:HE3	1:19:A:ARG:H	16	0.24
(1,860)	1:16:A:VAL:HB	1:19:A:ARG:H	7	0.24
(1,859)	1:3:A:CYS:HB2	1:18:A:SER:H	8	0.24
(1,859)	1:3:A:CYS:HB3	1:18:A:SER:H	8	0.24
(1,849)	1:33:A:ASP:H	1:11:A:ASN:H	11	0.24
(1,842)	1:80:A:CYS:HA	1:84:A:THR:H	9	0.24
(1,838)	1:58:A:CYS:HA	1:52:A:GLY:H	18	0.24
(1,809)	1:106:A:GLY:H	1:104:A:CYS:H	7	0.24
(1,803)	1:101:A:ASN:HD21	1:99:A:SER:H	11	0.24
(1,803)	1:101:A:ASN:HD21	1:99:A:SER:H	15	0.24
(1,801)	1:102:A:PHE:HB2	1:98:A:ILE:H	14	0.24
(1,801)	1:102:A:PHE:HB3	1:98:A:ILE:H	14	0.24
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG21	3	0.24
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG22	3	0.24
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG23	3	0.24
(1,794)	1:82:A:ASN:HD22	1:94:A:SER:H	2	0.24
(1,791)	1:85:A:CYS:HB2	1:89:A:GLU:H	15	0.24
(1,791)	1:85:A:CYS:HB3	1:89:A:GLU:H	15	0.24
(1,783)	1:71:A:CYS:HB2	1:74:A:GLY:H	6	0.24
(1,783)	1:71:A:CYS:HB3	1:74:A:GLY:H	6	0.24
(1,768)	1:58:A:CYS:HA	1:59:A:ILE:H	1	0.24
(1,768)	1:58:A:CYS:HA	1:59:A:ILE:H	17	0.24
(1,766)	1:48:A:GLU:HB2	1:58:A:CYS:H	9	0.24
(1,766)	1:48:A:GLU:HB3	1:58:A:CYS:H	9	0.24
(1,761)	1:72:A:ASP:H	1:57:A:GLN:HE21	1	0.24
(1,761)	1:72:A:ASP:H	1:57:A:GLN:HE21	16	0.24
(1,734)	1:32:A:SER:H	1:11:A:ASN:H	5	0.24
(1,733)	1:32:A:SER:H	1:28:A:CYS:H	12	0.24
(1,731)	1:28:A:CYS:HB2	1:32:A:SER:H	15	0.24
(1,731)	1:28:A:CYS:HB3	1:32:A:SER:H	15	0.24
(1,729)	1:32:A:SER:H	1:28:A:CYS:H	12	0.24
(1,726)	1:34:A:GLU:HG2	1:27:A:ASP:H	14	0.24
(1,726)	1:34:A:GLU:HG3	1:27:A:ASP:H	14	0.24
(1,724)	1:34:A:GLU:HB2	1:25:A:ASP:H	3	0.24
(1,724)	1:34:A:GLU:HB3	1:25:A:ASP:H	3	0.24
(1,724)	1:34:A:GLU:HB2	1:25:A:ASP:H	8	0.24
(1,724)	1:34:A:GLU:HB3	1:25:A:ASP:H	8	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,718)	1:16:A:VAL:HB	1:20:A:TRP:HE1	7	0.24
(1,712)	1:32:A:SER:H	1:11:A:ASN:H	5	0.24
(1,711)	1:10:A:CYS:HB2	1:11:A:ASN:H	12	0.24
(1,711)	1:10:A:CYS:HB3	1:11:A:ASN:H	12	0.24
(1,690)	1:61:A:VAL:HG11	1:49:A:ILE:H	13	0.24
(1,690)	1:61:A:VAL:HG12	1:49:A:ILE:H	13	0.24
(1,690)	1:61:A:VAL:HG13	1:49:A:ILE:H	13	0.24
(1,690)	1:61:A:VAL:HG21	1:49:A:ILE:H	13	0.24
(1,690)	1:61:A:VAL:HG22	1:49:A:ILE:H	13	0.24
(1,690)	1:61:A:VAL:HG23	1:49:A:ILE:H	13	0.24
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD2	20	0.24
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD3	20	0.24
(1,667)	1:107:A:GLN:HG2	1:105:A:ASN:HD22	4	0.24
(1,667)	1:107:A:GLN:HG2	1:105:A:ASN:HD22	4	0.24
(1,667)	1:107:A:GLN:HG3	1:105:A:ASN:HD22	4	0.24
(1,667)	1:107:A:GLN:HG3	1:105:A:ASN:HD22	4	0.24
(1,658)	1:102:A:PHE:HA	1:105:A:ASN:HD22	3	0.24
(1,658)	1:102:A:PHE:HA	1:105:A:ASN:HD22	5	0.24
(1,639)	1:82:A:ASN:H	1:82:A:ASN:HD21	15	0.24
(1,596)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	3	0.24
(1,596)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	3	0.24
(1,592)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	1	0.24
(1,592)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	1	0.24
(1,592)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	5	0.24
(1,592)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	5	0.24
(1,591)	1:69:A:ASN:HB2	1:69:A:ASN:HD21	17	0.24
(1,591)	1:69:A:ASN:HB3	1:69:A:ASN:HD21	17	0.24
(1,585)	1:28:A:CYS:H	1:27:A:ASP:H	4	0.24
(1,585)	1:28:A:CYS:H	1:27:A:ASP:H	7	0.24
(1,569)	1:85:A:CYS:H	1:84:A:THR:H	20	0.24
(1,560)	1:90:A:PHE:H	1:99:A:SER:H	12	0.24
(1,560)	1:90:A:PHE:H	1:99:A:SER:H	15	0.24
(1,549)	1:115:A:ASP:HA	1:104:A:CYS:H	1	0.24
(1,545)	1:103:A:VAL:HA	1:105:A:ASN:H	11	0.24
(1,518)	1:49:A:ILE:H	1:61:A:VAL:H	20	0.24
(1,516)	1:49:A:ILE:H	1:59:A:ILE:H	6	0.24
(1,516)	1:49:A:ILE:H	1:59:A:ILE:H	18	0.24
(1,510)	1:48:A:GLU:HB2	1:48:A:GLU:H	9	0.24
(1,510)	1:48:A:GLU:HB3	1:48:A:GLU:H	9	0.24
(1,504)	1:39:A:CYS:HB2	1:39:A:CYS:H	5	0.24
(1,504)	1:39:A:CYS:HB3	1:39:A:CYS:H	5	0.24
(1,504)	1:39:A:CYS:HB2	1:39:A:CYS:H	9	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,504)	1:39:A:CYS:HB3	1:39:A:CYS:H	9	0.24
(1,504)	1:39:A:CYS:HB2	1:39:A:CYS:H	16	0.24
(1,504)	1:39:A:CYS:HB3	1:39:A:CYS:H	16	0.24
(1,504)	1:39:A:CYS:HB2	1:39:A:CYS:H	17	0.24
(1,504)	1:39:A:CYS:HB3	1:39:A:CYS:H	17	0.24
(1,504)	1:39:A:CYS:HB2	1:39:A:CYS:H	20	0.24
(1,504)	1:39:A:CYS:HB3	1:39:A:CYS:H	20	0.24
(1,501)	1:34:A:GLU:HB2	1:34:A:GLU:H	4	0.24
(1,501)	1:34:A:GLU:HB3	1:34:A:GLU:H	4	0.24
(1,499)	1:33:A:ASP:HB2	1:33:A:ASP:H	12	0.24
(1,499)	1:33:A:ASP:HB3	1:33:A:ASP:H	12	0.24
(1,476)	1:7:A:ASP:H	1:3:A:CYS:HB2	9	0.24
(1,476)	1:7:A:ASP:H	1:3:A:CYS:HB3	9	0.24
(1,454)	1:78:A:GLU:HG2	1:76:A:ASP:H	16	0.24
(1,454)	1:78:A:GLU:HG3	1:76:A:ASP:H	16	0.24
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB2	9	0.24
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB3	9	0.24
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB2	19	0.24
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB3	19	0.24
(1,437)	1:72:A:ASP:H	1:71:A:CYS:H	15	0.24
(1,418)	1:64:A:ARG:HA	1:66:A:ASP:H	16	0.24
(1,418)	1:64:A:ARG:HA	1:66:A:ASP:H	20	0.24
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB1	20	0.24
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB2	20	0.24
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB3	20	0.24
(1,375)	1:48:A:GLU:HA	1:49:A:ILE:H	2	0.24
(1,375)	1:48:A:GLU:HA	1:49:A:ILE:H	3	0.24
(1,375)	1:48:A:GLU:HA	1:49:A:ILE:H	7	0.24
(1,372)	1:48:A:GLU:H	1:48:A:GLU:HA	2	0.24
(1,347)	1:31:A:GLY:H	1:28:A:CYS:H	20	0.24
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB2	3	0.24
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB3	3	0.24
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB2	6	0.24
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB3	6	0.24
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB2	18	0.24
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB3	18	0.24
(1,328)	1:22:A:CYS:HB2	1:22:A:CYS:H	11	0.24
(1,328)	1:22:A:CYS:HB3	1:22:A:CYS:H	11	0.24
(1,328)	1:22:A:CYS:HB2	1:22:A:CYS:H	12	0.24
(1,328)	1:22:A:CYS:HB3	1:22:A:CYS:H	12	0.24
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB2	14	0.24
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB3	14	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,319)	1:16:A:VAL:H	1:9:A:VAL:HA	4	0.24
(1,312)	1:14:A:GLN:HG2	1:14:A:GLN:H	13	0.24
(1,312)	1:14:A:GLN:HG3	1:14:A:GLN:H	13	0.24
(1,298)	1:14:A:GLN:H	1:11:A:ASN:H	1	0.24
(1,283)	1:8:A:PHE:H	1:7:A:ASP:H	1	0.24
(1,279)	1:6:A:SER:HB2	1:6:A:SER:H	16	0.24
(1,279)	1:6:A:SER:HB3	1:6:A:SER:H	16	0.24
(1,277)	1:6:A:SER:HB2	1:6:A:SER:H	16	0.24
(1,277)	1:6:A:SER:HB3	1:6:A:SER:H	16	0.24
(1,248)	1:83:A:ILE:HB	1:84:A:THR:H	18	0.24
(1,228)	1:92:A:CYS:HB2	1:93:A:SER:H	7	0.24
(1,228)	1:92:A:CYS:HB3	1:93:A:SER:H	7	0.24
(1,205)	1:98:A:ILE:HG12	1:98:A:ILE:H	5	0.24
(1,205)	1:98:A:ILE:HG13	1:98:A:ILE:H	5	0.24
(1,205)	1:98:A:ILE:HG12	1:98:A:ILE:H	18	0.24
(1,205)	1:98:A:ILE:HG13	1:98:A:ILE:H	18	0.24
(1,204)	1:98:A:ILE:HG12	1:98:A:ILE:H	2	0.24
(1,204)	1:98:A:ILE:HG13	1:98:A:ILE:H	2	0.24
(1,204)	1:98:A:ILE:HG12	1:98:A:ILE:H	3	0.24
(1,204)	1:98:A:ILE:HG13	1:98:A:ILE:H	3	0.24
(1,203)	1:89:A:GLU:HB2	1:98:A:ILE:H	5	0.24
(1,203)	1:89:A:GLU:HB3	1:98:A:ILE:H	5	0.24
(1,203)	1:89:A:GLU:HB2	1:98:A:ILE:H	13	0.24
(1,203)	1:89:A:GLU:HB3	1:98:A:ILE:H	13	0.24
(1,165)	1:104:A:CYS:H	1:116:A:GLU:HA	19	0.24
(1,139)	1:109:A:ASP:H	1:109:A:ASP:HB2	5	0.24
(1,139)	1:109:A:ASP:H	1:109:A:ASP:HB3	5	0.24
(1,134)	1:110:A:CYS:H	1:109:A:ASP:HB2	7	0.24
(1,134)	1:110:A:CYS:H	1:109:A:ASP:HB2	7	0.24
(1,134)	1:110:A:CYS:H	1:109:A:ASP:HB3	7	0.24
(1,134)	1:110:A:CYS:H	1:109:A:ASP:HB3	7	0.24
(1,123)	1:115:A:ASP:HB2	1:115:A:ASP:H	5	0.24
(1,123)	1:115:A:ASP:HB3	1:115:A:ASP:H	5	0.24
(1,109)	1:119:A:CYS:H	1:117:A:LEU:HG	17	0.24
(1,96)	1:100:A:ARG:H	1:89:A:GLU:HA	9	0.24
(1,96)	1:100:A:ARG:H	1:89:A:GLU:HA	18	0.24
(1,94)	1:120:A:ALA:H	1:119:A:CYS:HB2	9	0.24
(1,94)	1:120:A:ALA:H	1:119:A:CYS:HB3	9	0.24
(1,92)	1:7:A:ASP:HB2	1:8:A:PHE:H	16	0.24
(1,92)	1:7:A:ASP:HB3	1:8:A:PHE:H	16	0.24
(1,85)	1:21:A:LYS:HG2	1:22:A:CYS:H	17	0.24
(1,85)	1:21:A:LYS:HG3	1:22:A:CYS:H	17	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,85)	1:21:A:LYS:HG2	1:22:A:CYS:H	19	0.24
(1,85)	1:21:A:LYS:HG3	1:22:A:CYS:H	19	0.24
(1,54)	1:73:A:SER:H	1:74:A:GLY:H	10	0.24
(1,51)	1:78:A:GLU:H	1:77:A:GLU:H	13	0.24
(1,49)	1:94:A:SER:H	1:93:A:SER:H	12	0.24
(1,17)	1:81:A:GLY:H	1:80:A:CYS:H	16	0.24
(1,15)	1:109:A:ASP:H	1:110:A:CYS:H	18	0.24
(1,15)	1:109:A:ASP:H	1:110:A:CYS:H	20	0.24
(1,9)	1:12:A:ASN:H	1:11:A:ASN:H	19	0.24
(4,6)	1:51:A:CYS:H	1:57:A:GLN:O	15	0.23
(3,7)	2:202:A:CA:CA	1:63:A:TRP:O	1	0.23
(2,382)	1:72:A:ASP:HB2	1:73:A:SER:H	6	0.23
(2,382)	1:72:A:ASP:HB3	1:73:A:SER:H	6	0.23
(2,376)	1:87:A:PRO:HB2	1:88:A:ASP:H	11	0.23
(2,329)	1:91:A:THR:HA	1:98:A:ILE:H	8	0.23
(2,327)	1:68:A:GLU:HG2	1:71:A:CYS:H	18	0.23
(2,304)	1:11:A:ASN:HD21	1:12:A:ASN:H	13	0.23
(2,253)	1:86:A:SER:HB2	1:89:A:GLU:H	6	0.23
(2,246)	1:90:A:PHE:HB2	1:100:A:ARG:H	15	0.23
(2,246)	1:90:A:PHE:HB3	1:100:A:ARG:H	15	0.23
(2,218)	1:36:A:PRO:HD2	1:37:A:GLU:H	11	0.23
(2,218)	1:36:A:PRO:HD2	1:37:A:GLU:H	19	0.23
(2,112)	1:84:A:THR:HG1	1:84:A:THR:H	12	0.23
(2,49)	1:35:A:SER:HB3	1:39:A:CYS:H	10	0.23
(2,46)	1:114:A:SER:HG	1:115:A:ASP:H	2	0.23
(2,44)	1:83:A:ILE:HG22	1:97:A:CYS:H	19	0.23
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG21	12	0.23
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG22	12	0.23
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG23	12	0.23
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG11	2	0.23
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG12	2	0.23
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG13	2	0.23
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG21	2	0.23
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG22	2	0.23
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG23	2	0.23
(1,916)	1:77:A:GLU:HB2	1:77:A:GLU:H	2	0.23
(1,916)	1:77:A:GLU:HB3	1:77:A:GLU:H	2	0.23
(1,900)	1:83:A:ILE:HG12	1:82:A:ASN:H	4	0.23
(1,900)	1:83:A:ILE:HG13	1:82:A:ASN:H	4	0.23
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB2	6	0.23
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB3	6	0.23
(1,886)	1:51:A:CYS:H	1:58:A:CYS:H	9	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,886)	1:51:A:CYS:H	1:58:A:CYS:H	11	0.23
(1,881)	1:48:A:GLU:H	1:45:A:ARG:H	20	0.23
(1,879)	1:48:A:GLU:H	1:45:A:ARG:H	20	0.23
(1,869)	1:14:A:GLN:HE22	1:28:A:CYS:H	20	0.23
(1,863)	1:17:A:PRO:HD2	1:20:A:TRP:HE1	20	0.23
(1,863)	1:17:A:PRO:HD3	1:20:A:TRP:HE1	20	0.23
(1,860)	1:16:A:VAL:HB	1:19:A:ARG:H	3	0.23
(1,860)	1:16:A:VAL:HB	1:19:A:ARG:H	13	0.23
(1,859)	1:3:A:CYS:HB2	1:18:A:SER:H	15	0.23
(1,859)	1:3:A:CYS:HB3	1:18:A:SER:H	15	0.23
(1,859)	1:3:A:CYS:HB2	1:18:A:SER:H	16	0.23
(1,859)	1:3:A:CYS:HB3	1:18:A:SER:H	16	0.23
(1,844)	1:79:A:ASN:HB2	1:92:A:CYS:H	11	0.23
(1,844)	1:79:A:ASN:HB3	1:92:A:CYS:H	11	0.23
(1,840)	1:71:A:CYS:HB2	1:77:A:GLU:H	10	0.23
(1,840)	1:71:A:CYS:HB3	1:77:A:GLU:H	10	0.23
(1,826)	1:114:A:SER:H	1:117:A:LEU:H	16	0.23
(1,810)	1:101:A:ASN:HD21	1:105:A:ASN:HD22	5	0.23
(1,810)	1:101:A:ASN:HD21	1:105:A:ASN:HD22	8	0.23
(1,810)	1:101:A:ASN:HD21	1:105:A:ASN:HD22	10	0.23
(1,809)	1:106:A:GLY:H	1:104:A:CYS:H	4	0.23
(1,806)	1:101:A:ASN:HD21	1:102:A:PHE:H	6	0.23
(1,806)	1:101:A:ASN:HD21	1:102:A:PHE:H	7	0.23
(1,799)	1:85:A:CYS:HA	1:97:A:CYS:H	7	0.23
(1,797)	1:91:A:THR:HG23	1:96:A:ARG:H	9	0.23
(1,797)	1:91:A:THR:HG23	1:96:A:ARG:H	16	0.23
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG21	9	0.23
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG22	9	0.23
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG23	9	0.23
(1,794)	1:82:A:ASN:HD22	1:94:A:SER:H	7	0.23
(1,794)	1:82:A:ASN:HD22	1:94:A:SER:H	9	0.23
(1,792)	1:97:A:CYS:HB2	1:91:A:THR:H	14	0.23
(1,792)	1:97:A:CYS:HB3	1:91:A:THR:H	14	0.23
(1,789)	1:85:A:CYS:H	1:84:A:THR:HB	18	0.23
(1,768)	1:58:A:CYS:HA	1:59:A:ILE:H	5	0.23
(1,768)	1:58:A:CYS:HA	1:59:A:ILE:H	6	0.23
(1,768)	1:58:A:CYS:HA	1:59:A:ILE:H	7	0.23
(1,768)	1:58:A:CYS:HA	1:59:A:ILE:H	19	0.23
(1,766)	1:48:A:GLU:HB2	1:58:A:CYS:H	5	0.23
(1,766)	1:48:A:GLU:HB3	1:58:A:CYS:H	5	0.23
(1,761)	1:72:A:ASP:H	1:57:A:GLN:HE21	7	0.23
(1,761)	1:72:A:ASP:H	1:57:A:GLN:HE21	11	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,745)	1:48:A:GLU:HB2	1:49:A:ILE:H	9	0.23
(1,745)	1:48:A:GLU:HB3	1:49:A:ILE:H	9	0.23
(1,745)	1:48:A:GLU:HB2	1:49:A:ILE:H	15	0.23
(1,745)	1:48:A:GLU:HB3	1:49:A:ILE:H	15	0.23
(1,744)	1:48:A:GLU:H	1:47:A:HIS:H	12	0.23
(1,734)	1:32:A:SER:H	1:11:A:ASN:H	1	0.23
(1,724)	1:34:A:GLU:HB2	1:25:A:ASP:H	2	0.23
(1,724)	1:34:A:GLU:HB3	1:25:A:ASP:H	2	0.23
(1,722)	1:23:A:ASP:H	1:45:A:ARG:HB2	5	0.23
(1,722)	1:23:A:ASP:H	1:45:A:ARG:HB3	5	0.23
(1,712)	1:32:A:SER:H	1:11:A:ASN:H	1	0.23
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD2	12	0.23
(1,710)	1:8:A:PHE:H	1:21:A:LYS:HD3	12	0.23
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG2	2	0.23
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG3	2	0.23
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG2	3	0.23
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG3	3	0.23
(1,693)	1:21:A:LYS:HD2	1:21:A:LYS:H	11	0.23
(1,693)	1:21:A:LYS:HD3	1:21:A:LYS:H	11	0.23
(1,693)	1:21:A:LYS:HD2	1:21:A:LYS:H	15	0.23
(1,693)	1:21:A:LYS:HD3	1:21:A:LYS:H	15	0.23
(1,693)	1:21:A:LYS:HD2	1:21:A:LYS:H	20	0.23
(1,693)	1:21:A:LYS:HD3	1:21:A:LYS:H	20	0.23
(1,685)	1:107:A:GLN:HG2	1:107:A:GLN:HE21	9	0.23
(1,685)	1:107:A:GLN:HG2	1:107:A:GLN:HE21	9	0.23
(1,685)	1:107:A:GLN:HG3	1:107:A:GLN:HE21	9	0.23
(1,685)	1:107:A:GLN:HG3	1:107:A:GLN:HE21	9	0.23
(1,591)	1:69:A:ASN:HB2	1:69:A:ASN:HD21	2	0.23
(1,591)	1:69:A:ASN:HB3	1:69:A:ASN:HD21	2	0.23
(1,585)	1:28:A:CYS:H	1:27:A:ASP:H	2	0.23
(1,569)	1:85:A:CYS:H	1:84:A:THR:H	5	0.23
(1,562)	1:102:A:PHE:HB2	1:99:A:SER:H	16	0.23
(1,562)	1:102:A:PHE:HB3	1:99:A:SER:H	16	0.23
(1,553)	1:115:A:ASP:HB2	1:104:A:CYS:H	6	0.23
(1,553)	1:115:A:ASP:HB3	1:104:A:CYS:H	6	0.23
(1,551)	1:104:A:CYS:HB2	1:104:A:CYS:H	11	0.23
(1,551)	1:104:A:CYS:HB3	1:104:A:CYS:H	11	0.23
(1,550)	1:104:A:CYS:HB2	1:104:A:CYS:H	11	0.23
(1,550)	1:104:A:CYS:HB3	1:104:A:CYS:H	11	0.23
(1,545)	1:103:A:VAL:HA	1:105:A:ASN:H	9	0.23
(1,543)	1:112:A:ASP:HB2	1:114:A:SER:H	14	0.23
(1,543)	1:112:A:ASP:HB3	1:114:A:SER:H	14	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,510)	1:48:A:GLU:HB2	1:48:A:GLU:H	20	0.23
(1,510)	1:48:A:GLU:HB3	1:48:A:GLU:H	20	0.23
(1,504)	1:39:A:CYS:HB2	1:39:A:CYS:H	1	0.23
(1,504)	1:39:A:CYS:HB3	1:39:A:CYS:H	1	0.23
(1,504)	1:39:A:CYS:HB2	1:39:A:CYS:H	3	0.23
(1,504)	1:39:A:CYS:HB3	1:39:A:CYS:H	3	0.23
(1,504)	1:39:A:CYS:HB2	1:39:A:CYS:H	6	0.23
(1,504)	1:39:A:CYS:HB3	1:39:A:CYS:H	6	0.23
(1,504)	1:39:A:CYS:HB2	1:39:A:CYS:H	7	0.23
(1,504)	1:39:A:CYS:HB3	1:39:A:CYS:H	7	0.23
(1,501)	1:34:A:GLU:HB2	1:34:A:GLU:H	16	0.23
(1,501)	1:34:A:GLU:HB3	1:34:A:GLU:H	16	0.23
(1,486)	1:7:A:ASP:HA	1:19:A:ARG:H	13	0.23
(1,486)	1:7:A:ASP:HA	1:19:A:ARG:H	15	0.23
(1,476)	1:7:A:ASP:H	1:3:A:CYS:HB2	11	0.23
(1,476)	1:7:A:ASP:H	1:3:A:CYS:HB3	11	0.23
(1,433)	1:74:A:GLY:HA2	1:71:A:CYS:H	10	0.23
(1,433)	1:74:A:GLY:HA3	1:71:A:CYS:H	10	0.23
(1,418)	1:64:A:ARG:HA	1:66:A:ASP:H	10	0.23
(1,418)	1:64:A:ARG:HA	1:66:A:ASP:H	11	0.23
(1,415)	1:64:A:ARG:HA	1:65:A:CYS:H	4	0.23
(1,415)	1:64:A:ARG:HA	1:65:A:CYS:H	14	0.23
(1,415)	1:64:A:ARG:HA	1:65:A:CYS:H	16	0.23
(1,415)	1:64:A:ARG:HA	1:65:A:CYS:H	20	0.23
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB2	9	0.23
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB3	9	0.23
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB1	9	0.23
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB2	9	0.23
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB3	9	0.23
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB1	19	0.23
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB2	19	0.23
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB3	19	0.23
(1,379)	1:50:A:SER:H	1:50:A:SER:HA	15	0.23
(1,379)	1:50:A:SER:H	1:50:A:SER:HA	18	0.23
(1,375)	1:48:A:GLU:HA	1:49:A:ILE:H	13	0.23
(1,365)	1:43:A:THR:HB	1:43:A:THR:H	11	0.23
(1,347)	1:31:A:GLY:H	1:28:A:CYS:H	13	0.23
(1,343)	1:28:A:CYS:HB2	1:28:A:CYS:H	17	0.23
(1,343)	1:28:A:CYS:HB3	1:28:A:CYS:H	17	0.23
(1,341)	1:31:A:GLY:H	1:28:A:CYS:H	19	0.23
(1,335)	1:45:A:ARG:HD2	1:24:A:GLY:H	14	0.23
(1,335)	1:45:A:ARG:HD3	1:24:A:GLY:H	14	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,328)	1:22:A:CYS:HB2	1:22:A:CYS:H	4	0.23
(1,328)	1:22:A:CYS:HB3	1:22:A:CYS:H	4	0.23
(1,328)	1:22:A:CYS:HB2	1:22:A:CYS:H	16	0.23
(1,328)	1:22:A:CYS:HB3	1:22:A:CYS:H	16	0.23
(1,290)	1:8:A:PHE:HA	1:9:A:VAL:H	10	0.23
(1,283)	1:8:A:PHE:H	1:7:A:ASP:H	3	0.23
(1,248)	1:83:A:ILE:HB	1:84:A:THR:H	20	0.23
(1,228)	1:92:A:CYS:HB2	1:93:A:SER:H	20	0.23
(1,228)	1:92:A:CYS:HB3	1:93:A:SER:H	20	0.23
(1,220)	1:92:A:CYS:HB2	1:95:A:GLY:H	10	0.23
(1,220)	1:92:A:CYS:HB3	1:95:A:GLY:H	10	0.23
(1,215)	1:96:A:ARG:H	1:92:A:CYS:HB2	1	0.23
(1,215)	1:96:A:ARG:H	1:92:A:CYS:HB3	1	0.23
(1,187)	1:103:A:VAL:HG11	1:102:A:PHE:H	11	0.23
(1,187)	1:103:A:VAL:HG12	1:102:A:PHE:H	11	0.23
(1,187)	1:103:A:VAL:HG13	1:102:A:PHE:H	11	0.23
(1,187)	1:103:A:VAL:HG21	1:102:A:PHE:H	11	0.23
(1,187)	1:103:A:VAL:HG22	1:102:A:PHE:H	11	0.23
(1,187)	1:103:A:VAL:HG23	1:102:A:PHE:H	11	0.23
(1,187)	1:103:A:VAL:HG11	1:102:A:PHE:H	12	0.23
(1,187)	1:103:A:VAL:HG12	1:102:A:PHE:H	12	0.23
(1,187)	1:103:A:VAL:HG13	1:102:A:PHE:H	12	0.23
(1,187)	1:103:A:VAL:HG21	1:102:A:PHE:H	12	0.23
(1,187)	1:103:A:VAL:HG22	1:102:A:PHE:H	12	0.23
(1,187)	1:103:A:VAL:HG23	1:102:A:PHE:H	12	0.23
(1,184)	1:103:A:VAL:HB	1:102:A:PHE:H	20	0.23
(1,128)	1:114:A:SER:HA	1:114:A:SER:H	1	0.23
(1,128)	1:114:A:SER:HA	1:114:A:SER:H	5	0.23
(1,128)	1:114:A:SER:HA	1:114:A:SER:H	10	0.23
(1,109)	1:119:A:CYS:H	1:117:A:LEU:HG	19	0.23
(1,98)	1:98:A:ILE:HG12	1:99:A:SER:H	20	0.23
(1,98)	1:98:A:ILE:HG13	1:99:A:SER:H	20	0.23
(1,94)	1:120:A:ALA:H	1:119:A:CYS:HB2	6	0.23
(1,94)	1:120:A:ALA:H	1:119:A:CYS:HB3	6	0.23
(1,66)	1:23:A:ASP:H	1:24:A:GLY:H	17	0.23
(1,60)	1:56:A:THR:H	1:57:A:GLN:H	3	0.23
(1,55)	1:71:A:CYS:H	1:70:A:ASP:H	5	0.23
(1,49)	1:94:A:SER:H	1:93:A:SER:H	15	0.23
(1,28)	1:118:A:ASP:H	1:117:A:LEU:H	9	0.23
(1,24)	1:104:A:CYS:H	1:105:A:ASN:H	2	0.23
(1,24)	1:104:A:CYS:H	1:105:A:ASN:H	19	0.23
(1,23)	1:104:A:CYS:H	1:105:A:ASN:H	2	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,23)	1:104:A:CYS:H	1:105:A:ASN:H	19	0.23
(1,14)	1:110:A:CYS:H	1:109:A:ASP:H	14	0.23
(1,6)	1:23:A:ASP:H	1:24:A:GLY:H	19	0.23
(4,7)	1:8:A:PHE:H	1:16:A:VAL:O	16	0.22
(2,368)	1:87:A:PRO:HD2	1:88:A:ASP:H	15	0.22
(2,362)	1:14:A:GLN:HB2	1:10:A:CYS:H	19	0.22
(2,362)	1:14:A:GLN:HB3	1:10:A:CYS:H	19	0.22
(2,304)	1:11:A:ASN:HD21	1:12:A:ASN:H	20	0.22
(2,245)	1:36:A:PRO:HA	1:39:A:CYS:H	1	0.22
(2,226)	1:92:A:CYS:H	1:97:A:CYS:H	6	0.22
(2,188)	1:16:A:VAL:HG11	1:19:A:ARG:H	2	0.22
(2,188)	1:16:A:VAL:HG12	1:19:A:ARG:H	2	0.22
(2,188)	1:16:A:VAL:HG13	1:19:A:ARG:H	2	0.22
(2,188)	1:16:A:VAL:HG21	1:19:A:ARG:H	2	0.22
(2,188)	1:16:A:VAL:HG22	1:19:A:ARG:H	2	0.22
(2,188)	1:16:A:VAL:HG23	1:19:A:ARG:H	2	0.22
(2,188)	1:16:A:VAL:HG11	1:19:A:ARG:H	5	0.22
(2,188)	1:16:A:VAL:HG12	1:19:A:ARG:H	5	0.22
(2,188)	1:16:A:VAL:HG13	1:19:A:ARG:H	5	0.22
(2,188)	1:16:A:VAL:HG21	1:19:A:ARG:H	5	0.22
(2,188)	1:16:A:VAL:HG22	1:19:A:ARG:H	5	0.22
(2,188)	1:16:A:VAL:HG23	1:19:A:ARG:H	5	0.22
(2,187)	1:118:A:ASP:HA	1:119:A:CYS:H	18	0.22
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	11	0.22
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	11	0.22
(2,184)	1:16:A:VAL:HG11	1:15:A:CYS:H	11	0.22
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	11	0.22
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	11	0.22
(2,184)	1:16:A:VAL:HG12	1:15:A:CYS:H	11	0.22
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	11	0.22
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	11	0.22
(2,184)	1:16:A:VAL:HG13	1:15:A:CYS:H	11	0.22
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	11	0.22
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	11	0.22
(2,184)	1:16:A:VAL:HG21	1:15:A:CYS:H	11	0.22
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	11	0.22
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	11	0.22
(2,184)	1:16:A:VAL:HG22	1:15:A:CYS:H	11	0.22
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	11	0.22
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	11	0.22
(2,184)	1:16:A:VAL:HG23	1:15:A:CYS:H	11	0.22
(2,174)	1:117:A:LEU:HB2	1:116:A:GLU:H	7	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,173)	1:69:A:ASN:HD21	1:69:A:ASN:H	12	0.22
(2,104)	1:80:A:CYS:HB3	1:80:A:CYS:H	14	0.22
(2,104)	1:80:A:CYS:HB3	1:80:A:CYS:H	18	0.22
(2,83)	1:35:A:SER:HB3	1:38:A:GLN:H	2	0.22
(2,80)	1:41:A:MET:HA	1:56:A:THR:H	4	0.22
(2,31)	1:59:A:ILE:HD11	1:71:A:CYS:H	4	0.22
(2,29)	1:28:A:CYS:HA	1:29:A:GLU:H	16	0.22
(2,25)	1:79:A:ASN:HD22	1:80:A:CYS:HA	14	0.22
(2,25)	1:79:A:ASN:HD22	1:80:A:CYS:HA	18	0.22
(2,22)	1:75:A:GLU:HA	1:78:A:GLU:H	10	0.22
(2,22)	1:75:A:GLU:HA	1:78:A:GLU:H	12	0.22
(1,926)	1:16:A:VAL:HG11	1:20:A:TRP:HZ3	8	0.22
(1,926)	1:16:A:VAL:HG12	1:20:A:TRP:HZ3	8	0.22
(1,926)	1:16:A:VAL:HG13	1:20:A:TRP:HZ3	8	0.22
(1,921)	1:8:A:PHE:HA	1:16:A:VAL:HG21	11	0.22
(1,921)	1:8:A:PHE:HA	1:16:A:VAL:HG22	11	0.22
(1,921)	1:8:A:PHE:HA	1:16:A:VAL:HG23	11	0.22
(1,921)	1:8:A:PHE:HA	1:16:A:VAL:HG21	16	0.22
(1,921)	1:8:A:PHE:HA	1:16:A:VAL:HG22	16	0.22
(1,921)	1:8:A:PHE:HA	1:16:A:VAL:HG23	16	0.22
(1,905)	1:101:A:ASN:HD21	1:105:A:ASN:HD21	10	0.22
(1,884)	1:50:A:SER:H	1:59:A:ILE:H	9	0.22
(1,884)	1:50:A:SER:H	1:59:A:ILE:H	16	0.22
(1,873)	1:34:A:GLU:HB2	1:33:A:ASP:H	6	0.22
(1,873)	1:34:A:GLU:HB3	1:33:A:ASP:H	6	0.22
(1,869)	1:14:A:GLN:HE22	1:28:A:CYS:H	18	0.22
(1,860)	1:16:A:VAL:HB	1:19:A:ARG:H	12	0.22
(1,860)	1:16:A:VAL:HB	1:19:A:ARG:H	18	0.22
(1,856)	1:14:A:GLN:H	1:12:A:ASN:HD22	2	0.22
(1,842)	1:80:A:CYS:HA	1:84:A:THR:H	14	0.22
(1,842)	1:80:A:CYS:HA	1:84:A:THR:H	19	0.22
(1,838)	1:58:A:CYS:HA	1:52:A:GLY:H	4	0.22
(1,837)	1:50:A:SER:H	1:45:A:ARG:HD2	17	0.22
(1,837)	1:50:A:SER:H	1:45:A:ARG:HD3	17	0.22
(1,826)	1:114:A:SER:H	1:117:A:LEU:H	2	0.22
(1,816)	1:109:A:ASP:H	1:116:A:GLU:HG2	14	0.22
(1,816)	1:109:A:ASP:H	1:116:A:GLU:HG3	14	0.22
(1,811)	1:107:A:GLN:H	1:105:A:ASN:HD21	8	0.22
(1,811)	1:107:A:GLN:H	1:105:A:ASN:HD21	10	0.22
(1,810)	1:101:A:ASN:HD21	1:105:A:ASN:HD22	1	0.22
(1,810)	1:101:A:ASN:HD21	1:105:A:ASN:HD22	18	0.22
(1,807)	1:98:A:ILE:HG12	1:103:A:VAL:H	3	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,807)	1:98:A:ILE:HG13	1:103:A:VAL:H	3	0.22
(1,791)	1:85:A:CYS:HB2	1:89:A:GLU:H	3	0.22
(1,791)	1:85:A:CYS:HB3	1:89:A:GLU:H	3	0.22
(1,791)	1:85:A:CYS:HB2	1:89:A:GLU:H	11	0.22
(1,791)	1:85:A:CYS:HB3	1:89:A:GLU:H	11	0.22
(1,791)	1:85:A:CYS:HB2	1:89:A:GLU:H	19	0.22
(1,791)	1:85:A:CYS:HB3	1:89:A:GLU:H	19	0.22
(1,788)	1:80:A:CYS:H	1:78:A:GLU:H	19	0.22
(1,783)	1:71:A:CYS:HB2	1:74:A:GLY:H	8	0.22
(1,783)	1:71:A:CYS:HB3	1:74:A:GLY:H	8	0.22
(1,768)	1:58:A:CYS:HA	1:59:A:ILE:H	13	0.22
(1,734)	1:32:A:SER:H	1:11:A:ASN:H	19	0.22
(1,726)	1:34:A:GLU:HG2	1:27:A:ASP:H	18	0.22
(1,726)	1:34:A:GLU:HG3	1:27:A:ASP:H	18	0.22
(1,712)	1:32:A:SER:H	1:11:A:ASN:H	19	0.22
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG2	12	0.22
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG3	12	0.22
(1,689)	1:69:A:ASN:HD21	1:69:A:ASN:H	12	0.22
(1,683)	1:78:A:GLU:HG2	1:79:A:ASN:HD21	19	0.22
(1,683)	1:78:A:GLU:HG3	1:79:A:ASN:HD21	19	0.22
(1,639)	1:82:A:ASN:H	1:82:A:ASN:HD21	17	0.22
(1,592)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	11	0.22
(1,592)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	11	0.22
(1,592)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	16	0.22
(1,592)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	16	0.22
(1,585)	1:28:A:CYS:H	1:27:A:ASP:H	17	0.22
(1,569)	1:85:A:CYS:H	1:84:A:THR:H	3	0.22
(1,569)	1:85:A:CYS:H	1:84:A:THR:H	6	0.22
(1,551)	1:104:A:CYS:HB2	1:104:A:CYS:H	17	0.22
(1,551)	1:104:A:CYS:HB3	1:104:A:CYS:H	17	0.22
(1,550)	1:104:A:CYS:HB2	1:104:A:CYS:H	17	0.22
(1,550)	1:104:A:CYS:HB3	1:104:A:CYS:H	17	0.22
(1,545)	1:103:A:VAL:HA	1:105:A:ASN:H	7	0.22
(1,545)	1:103:A:VAL:HA	1:105:A:ASN:H	16	0.22
(1,541)	1:115:A:ASP:HB2	1:116:A:GLU:H	12	0.22
(1,541)	1:115:A:ASP:HB3	1:116:A:GLU:H	12	0.22
(1,534)	1:77:A:GLU:HB2	1:77:A:GLU:H	1	0.22
(1,534)	1:77:A:GLU:HB3	1:77:A:GLU:H	1	0.22
(1,518)	1:49:A:ILE:H	1:61:A:VAL:H	1	0.22
(1,501)	1:34:A:GLU:HB2	1:34:A:GLU:H	3	0.22
(1,501)	1:34:A:GLU:HB3	1:34:A:GLU:H	3	0.22
(1,476)	1:7:A:ASP:H	1:3:A:CYS:HB2	19	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,476)	1:7:A:ASP:H	1:3:A:CYS:HB3	19	0.22
(1,475)	1:75:A:GLU:H	1:76:A:ASP:H	7	0.22
(1,468)	1:78:A:GLU:HG2	1:79:A:ASN:H	19	0.22
(1,468)	1:78:A:GLU:HG3	1:79:A:ASN:H	19	0.22
(1,454)	1:78:A:GLU:HG2	1:76:A:ASP:H	14	0.22
(1,454)	1:78:A:GLU:HG3	1:76:A:ASP:H	14	0.22
(1,451)	1:75:A:GLU:H	1:76:A:ASP:H	7	0.22
(1,433)	1:74:A:GLY:HA2	1:71:A:CYS:H	18	0.22
(1,433)	1:74:A:GLY:HA3	1:71:A:CYS:H	18	0.22
(1,432)	1:70:A:ASP:HB2	1:70:A:ASP:H	6	0.22
(1,432)	1:70:A:ASP:HB3	1:70:A:ASP:H	6	0.22
(1,418)	1:64:A:ARG:HA	1:66:A:ASP:H	5	0.22
(1,418)	1:64:A:ARG:HA	1:66:A:ASP:H	7	0.22
(1,418)	1:64:A:ARG:HA	1:66:A:ASP:H	8	0.22
(1,418)	1:64:A:ARG:HA	1:66:A:ASP:H	12	0.22
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB2	20	0.22
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB3	20	0.22
(1,386)	1:51:A:CYS:HB2	1:51:A:CYS:H	2	0.22
(1,386)	1:51:A:CYS:HB3	1:51:A:CYS:H	2	0.22
(1,383)	1:51:A:CYS:H	1:50:A:SER:HA	4	0.22
(1,374)	1:61:A:VAL:H	1:49:A:ILE:H	9	0.22
(1,369)	1:43:A:THR:HB	1:44:A:CYS:H	18	0.22
(1,351)	1:32:A:SER:H	1:33:A:ASP:H	7	0.22
(1,351)	1:32:A:SER:H	1:33:A:ASP:H	17	0.22
(1,349)	1:32:A:SER:H	1:33:A:ASP:H	7	0.22
(1,349)	1:32:A:SER:H	1:33:A:ASP:H	17	0.22
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB2	10	0.22
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB3	10	0.22
(1,335)	1:45:A:ARG:HD2	1:24:A:GLY:H	7	0.22
(1,335)	1:45:A:ARG:HD3	1:24:A:GLY:H	7	0.22
(1,328)	1:22:A:CYS:HB2	1:22:A:CYS:H	3	0.22
(1,328)	1:22:A:CYS:HB3	1:22:A:CYS:H	3	0.22
(1,328)	1:22:A:CYS:HB2	1:22:A:CYS:H	5	0.22
(1,328)	1:22:A:CYS:HB3	1:22:A:CYS:H	5	0.22
(1,328)	1:22:A:CYS:HB2	1:22:A:CYS:H	6	0.22
(1,328)	1:22:A:CYS:HB3	1:22:A:CYS:H	6	0.22
(1,328)	1:22:A:CYS:HB2	1:22:A:CYS:H	19	0.22
(1,328)	1:22:A:CYS:HB3	1:22:A:CYS:H	19	0.22
(1,320)	1:7:A:ASP:HA	1:18:A:SER:H	7	0.22
(1,319)	1:16:A:VAL:H	1:9:A:VAL:HA	12	0.22
(1,312)	1:14:A:GLN:HG2	1:14:A:GLN:H	9	0.22
(1,312)	1:14:A:GLN:HG3	1:14:A:GLN:H	9	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,312)	1:14:A:GLN:HG2	1:14:A:GLN:H	19	0.22
(1,312)	1:14:A:GLN:HG3	1:14:A:GLN:H	19	0.22
(1,299)	1:11:A:ASN:H	1:12:A:ASN:H	17	0.22
(1,283)	1:8:A:PHE:H	1:7:A:ASP:H	2	0.22
(1,283)	1:8:A:PHE:H	1:7:A:ASP:H	4	0.22
(1,283)	1:8:A:PHE:H	1:7:A:ASP:H	6	0.22
(1,283)	1:8:A:PHE:H	1:7:A:ASP:H	9	0.22
(1,283)	1:8:A:PHE:H	1:7:A:ASP:H	10	0.22
(1,283)	1:8:A:PHE:H	1:7:A:ASP:H	16	0.22
(1,283)	1:8:A:PHE:H	1:7:A:ASP:H	18	0.22
(1,281)	1:5:A:GLU:HB2	1:6:A:SER:H	9	0.22
(1,281)	1:5:A:GLU:HB2	1:6:A:SER:H	9	0.22
(1,281)	1:5:A:GLU:HB3	1:6:A:SER:H	9	0.22
(1,281)	1:5:A:GLU:HB3	1:6:A:SER:H	9	0.22
(1,248)	1:83:A:ILE:HB	1:84:A:THR:H	16	0.22
(1,228)	1:92:A:CYS:HB2	1:93:A:SER:H	12	0.22
(1,228)	1:92:A:CYS:HB3	1:93:A:SER:H	12	0.22
(1,205)	1:98:A:ILE:HG12	1:98:A:ILE:H	19	0.22
(1,205)	1:98:A:ILE:HG13	1:98:A:ILE:H	19	0.22
(1,187)	1:103:A:VAL:HG11	1:102:A:PHE:H	15	0.22
(1,187)	1:103:A:VAL:HG12	1:102:A:PHE:H	15	0.22
(1,187)	1:103:A:VAL:HG13	1:102:A:PHE:H	15	0.22
(1,187)	1:103:A:VAL:HG21	1:102:A:PHE:H	15	0.22
(1,187)	1:103:A:VAL:HG22	1:102:A:PHE:H	15	0.22
(1,187)	1:103:A:VAL:HG23	1:102:A:PHE:H	15	0.22
(1,184)	1:103:A:VAL:HB	1:102:A:PHE:H	12	0.22
(1,136)	1:112:A:ASP:H	1:110:A:CYS:H	4	0.22
(1,128)	1:114:A:SER:HA	1:114:A:SER:H	8	0.22
(1,109)	1:119:A:CYS:H	1:117:A:LEU:HG	4	0.22
(1,98)	1:98:A:ILE:HG12	1:99:A:SER:H	15	0.22
(1,98)	1:98:A:ILE:HG13	1:99:A:SER:H	15	0.22
(1,96)	1:100:A:ARG:H	1:89:A:GLU:HA	4	0.22
(1,92)	1:7:A:ASP:HB2	1:8:A:PHE:H	11	0.22
(1,92)	1:7:A:ASP:HB3	1:8:A:PHE:H	11	0.22
(1,74)	1:65:A:CYS:H	1:65:A:CYS:HB2	5	0.22
(1,74)	1:65:A:CYS:H	1:65:A:CYS:HB3	5	0.22
(1,74)	1:65:A:CYS:H	1:65:A:CYS:HB2	20	0.22
(1,74)	1:65:A:CYS:H	1:65:A:CYS:HB3	20	0.22
(1,70)	1:77:A:GLU:HB2	1:78:A:GLU:H	6	0.22
(1,70)	1:77:A:GLU:HB3	1:78:A:GLU:H	6	0.22
(1,55)	1:71:A:CYS:H	1:70:A:ASP:H	20	0.22
(1,33)	1:115:A:ASP:H	1:114:A:SER:H	19	0.22

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,9)	1:12:A:ASN:H	1:11:A:ASN:H	5	0.22
(4,5)	1:49:A:ILE:O	1:59:A:ILE:H	1	0.21
(4,5)	1:49:A:ILE:O	1:59:A:ILE:H	2	0.21
(4,5)	1:49:A:ILE:O	1:59:A:ILE:H	15	0.21
(4,2)	1:90:A:PHE:O	1:98:A:ILE:H	11	0.21
(3,7)	2:202:A:CA:CA	1:63:A:TRP:O	17	0.21
(2,366)	1:107:A:GLN:HA	1:106:A:GLY:H	7	0.21
(2,359)	1:98:A:ILE:HD12	1:98:A:ILE:H	18	0.21
(2,357)	1:69:A:ASN:HA	1:69:A:ASN:HD21	6	0.21
(2,320)	1:59:A:ILE:HA	1:58:A:CYS:H	4	0.21
(2,304)	1:11:A:ASN:HD21	1:12:A:ASN:H	16	0.21
(2,301)	1:11:A:ASN:HD22	1:32:A:SER:H	17	0.21
(2,276)	1:43:A:THR:HA	1:57:A:GLN:H	17	0.21
(2,270)	1:113:A:GLY:HA2	1:110:A:CYS:H	19	0.21
(2,263)	1:62:A:SER:HB2	1:63:A:TRP:H	12	0.21
(2,226)	1:98:A:ILE:H	1:97:A:CYS:H	19	0.21
(2,181)	1:39:A:CYS:HB3	1:41:A:MET:H	6	0.21
(2,180)	1:11:A:ASN:HA	1:11:A:ASN:HD21	12	0.21
(2,123)	1:16:A:VAL:HG11	1:33:A:ASP:H	7	0.21
(2,123)	1:16:A:VAL:HG12	1:33:A:ASP:H	7	0.21
(2,123)	1:16:A:VAL:HG13	1:33:A:ASP:H	7	0.21
(2,123)	1:16:A:VAL:HG21	1:33:A:ASP:H	7	0.21
(2,123)	1:16:A:VAL:HG22	1:33:A:ASP:H	7	0.21
(2,123)	1:16:A:VAL:HG23	1:33:A:ASP:H	7	0.21
(2,89)	1:107:A:GLN:HB2	1:108:A:ASP:H	7	0.21
(2,89)	1:107:A:GLN:HB3	1:108:A:ASP:H	7	0.21
(2,49)	1:35:A:SER:HB3	1:39:A:CYS:H	6	0.21
(2,44)	1:83:A:ILE:HG21	1:97:A:CYS:H	7	0.21
(1,917)	1:28:A:CYS:H	1:14:A:GLN:HG2	1	0.21
(1,905)	1:101:A:ASN:HD21	1:105:A:ASN:HD21	1	0.21
(1,890)	1:81:A:GLY:HA2	1:63:A:TRP:HE1	2	0.21
(1,890)	1:81:A:GLY:HA2	1:63:A:TRP:HE1	2	0.21
(1,890)	1:81:A:GLY:HA3	1:63:A:TRP:HE1	2	0.21
(1,890)	1:81:A:GLY:HA3	1:63:A:TRP:HE1	2	0.21
(1,886)	1:51:A:CYS:H	1:58:A:CYS:H	4	0.21
(1,886)	1:51:A:CYS:H	1:58:A:CYS:H	15	0.21
(1,869)	1:14:A:GLN:HE22	1:28:A:CYS:H	8	0.21
(1,863)	1:17:A:PRO:HD2	1:20:A:TRP:HE1	7	0.21
(1,863)	1:17:A:PRO:HD3	1:20:A:TRP:HE1	7	0.21
(1,863)	1:17:A:PRO:HD2	1:20:A:TRP:HE1	13	0.21
(1,863)	1:17:A:PRO:HD3	1:20:A:TRP:HE1	13	0.21
(1,856)	1:14:A:GLN:H	1:12:A:ASN:HD22	5	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,851)	1:32:A:SER:H	1:11:A:ASN:HD22	17	0.21
(1,849)	1:33:A:ASP:H	1:11:A:ASN:H	16	0.21
(1,844)	1:79:A:ASN:HB2	1:92:A:CYS:H	18	0.21
(1,844)	1:79:A:ASN:HB3	1:92:A:CYS:H	18	0.21
(1,842)	1:80:A:CYS:HA	1:84:A:THR:H	3	0.21
(1,842)	1:80:A:CYS:HA	1:84:A:THR:H	10	0.21
(1,842)	1:80:A:CYS:HA	1:84:A:THR:H	18	0.21
(1,840)	1:71:A:CYS:HB2	1:77:A:GLU:H	6	0.21
(1,840)	1:71:A:CYS:HB3	1:77:A:GLU:H	6	0.21
(1,822)	1:113:A:GLY:HA2	1:116:A:GLU:H	3	0.21
(1,822)	1:113:A:GLY:HA3	1:116:A:GLU:H	3	0.21
(1,809)	1:106:A:GLY:H	1:104:A:CYS:H	6	0.21
(1,809)	1:106:A:GLY:H	1:104:A:CYS:H	10	0.21
(1,801)	1:102:A:PHE:HB2	1:98:A:ILE:H	9	0.21
(1,801)	1:102:A:PHE:HB3	1:98:A:ILE:H	9	0.21
(1,791)	1:85:A:CYS:HB2	1:89:A:GLU:H	6	0.21
(1,791)	1:85:A:CYS:HB3	1:89:A:GLU:H	6	0.21
(1,789)	1:85:A:CYS:H	1:84:A:THR:HB	15	0.21
(1,789)	1:85:A:CYS:H	1:84:A:THR:HB	16	0.21
(1,788)	1:80:A:CYS:H	1:78:A:GLU:H	15	0.21
(1,786)	1:71:A:CYS:H	1:76:A:ASP:H	14	0.21
(1,776)	1:77:A:GLU:HG2	1:70:A:ASP:H	8	0.21
(1,776)	1:77:A:GLU:HG3	1:70:A:ASP:H	8	0.21
(1,772)	1:68:A:GLU:H	1:64:A:ARG:H	17	0.21
(1,768)	1:58:A:CYS:HA	1:59:A:ILE:H	2	0.21
(1,761)	1:72:A:ASP:H	1:57:A:GLN:HE21	18	0.21
(1,759)	1:57:A:GLN:HE21	1:71:A:CYS:HA	10	0.21
(1,734)	1:32:A:SER:H	1:11:A:ASN:H	17	0.21
(1,724)	1:34:A:GLU:HB2	1:25:A:ASP:H	6	0.21
(1,724)	1:34:A:GLU:HB3	1:25:A:ASP:H	6	0.21
(1,712)	1:32:A:SER:H	1:11:A:ASN:H	17	0.21
(1,705)	1:100:A:ARG:H	1:100:A:ARG:HD2	16	0.21
(1,705)	1:100:A:ARG:H	1:100:A:ARG:HD3	16	0.21
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG2	9	0.21
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG3	9	0.21
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG2	14	0.21
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG3	14	0.21
(1,694)	1:21:A:LYS:HE2	1:21:A:LYS:H	10	0.21
(1,694)	1:21:A:LYS:HE3	1:21:A:LYS:H	10	0.21
(1,687)	1:69:A:ASN:HD21	1:74:A:GLY:H	6	0.21
(1,686)	1:74:A:GLY:H	1:69:A:ASN:HD22	17	0.21
(1,679)	1:78:A:GLU:HG2	1:79:A:ASN:HD22	1	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,679)	1:78:A:GLU:HG3	1:79:A:ASN:HD22	1	0.21
(1,645)	1:101:A:ASN:HD22	1:101:A:ASN:H	2	0.21
(1,639)	1:82:A:ASN:H	1:82:A:ASN:HD21	13	0.21
(1,639)	1:82:A:ASN:H	1:82:A:ASN:HD21	19	0.21
(1,628)	1:71:A:CYS:HB2	1:57:A:GLN:HE22	3	0.21
(1,628)	1:71:A:CYS:HB3	1:57:A:GLN:HE22	3	0.21
(1,628)	1:71:A:CYS:HB2	1:57:A:GLN:HE22	11	0.21
(1,628)	1:71:A:CYS:HB3	1:57:A:GLN:HE22	11	0.21
(1,628)	1:71:A:CYS:HB2	1:57:A:GLN:HE22	16	0.21
(1,628)	1:71:A:CYS:HB3	1:57:A:GLN:HE22	16	0.21
(1,626)	1:71:A:CYS:HA	1:57:A:GLN:HE22	14	0.21
(1,612)	1:15:A:CYS:H	1:14:A:GLN:HE22	2	0.21
(1,603)	1:32:A:SER:HB2	1:11:A:ASN:HD22	17	0.21
(1,603)	1:32:A:SER:HB3	1:11:A:ASN:HD22	17	0.21
(1,598)	1:74:A:GLY:HA2	1:69:A:ASN:HD22	6	0.21
(1,598)	1:74:A:GLY:HA3	1:69:A:ASN:HD22	6	0.21
(1,597)	1:74:A:GLY:HA2	1:69:A:ASN:HD22	6	0.21
(1,597)	1:74:A:GLY:HA3	1:69:A:ASN:HD22	6	0.21
(1,585)	1:28:A:CYS:H	1:27:A:ASP:H	10	0.21
(1,585)	1:28:A:CYS:H	1:27:A:ASP:H	14	0.21
(1,569)	1:85:A:CYS:H	1:84:A:THR:H	2	0.21
(1,569)	1:85:A:CYS:H	1:84:A:THR:H	4	0.21
(1,569)	1:85:A:CYS:H	1:84:A:THR:H	10	0.21
(1,569)	1:85:A:CYS:H	1:84:A:THR:H	11	0.21
(1,562)	1:102:A:PHE:HB2	1:99:A:SER:H	2	0.21
(1,562)	1:102:A:PHE:HB3	1:99:A:SER:H	2	0.21
(1,562)	1:102:A:PHE:HB2	1:99:A:SER:H	20	0.21
(1,562)	1:102:A:PHE:HB3	1:99:A:SER:H	20	0.21
(1,560)	1:90:A:PHE:H	1:99:A:SER:H	14	0.21
(1,560)	1:90:A:PHE:H	1:99:A:SER:H	19	0.21
(1,553)	1:115:A:ASP:HB2	1:104:A:CYS:H	13	0.21
(1,553)	1:115:A:ASP:HB3	1:104:A:CYS:H	13	0.21
(1,545)	1:103:A:VAL:HA	1:105:A:ASN:H	3	0.21
(1,541)	1:115:A:ASP:HB2	1:116:A:GLU:H	4	0.21
(1,541)	1:115:A:ASP:HB3	1:116:A:GLU:H	4	0.21
(1,534)	1:77:A:GLU:HB2	1:77:A:GLU:H	5	0.21
(1,534)	1:77:A:GLU:HB3	1:77:A:GLU:H	5	0.21
(1,518)	1:49:A:ILE:H	1:61:A:VAL:H	17	0.21
(1,516)	1:49:A:ILE:H	1:59:A:ILE:H	1	0.21
(1,510)	1:48:A:GLU:HB2	1:48:A:GLU:H	4	0.21
(1,510)	1:48:A:GLU:HB3	1:48:A:GLU:H	4	0.21
(1,510)	1:48:A:GLU:HB2	1:48:A:GLU:H	12	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,510)	1:48:A:GLU:HB3	1:48:A:GLU:H	12	0.21
(1,504)	1:39:A:CYS:HB2	1:39:A:CYS:H	4	0.21
(1,504)	1:39:A:CYS:HB3	1:39:A:CYS:H	4	0.21
(1,499)	1:33:A:ASP:HB2	1:33:A:ASP:H	15	0.21
(1,499)	1:33:A:ASP:HB3	1:33:A:ASP:H	15	0.21
(1,499)	1:33:A:ASP:HB2	1:33:A:ASP:H	20	0.21
(1,499)	1:33:A:ASP:HB3	1:33:A:ASP:H	20	0.21
(1,486)	1:7:A:ASP:HA	1:19:A:ARG:H	6	0.21
(1,483)	1:10:A:CYS:HB2	1:14:A:GLN:H	11	0.21
(1,483)	1:10:A:CYS:HB3	1:14:A:GLN:H	11	0.21
(1,482)	1:11:A:ASN:HD21	1:11:A:ASN:H	8	0.21
(1,482)	1:11:A:ASN:HD21	1:11:A:ASN:H	20	0.21
(1,462)	1:79:A:ASN:H	1:78:A:GLU:H	14	0.21
(1,460)	1:74:A:GLY:HA2	1:77:A:GLU:H	13	0.21
(1,460)	1:74:A:GLY:HA3	1:77:A:GLU:H	13	0.21
(1,445)	1:75:A:GLU:H	1:74:A:GLY:H	15	0.21
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB2	3	0.21
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB3	3	0.21
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB2	5	0.21
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB3	5	0.21
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB2	16	0.21
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB3	16	0.21
(1,415)	1:64:A:ARG:HA	1:65:A:CYS:H	2	0.21
(1,415)	1:64:A:ARG:HA	1:65:A:CYS:H	5	0.21
(1,415)	1:64:A:ARG:HA	1:65:A:CYS:H	10	0.21
(1,415)	1:64:A:ARG:HA	1:65:A:CYS:H	18	0.21
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB2	11	0.21
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB3	11	0.21
(1,390)	1:51:A:CYS:HB2	1:52:A:GLY:H	9	0.21
(1,390)	1:51:A:CYS:HB3	1:52:A:GLY:H	9	0.21
(1,386)	1:51:A:CYS:HB2	1:51:A:CYS:H	7	0.21
(1,386)	1:51:A:CYS:HB3	1:51:A:CYS:H	7	0.21
(1,386)	1:51:A:CYS:HB2	1:51:A:CYS:H	17	0.21
(1,386)	1:51:A:CYS:HB3	1:51:A:CYS:H	17	0.21
(1,383)	1:51:A:CYS:H	1:50:A:SER:HA	12	0.21
(1,372)	1:48:A:GLU:H	1:48:A:GLU:HA	6	0.21
(1,372)	1:48:A:GLU:H	1:48:A:GLU:HA	7	0.21
(1,372)	1:48:A:GLU:H	1:48:A:GLU:HA	13	0.21
(1,367)	1:42:A:ARG:HG2	1:43:A:THR:H	1	0.21
(1,367)	1:42:A:ARG:HG2	1:43:A:THR:H	1	0.21
(1,367)	1:42:A:ARG:HG3	1:43:A:THR:H	1	0.21
(1,367)	1:42:A:ARG:HG3	1:43:A:THR:H	1	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,343)	1:28:A:CYS:HB2	1:28:A:CYS:H	3	0.21
(1,343)	1:28:A:CYS:HB3	1:28:A:CYS:H	3	0.21
(1,328)	1:22:A:CYS:HB2	1:22:A:CYS:H	1	0.21
(1,328)	1:22:A:CYS:HB3	1:22:A:CYS:H	1	0.21
(1,328)	1:22:A:CYS:HB2	1:22:A:CYS:H	17	0.21
(1,328)	1:22:A:CYS:HB3	1:22:A:CYS:H	17	0.21
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB2	15	0.21
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB3	15	0.21
(1,320)	1:7:A:ASP:HA	1:18:A:SER:H	16	0.21
(1,319)	1:16:A:VAL:H	1:9:A:VAL:HA	9	0.21
(1,312)	1:14:A:GLN:HG2	1:14:A:GLN:H	6	0.21
(1,312)	1:14:A:GLN:HG3	1:14:A:GLN:H	6	0.21
(1,312)	1:14:A:GLN:HG2	1:14:A:GLN:H	12	0.21
(1,312)	1:14:A:GLN:HG3	1:14:A:GLN:H	12	0.21
(1,308)	1:13:A:GLY:H	1:14:A:GLN:H	3	0.21
(1,308)	1:13:A:GLY:H	1:14:A:GLN:H	4	0.21
(1,308)	1:13:A:GLY:H	1:14:A:GLN:H	8	0.21
(1,308)	1:13:A:GLY:H	1:14:A:GLN:H	18	0.21
(1,290)	1:8:A:PHE:HA	1:9:A:VAL:H	9	0.21
(1,290)	1:8:A:PHE:HA	1:9:A:VAL:H	14	0.21
(1,290)	1:8:A:PHE:HA	1:9:A:VAL:H	16	0.21
(1,286)	1:7:A:ASP:HB2	1:7:A:ASP:H	1	0.21
(1,286)	1:7:A:ASP:HB3	1:7:A:ASP:H	1	0.21
(1,286)	1:7:A:ASP:HB2	1:7:A:ASP:H	5	0.21
(1,286)	1:7:A:ASP:HB3	1:7:A:ASP:H	5	0.21
(1,283)	1:8:A:PHE:H	1:7:A:ASP:H	7	0.21
(1,283)	1:8:A:PHE:H	1:7:A:ASP:H	12	0.21
(1,283)	1:8:A:PHE:H	1:7:A:ASP:H	15	0.21
(1,283)	1:8:A:PHE:H	1:7:A:ASP:H	19	0.21
(1,281)	1:5:A:GLU:HB2	1:6:A:SER:H	12	0.21
(1,281)	1:5:A:GLU:HB2	1:6:A:SER:H	12	0.21
(1,281)	1:5:A:GLU:HB3	1:6:A:SER:H	12	0.21
(1,281)	1:5:A:GLU:HB3	1:6:A:SER:H	12	0.21
(1,273)	1:7:A:ASP:HB2	1:4:A:ALA:H	6	0.21
(1,273)	1:7:A:ASP:HB3	1:4:A:ALA:H	6	0.21
(1,248)	1:83:A:ILE:HB	1:84:A:THR:H	2	0.21
(1,232)	1:95:A:GLY:H	1:92:A:CYS:H	4	0.21
(1,226)	1:92:A:CYS:HB2	1:94:A:SER:H	7	0.21
(1,226)	1:92:A:CYS:HB3	1:94:A:SER:H	7	0.21
(1,205)	1:98:A:ILE:HG12	1:98:A:ILE:H	1	0.21
(1,205)	1:98:A:ILE:HG13	1:98:A:ILE:H	1	0.21
(1,205)	1:98:A:ILE:HG12	1:98:A:ILE:H	17	0.21

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,205)	1:98:A:ILE:HG13	1:98:A:ILE:H	17	0.21
(1,204)	1:98:A:ILE:HG12	1:98:A:ILE:H	4	0.21
(1,204)	1:98:A:ILE:HG13	1:98:A:ILE:H	4	0.21
(1,204)	1:98:A:ILE:HG12	1:98:A:ILE:H	7	0.21
(1,204)	1:98:A:ILE:HG13	1:98:A:ILE:H	7	0.21
(1,204)	1:98:A:ILE:HG12	1:98:A:ILE:H	12	0.21
(1,204)	1:98:A:ILE:HG13	1:98:A:ILE:H	12	0.21
(1,184)	1:103:A:VAL:HB	1:102:A:PHE:H	13	0.21
(1,180)	1:99:A:SER:HB2	1:102:A:PHE:H	12	0.21
(1,180)	1:99:A:SER:HB3	1:102:A:PHE:H	12	0.21
(1,136)	1:112:A:ASP:H	1:110:A:CYS:H	6	0.21
(1,128)	1:114:A:SER:HA	1:114:A:SER:H	2	0.21
(1,128)	1:114:A:SER:HA	1:114:A:SER:H	6	0.21
(1,128)	1:114:A:SER:HA	1:114:A:SER:H	17	0.21
(1,128)	1:114:A:SER:HA	1:114:A:SER:H	19	0.21
(1,123)	1:115:A:ASP:HB2	1:115:A:ASP:H	4	0.21
(1,123)	1:115:A:ASP:HB3	1:115:A:ASP:H	4	0.21
(1,123)	1:115:A:ASP:HB2	1:115:A:ASP:H	7	0.21
(1,123)	1:115:A:ASP:HB3	1:115:A:ASP:H	7	0.21
(1,116)	1:116:A:GLU:HG2	1:116:A:GLU:H	5	0.21
(1,116)	1:116:A:GLU:HG3	1:116:A:GLU:H	5	0.21
(1,109)	1:119:A:CYS:H	1:117:A:LEU:HG	3	0.21
(1,109)	1:119:A:CYS:H	1:117:A:LEU:HG	7	0.21
(1,109)	1:119:A:CYS:H	1:117:A:LEU:HG	20	0.21
(1,96)	1:100:A:ARG:H	1:89:A:GLU:HA	12	0.21
(1,92)	1:7:A:ASP:HB2	1:8:A:PHE:H	9	0.21
(1,92)	1:7:A:ASP:HB3	1:8:A:PHE:H	9	0.21
(1,91)	1:14:A:GLN:HG2	1:15:A:CYS:H	5	0.21
(1,91)	1:14:A:GLN:HG3	1:15:A:CYS:H	5	0.21
(1,55)	1:71:A:CYS:H	1:70:A:ASP:H	3	0.21
(1,49)	1:94:A:SER:H	1:93:A:SER:H	1	0.21
(1,28)	1:118:A:ASP:H	1:117:A:LEU:H	6	0.21
(1,17)	1:81:A:GLY:H	1:80:A:CYS:H	6	0.21
(1,15)	1:109:A:ASP:H	1:110:A:CYS:H	15	0.21
(1,14)	1:110:A:CYS:H	1:109:A:ASP:H	9	0.21
(1,6)	1:23:A:ASP:H	1:24:A:GLY:H	8	0.21
(4,7)	1:8:A:PHE:H	1:16:A:VAL:O	11	0.2
(4,6)	1:51:A:CYS:H	1:57:A:GLN:O	12	0.2
(4,5)	1:49:A:ILE:O	1:59:A:ILE:H	9	0.2
(3,7)	2:202:A:CA:CA	1:63:A:TRP:O	9	0.2
(2,376)	1:87:A:PRO:HB2	1:88:A:ASP:H	20	0.2
(2,370)	1:38:A:GLN:HG2	1:38:A:GLN:HE22	12	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,353)	1:99:A:SER:HG	1:101:A:ASN:HD22	20	0.2
(2,331)	1:101:A:ASN:H	1:99:A:SER:H	3	0.2
(2,329)	1:90:A:PHE:HA	1:98:A:ILE:H	16	0.2
(2,304)	1:11:A:ASN:HD21	1:12:A:ASN:H	11	0.2
(2,298)	1:28:A:CYS:HB2	1:14:A:GLN:HE22	14	0.2
(2,298)	1:28:A:CYS:HB3	1:14:A:GLN:HE22	16	0.2
(2,293)	1:18:A:SER:HB3	1:8:A:PHE:H	16	0.2
(2,280)	1:92:A:CYS:H	1:91:A:THR:H	7	0.2
(2,280)	1:92:A:CYS:H	1:91:A:THR:H	13	0.2
(2,280)	1:92:A:CYS:H	1:91:A:THR:H	17	0.2
(2,235)	1:80:A:CYS:HA	1:85:A:CYS:H	3	0.2
(2,235)	1:86:A:SER:HA	1:85:A:CYS:H	16	0.2
(2,226)	1:98:A:ILE:H	1:97:A:CYS:H	2	0.2
(2,218)	1:36:A:PRO:HD2	1:37:A:GLU:H	15	0.2
(2,218)	1:36:A:PRO:HD2	1:37:A:GLU:H	18	0.2
(2,174)	1:117:A:LEU:HB2	1:116:A:GLU:H	3	0.2
(2,168)	1:38:A:GLN:HG3	1:38:A:GLN:H	18	0.2
(2,164)	1:14:A:GLN:HB2	1:14:A:GLN:H	8	0.2
(2,164)	1:14:A:GLN:HB3	1:14:A:GLN:H	8	0.2
(2,89)	1:107:A:GLN:HB2	1:108:A:ASP:H	9	0.2
(2,89)	1:107:A:GLN:HB3	1:108:A:ASP:H	9	0.2
(2,49)	1:35:A:SER:HB3	1:39:A:CYS:H	17	0.2
(2,29)	1:28:A:CYS:HA	1:29:A:GLU:H	11	0.2
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG21	5	0.2
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG22	5	0.2
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG23	5	0.2
(1,900)	1:83:A:ILE:HG12	1:82:A:ASN:H	7	0.2
(1,900)	1:83:A:ILE:HG13	1:82:A:ASN:H	7	0.2
(1,900)	1:83:A:ILE:HG12	1:82:A:ASN:H	12	0.2
(1,900)	1:83:A:ILE:HG13	1:82:A:ASN:H	12	0.2
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB2	18	0.2
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB3	18	0.2
(1,886)	1:51:A:CYS:H	1:58:A:CYS:H	6	0.2
(1,884)	1:50:A:SER:H	1:59:A:ILE:H	17	0.2
(1,882)	1:58:A:CYS:HA	1:50:A:SER:H	6	0.2
(1,876)	1:39:A:CYS:HB2	1:43:A:THR:H	1	0.2
(1,876)	1:39:A:CYS:HB3	1:43:A:THR:H	1	0.2
(1,875)	1:38:A:GLN:HE22	1:38:A:GLN:H	10	0.2
(1,869)	1:14:A:GLN:HE22	1:28:A:CYS:H	14	0.2
(1,864)	1:20:A:TRP:HA	1:20:A:TRP:HE1	4	0.2
(1,864)	1:20:A:TRP:HA	1:20:A:TRP:HE1	12	0.2
(1,864)	1:20:A:TRP:HA	1:20:A:TRP:HE1	15	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,860)	1:16:A:VAL:HB	1:19:A:ARG:H	17	0.2
(1,853)	1:10:A:CYS:HB2	1:12:A:ASN:H	4	0.2
(1,853)	1:10:A:CYS:HB3	1:12:A:ASN:H	4	0.2
(1,844)	1:79:A:ASN:HB2	1:92:A:CYS:H	10	0.2
(1,844)	1:79:A:ASN:HB3	1:92:A:CYS:H	10	0.2
(1,840)	1:71:A:CYS:HB2	1:77:A:GLU:H	11	0.2
(1,840)	1:71:A:CYS:HB3	1:77:A:GLU:H	11	0.2
(1,838)	1:58:A:CYS:HA	1:52:A:GLY:H	7	0.2
(1,822)	1:113:A:GLY:HA2	1:116:A:GLU:H	4	0.2
(1,822)	1:113:A:GLY:HA3	1:116:A:GLU:H	4	0.2
(1,811)	1:107:A:GLN:H	1:105:A:ASN:HD21	1	0.2
(1,811)	1:107:A:GLN:H	1:105:A:ASN:HD21	14	0.2
(1,811)	1:107:A:GLN:H	1:105:A:ASN:HD21	15	0.2
(1,810)	1:101:A:ASN:HD21	1:105:A:ASN:HD22	6	0.2
(1,806)	1:101:A:ASN:HD21	1:102:A:PHE:H	4	0.2
(1,803)	1:101:A:ASN:HD21	1:99:A:SER:H	20	0.2
(1,801)	1:102:A:PHE:HB2	1:98:A:ILE:H	3	0.2
(1,801)	1:102:A:PHE:HB3	1:98:A:ILE:H	3	0.2
(1,799)	1:85:A:CYS:HA	1:97:A:CYS:H	6	0.2
(1,799)	1:85:A:CYS:HA	1:97:A:CYS:H	15	0.2
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG21	20	0.2
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG22	20	0.2
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG23	20	0.2
(1,795)	1:91:A:THR:HG23	1:95:A:GLY:H	16	0.2
(1,792)	1:97:A:CYS:HB2	1:91:A:THR:H	12	0.2
(1,792)	1:97:A:CYS:HB3	1:91:A:THR:H	12	0.2
(1,792)	1:97:A:CYS:HB2	1:91:A:THR:H	13	0.2
(1,792)	1:97:A:CYS:HB3	1:91:A:THR:H	13	0.2
(1,789)	1:85:A:CYS:H	1:84:A:THR:HB	4	0.2
(1,787)	1:73:A:SER:H	1:76:A:ASP:H	4	0.2
(1,784)	1:71:A:CYS:HB2	1:76:A:ASP:H	15	0.2
(1,784)	1:71:A:CYS:HB3	1:76:A:ASP:H	15	0.2
(1,778)	1:77:A:GLU:HG2	1:71:A:CYS:H	3	0.2
(1,778)	1:77:A:GLU:HG3	1:71:A:CYS:H	3	0.2
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	18	0.2
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	18	0.2
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	18	0.2
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	18	0.2
(1,751)	1:52:A:GLY:H	1:57:A:GLN:HG2	6	0.2
(1,751)	1:52:A:GLY:H	1:57:A:GLN:HG3	6	0.2
(1,744)	1:48:A:GLU:H	1:47:A:HIS:H	6	0.2
(1,744)	1:48:A:GLU:H	1:47:A:HIS:H	20	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,737)	1:33:A:ASP:HB2	1:34:A:GLU:H	6	0.2
(1,737)	1:33:A:ASP:HB3	1:34:A:GLU:H	6	0.2
(1,726)	1:34:A:GLU:HG2	1:27:A:ASP:H	1	0.2
(1,726)	1:34:A:GLU:HG3	1:27:A:ASP:H	1	0.2
(1,726)	1:34:A:GLU:HG2	1:27:A:ASP:H	17	0.2
(1,726)	1:34:A:GLU:HG3	1:27:A:ASP:H	17	0.2
(1,724)	1:34:A:GLU:HB2	1:25:A:ASP:H	12	0.2
(1,724)	1:34:A:GLU:HB3	1:25:A:ASP:H	12	0.2
(1,716)	1:28:A:CYS:HB2	1:14:A:GLN:HE22	2	0.2
(1,716)	1:28:A:CYS:HB3	1:14:A:GLN:HE22	2	0.2
(1,711)	1:10:A:CYS:HB2	1:11:A:ASN:H	8	0.2
(1,711)	1:10:A:CYS:HB3	1:11:A:ASN:H	8	0.2
(1,711)	1:10:A:CYS:HB2	1:11:A:ASN:H	19	0.2
(1,711)	1:10:A:CYS:HB3	1:11:A:ASN:H	19	0.2
(1,709)	1:45:A:ARG:HD2	1:45:A:ARG:H	11	0.2
(1,709)	1:45:A:ARG:HD3	1:45:A:ARG:H	11	0.2
(1,708)	1:44:A:CYS:HB2	1:45:A:ARG:H	10	0.2
(1,708)	1:44:A:CYS:HB3	1:45:A:ARG:H	10	0.2
(1,707)	1:45:A:ARG:HD2	1:45:A:ARG:H	11	0.2
(1,707)	1:45:A:ARG:HD3	1:45:A:ARG:H	11	0.2
(1,705)	1:100:A:ARG:H	1:100:A:ARG:HD2	11	0.2
(1,705)	1:100:A:ARG:H	1:100:A:ARG:HD3	11	0.2
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG2	13	0.2
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG3	13	0.2
(1,696)	1:44:A:CYS:HB2	1:34:A:GLU:H	14	0.2
(1,696)	1:44:A:CYS:HB3	1:34:A:GLU:H	14	0.2
(1,694)	1:21:A:LYS:HE2	1:21:A:LYS:H	11	0.2
(1,694)	1:21:A:LYS:HE3	1:21:A:LYS:H	11	0.2
(1,670)	1:107:A:GLN:HB2	1:105:A:ASN:HD22	2	0.2
(1,670)	1:107:A:GLN:HB2	1:105:A:ASN:HD22	2	0.2
(1,670)	1:107:A:GLN:HB3	1:105:A:ASN:HD22	2	0.2
(1,670)	1:107:A:GLN:HB3	1:105:A:ASN:HD22	2	0.2
(1,664)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	14	0.2
(1,664)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	14	0.2
(1,658)	1:102:A:PHE:HA	1:105:A:ASN:HD22	1	0.2
(1,645)	1:101:A:ASN:HD22	1:101:A:ASN:H	8	0.2
(1,630)	1:57:A:GLN:HB2	1:57:A:GLN:HE22	20	0.2
(1,630)	1:57:A:GLN:HB2	1:57:A:GLN:HE22	20	0.2
(1,630)	1:57:A:GLN:HB3	1:57:A:GLN:HE22	20	0.2
(1,630)	1:57:A:GLN:HB3	1:57:A:GLN:HE22	20	0.2
(1,603)	1:32:A:SER:HB2	1:11:A:ASN:HD22	13	0.2
(1,603)	1:32:A:SER:HB3	1:11:A:ASN:HD22	13	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,586)	1:69:A:ASN:HA	1:64:A:ARG:H	2	0.2
(1,580)	1:48:A:GLU:HG2	1:49:A:ILE:H	14	0.2
(1,580)	1:48:A:GLU:HG3	1:49:A:ILE:H	14	0.2
(1,580)	1:48:A:GLU:HG2	1:49:A:ILE:H	19	0.2
(1,580)	1:48:A:GLU:HG3	1:49:A:ILE:H	19	0.2
(1,553)	1:115:A:ASP:HB2	1:104:A:CYS:H	14	0.2
(1,553)	1:115:A:ASP:HB3	1:104:A:CYS:H	14	0.2
(1,553)	1:115:A:ASP:HB2	1:104:A:CYS:H	16	0.2
(1,553)	1:115:A:ASP:HB3	1:104:A:CYS:H	16	0.2
(1,545)	1:103:A:VAL:HA	1:105:A:ASN:H	4	0.2
(1,545)	1:103:A:VAL:HA	1:105:A:ASN:H	6	0.2
(1,542)	1:112:A:ASP:H	1:114:A:SER:H	2	0.2
(1,541)	1:115:A:ASP:HB2	1:116:A:GLU:H	7	0.2
(1,541)	1:115:A:ASP:HB3	1:116:A:GLU:H	7	0.2
(1,518)	1:49:A:ILE:H	1:61:A:VAL:H	5	0.2
(1,518)	1:49:A:ILE:H	1:61:A:VAL:H	16	0.2
(1,516)	1:49:A:ILE:H	1:59:A:ILE:H	17	0.2
(1,509)	1:46:A:ILE:HA	1:46:A:ILE:H	3	0.2
(1,501)	1:34:A:GLU:HB2	1:34:A:GLU:H	6	0.2
(1,501)	1:34:A:GLU:HB3	1:34:A:GLU:H	6	0.2
(1,501)	1:34:A:GLU:HB2	1:34:A:GLU:H	9	0.2
(1,501)	1:34:A:GLU:HB3	1:34:A:GLU:H	9	0.2
(1,483)	1:10:A:CYS:HB2	1:14:A:GLN:H	9	0.2
(1,483)	1:10:A:CYS:HB3	1:14:A:GLN:H	9	0.2
(1,483)	1:10:A:CYS:HB2	1:14:A:GLN:H	16	0.2
(1,483)	1:10:A:CYS:HB3	1:14:A:GLN:H	16	0.2
(1,482)	1:11:A:ASN:HD21	1:11:A:ASN:H	11	0.2
(1,482)	1:11:A:ASN:HD21	1:11:A:ASN:H	13	0.2
(1,480)	1:10:A:CYS:HB2	1:10:A:CYS:H	12	0.2
(1,480)	1:10:A:CYS:HB3	1:10:A:CYS:H	12	0.2
(1,462)	1:79:A:ASN:H	1:78:A:GLU:H	18	0.2
(1,445)	1:75:A:GLU:H	1:74:A:GLY:H	14	0.2
(1,438)	1:72:A:ASP:H	1:73:A:SER:H	8	0.2
(1,436)	1:73:A:SER:H	1:72:A:ASP:H	20	0.2
(1,433)	1:74:A:GLY:HA2	1:71:A:CYS:H	4	0.2
(1,433)	1:74:A:GLY:HA3	1:71:A:CYS:H	4	0.2
(1,419)	1:65:A:CYS:HB2	1:66:A:ASP:H	17	0.2
(1,419)	1:65:A:CYS:HB3	1:66:A:ASP:H	17	0.2
(1,418)	1:64:A:ARG:HA	1:66:A:ASP:H	9	0.2
(1,415)	1:64:A:ARG:HA	1:65:A:CYS:H	1	0.2
(1,415)	1:64:A:ARG:HA	1:65:A:CYS:H	3	0.2
(1,415)	1:64:A:ARG:HA	1:65:A:CYS:H	8	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,415)	1:64:A:ARG:HA	1:65:A:CYS:H	9	0.2
(1,415)	1:64:A:ARG:HA	1:65:A:CYS:H	11	0.2
(1,415)	1:64:A:ARG:HA	1:65:A:CYS:H	13	0.2
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB2	3	0.2
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB3	3	0.2
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB2	16	0.2
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB3	16	0.2
(1,386)	1:51:A:CYS:HB2	1:51:A:CYS:H	14	0.2
(1,386)	1:51:A:CYS:HB3	1:51:A:CYS:H	14	0.2
(1,386)	1:51:A:CYS:HB2	1:51:A:CYS:H	18	0.2
(1,386)	1:51:A:CYS:HB3	1:51:A:CYS:H	18	0.2
(1,383)	1:51:A:CYS:H	1:50:A:SER:HA	15	0.2
(1,378)	1:48:A:GLU:HG2	1:49:A:ILE:H	14	0.2
(1,378)	1:48:A:GLU:HG3	1:49:A:ILE:H	14	0.2
(1,378)	1:48:A:GLU:HG2	1:49:A:ILE:H	19	0.2
(1,378)	1:48:A:GLU:HG3	1:49:A:ILE:H	19	0.2
(1,374)	1:61:A:VAL:H	1:49:A:ILE:H	15	0.2
(1,372)	1:48:A:GLU:H	1:48:A:GLU:HA	5	0.2
(1,351)	1:32:A:SER:H	1:33:A:ASP:H	11	0.2
(1,350)	1:31:A:GLY:H	1:32:A:SER:H	12	0.2
(1,349)	1:32:A:SER:H	1:33:A:ASP:H	11	0.2
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB2	16	0.2
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB3	16	0.2
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB2	19	0.2
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB3	19	0.2
(1,313)	1:14:A:GLN:HG2	1:14:A:GLN:H	18	0.2
(1,313)	1:14:A:GLN:HG3	1:14:A:GLN:H	18	0.2
(1,312)	1:14:A:GLN:HG2	1:14:A:GLN:H	10	0.2
(1,312)	1:14:A:GLN:HG3	1:14:A:GLN:H	10	0.2
(1,308)	1:13:A:GLY:H	1:14:A:GLN:H	14	0.2
(1,290)	1:8:A:PHE:HA	1:9:A:VAL:H	5	0.2
(1,283)	1:8:A:PHE:H	1:7:A:ASP:H	14	0.2
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	11	0.2
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	11	0.2
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	11	0.2
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	11	0.2
(1,226)	1:92:A:CYS:HB2	1:94:A:SER:H	13	0.2
(1,226)	1:92:A:CYS:HB3	1:94:A:SER:H	13	0.2
(1,203)	1:89:A:GLU:HB2	1:98:A:ILE:H	8	0.2
(1,203)	1:89:A:GLU:HB3	1:98:A:ILE:H	8	0.2
(1,196)	1:98:A:ILE:HA	1:99:A:SER:H	1	0.2
(1,196)	1:98:A:ILE:HA	1:99:A:SER:H	8	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,184)	1:103:A:VAL:HB	1:102:A:PHE:H	18	0.2
(1,137)	1:109:A:ASP:H	1:113:A:GLY:HA2	17	0.2
(1,137)	1:109:A:ASP:H	1:113:A:GLY:HA3	17	0.2
(1,136)	1:112:A:ASP:H	1:110:A:CYS:H	7	0.2
(1,123)	1:115:A:ASP:HB2	1:115:A:ASP:H	20	0.2
(1,123)	1:115:A:ASP:HB3	1:115:A:ASP:H	20	0.2
(1,99)	1:98:A:ILE:HG12	1:99:A:SER:H	9	0.2
(1,99)	1:98:A:ILE:HG13	1:99:A:SER:H	9	0.2
(1,96)	1:100:A:ARG:H	1:89:A:GLU:HA	16	0.2
(1,92)	1:7:A:ASP:HB2	1:8:A:PHE:H	20	0.2
(1,92)	1:7:A:ASP:HB3	1:8:A:PHE:H	20	0.2
(1,74)	1:65:A:CYS:H	1:65:A:CYS:HB2	16	0.2
(1,74)	1:65:A:CYS:H	1:65:A:CYS:HB3	16	0.2
(1,55)	1:71:A:CYS:H	1:70:A:ASP:H	7	0.2
(1,49)	1:94:A:SER:H	1:93:A:SER:H	3	0.2
(1,49)	1:94:A:SER:H	1:93:A:SER:H	6	0.2
(1,33)	1:115:A:ASP:H	1:114:A:SER:H	5	0.2
(1,28)	1:118:A:ASP:H	1:117:A:LEU:H	20	0.2
(1,24)	1:104:A:CYS:H	1:105:A:ASN:H	3	0.2
(1,24)	1:104:A:CYS:H	1:105:A:ASN:H	17	0.2
(1,23)	1:104:A:CYS:H	1:105:A:ASN:H	3	0.2
(1,23)	1:104:A:CYS:H	1:105:A:ASN:H	17	0.2
(1,22)	1:91:A:THR:H	1:92:A:CYS:H	7	0.2
(1,22)	1:91:A:THR:H	1:92:A:CYS:H	13	0.2
(1,22)	1:91:A:THR:H	1:92:A:CYS:H	17	0.2
(1,17)	1:81:A:GLY:H	1:80:A:CYS:H	2	0.2
(1,17)	1:81:A:GLY:H	1:80:A:CYS:H	18	0.2
(1,9)	1:12:A:ASN:H	1:11:A:ASN:H	10	0.2
(1,9)	1:12:A:ASN:H	1:11:A:ASN:H	14	0.2
(1,6)	1:23:A:ASP:H	1:24:A:GLY:H	9	0.2
(1,6)	1:23:A:ASP:H	1:24:A:GLY:H	11	0.2
(4,7)	1:8:A:PHE:H	1:16:A:VAL:O	1	0.19
(4,5)	1:49:A:ILE:O	1:59:A:ILE:H	6	0.19
(4,5)	1:49:A:ILE:O	1:59:A:ILE:H	16	0.19
(3,7)	2:202:A:CA:CA	1:63:A:TRP:O	5	0.19
(2,382)	1:72:A:ASP:HB2	1:73:A:SER:H	19	0.19
(2,382)	1:72:A:ASP:HB3	1:73:A:SER:H	19	0.19
(2,370)	1:38:A:GLN:HG3	1:38:A:GLN:HE22	3	0.19
(2,313)	1:17:A:PRO:HB2	1:20:A:TRP:H	10	0.19
(2,298)	1:28:A:CYS:HB2	1:14:A:GLN:HE22	7	0.19
(2,298)	1:28:A:CYS:HB3	1:14:A:GLN:HE22	13	0.19
(2,280)	1:92:A:CYS:H	1:91:A:THR:H	15	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,245)	1:36:A:PRO:HA	1:39:A:CYS:H	20	0.19
(2,218)	1:36:A:PRO:HD2	1:37:A:GLU:H	1	0.19
(2,218)	1:36:A:PRO:HD2	1:37:A:GLU:H	4	0.19
(2,210)	1:33:A:ASP:HA	1:38:A:GLN:HE21	19	0.19
(2,188)	1:16:A:VAL:HG11	1:19:A:ARG:H	17	0.19
(2,188)	1:16:A:VAL:HG12	1:19:A:ARG:H	17	0.19
(2,188)	1:16:A:VAL:HG13	1:19:A:ARG:H	17	0.19
(2,188)	1:16:A:VAL:HG21	1:19:A:ARG:H	17	0.19
(2,188)	1:16:A:VAL:HG22	1:19:A:ARG:H	17	0.19
(2,188)	1:16:A:VAL:HG23	1:19:A:ARG:H	17	0.19
(2,181)	1:41:A:MET:HG3	1:41:A:MET:H	1	0.19
(2,181)	1:39:A:CYS:HB3	1:41:A:MET:H	5	0.19
(2,174)	1:117:A:LEU:HB2	1:116:A:GLU:H	4	0.19
(2,173)	1:69:A:ASN:HD21	1:69:A:ASN:H	19	0.19
(2,164)	1:14:A:GLN:HB2	1:14:A:GLN:H	15	0.19
(2,164)	1:14:A:GLN:HB3	1:14:A:GLN:H	15	0.19
(2,164)	1:14:A:GLN:HB2	1:14:A:GLN:H	20	0.19
(2,164)	1:14:A:GLN:HB3	1:14:A:GLN:H	20	0.19
(2,123)	1:16:A:VAL:HG11	1:33:A:ASP:H	2	0.19
(2,123)	1:16:A:VAL:HG12	1:33:A:ASP:H	2	0.19
(2,123)	1:16:A:VAL:HG13	1:33:A:ASP:H	2	0.19
(2,123)	1:16:A:VAL:HG21	1:33:A:ASP:H	2	0.19
(2,123)	1:16:A:VAL:HG22	1:33:A:ASP:H	2	0.19
(2,123)	1:16:A:VAL:HG23	1:33:A:ASP:H	2	0.19
(2,114)	1:16:A:VAL:HG11	1:16:A:VAL:H	12	0.19
(2,114)	1:16:A:VAL:HG12	1:16:A:VAL:H	12	0.19
(2,114)	1:16:A:VAL:HG13	1:16:A:VAL:H	12	0.19
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	12	0.19
(2,114)	1:16:A:VAL:HG21	1:16:A:VAL:H	12	0.19
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	12	0.19
(2,114)	1:16:A:VAL:HG22	1:16:A:VAL:H	12	0.19
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	12	0.19
(2,114)	1:16:A:VAL:HG23	1:16:A:VAL:H	12	0.19
(2,89)	1:107:A:GLN:HB2	1:108:A:ASP:H	10	0.19
(2,89)	1:107:A:GLN:HB3	1:108:A:ASP:H	10	0.19
(2,83)	1:35:A:SER:HB3	1:38:A:GLN:H	6	0.19
(2,80)	1:42:A:ARG:HA	1:56:A:THR:H	11	0.19
(2,74)	1:46:A:ILE:HB	1:46:A:ILE:H	3	0.19
(2,56)	1:114:A:SER:HA	1:117:A:LEU:H	4	0.19
(2,29)	1:28:A:CYS:HA	1:29:A:GLU:H	12	0.19
(1,921)	1:8:A:PHE:HA	1:16:A:VAL:HG21	19	0.19
(1,921)	1:8:A:PHE:HA	1:16:A:VAL:HG22	19	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,921)	1:8:A:PHE:HA	1:16:A:VAL:HG23	19	0.19
(1,916)	1:77:A:GLU:HB2	1:77:A:GLU:H	20	0.19
(1,916)	1:77:A:GLU:HB3	1:77:A:GLU:H	20	0.19
(1,907)	1:39:A:CYS:H	1:41:A:MET:H	8	0.19
(1,905)	1:101:A:ASN:HD21	1:105:A:ASN:HD21	8	0.19
(1,905)	1:101:A:ASN:HD21	1:105:A:ASN:HD21	17	0.19
(1,900)	1:83:A:ILE:HG12	1:82:A:ASN:H	9	0.19
(1,900)	1:83:A:ILE:HG13	1:82:A:ASN:H	9	0.19
(1,900)	1:83:A:ILE:HG12	1:82:A:ASN:H	19	0.19
(1,900)	1:83:A:ILE:HG13	1:82:A:ASN:H	19	0.19
(1,897)	1:77:A:GLU:HB2	1:69:A:ASN:HD22	4	0.19
(1,897)	1:77:A:GLU:HB3	1:69:A:ASN:HD22	4	0.19
(1,884)	1:50:A:SER:H	1:59:A:ILE:H	15	0.19
(1,881)	1:48:A:GLU:H	1:45:A:ARG:H	6	0.19
(1,879)	1:48:A:GLU:H	1:45:A:ARG:H	6	0.19
(1,876)	1:39:A:CYS:HB2	1:43:A:THR:H	3	0.19
(1,876)	1:39:A:CYS:HB3	1:43:A:THR:H	3	0.19
(1,876)	1:39:A:CYS:HB2	1:43:A:THR:H	16	0.19
(1,876)	1:39:A:CYS:HB3	1:43:A:THR:H	16	0.19
(1,859)	1:3:A:CYS:HB2	1:18:A:SER:H	13	0.19
(1,859)	1:3:A:CYS:HB3	1:18:A:SER:H	13	0.19
(1,856)	1:14:A:GLN:H	1:12:A:ASN:HD22	1	0.19
(1,840)	1:71:A:CYS:HB2	1:77:A:GLU:H	5	0.19
(1,840)	1:71:A:CYS:HB3	1:77:A:GLU:H	5	0.19
(1,837)	1:50:A:SER:H	1:45:A:ARG:HD2	14	0.19
(1,837)	1:50:A:SER:H	1:45:A:ARG:HD3	14	0.19
(1,837)	1:50:A:SER:H	1:45:A:ARG:HD2	20	0.19
(1,837)	1:50:A:SER:H	1:45:A:ARG:HD3	20	0.19
(1,810)	1:101:A:ASN:HD21	1:105:A:ASN:HD22	2	0.19
(1,810)	1:101:A:ASN:HD21	1:105:A:ASN:HD22	19	0.19
(1,809)	1:106:A:GLY:H	1:104:A:CYS:H	9	0.19
(1,808)	1:116:A:GLU:HB2	1:104:A:CYS:H	13	0.19
(1,808)	1:116:A:GLU:HB3	1:104:A:CYS:H	13	0.19
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG21	10	0.19
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG22	10	0.19
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG23	10	0.19
(1,792)	1:97:A:CYS:HB2	1:91:A:THR:H	2	0.19
(1,792)	1:97:A:CYS:HB3	1:91:A:THR:H	2	0.19
(1,789)	1:85:A:CYS:H	1:84:A:THR:HB	17	0.19
(1,784)	1:71:A:CYS:HB2	1:76:A:ASP:H	19	0.19
(1,784)	1:71:A:CYS:HB3	1:76:A:ASP:H	19	0.19
(1,783)	1:71:A:CYS:HB2	1:74:A:GLY:H	2	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,783)	1:71:A:CYS:HB3	1:74:A:GLY:H	2	0.19
(1,751)	1:52:A:GLY:H	1:57:A:GLN:HG2	2	0.19
(1,751)	1:52:A:GLY:H	1:57:A:GLN:HG3	2	0.19
(1,744)	1:48:A:GLU:H	1:47:A:HIS:H	9	0.19
(1,744)	1:48:A:GLU:H	1:47:A:HIS:H	11	0.19
(1,734)	1:32:A:SER:H	1:11:A:ASN:H	2	0.19
(1,731)	1:28:A:CYS:HB2	1:32:A:SER:H	10	0.19
(1,731)	1:28:A:CYS:HB3	1:32:A:SER:H	10	0.19
(1,718)	1:16:A:VAL:HB	1:20:A:TRP:HE1	18	0.19
(1,716)	1:28:A:CYS:HB2	1:14:A:GLN:HE22	1	0.19
(1,716)	1:28:A:CYS:HB3	1:14:A:GLN:HE22	1	0.19
(1,712)	1:32:A:SER:H	1:11:A:ASN:H	2	0.19
(1,711)	1:10:A:CYS:HB2	1:11:A:ASN:H	2	0.19
(1,711)	1:10:A:CYS:HB3	1:11:A:ASN:H	2	0.19
(1,709)	1:45:A:ARG:HD2	1:45:A:ARG:H	18	0.19
(1,709)	1:45:A:ARG:HD3	1:45:A:ARG:H	18	0.19
(1,707)	1:45:A:ARG:HD2	1:45:A:ARG:H	18	0.19
(1,707)	1:45:A:ARG:HD3	1:45:A:ARG:H	18	0.19
(1,705)	1:100:A:ARG:H	1:100:A:ARG:HD2	13	0.19
(1,705)	1:100:A:ARG:H	1:100:A:ARG:HD3	13	0.19
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG2	17	0.19
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG3	17	0.19
(1,689)	1:69:A:ASN:HD21	1:69:A:ASN:H	19	0.19
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD2	4	0.19
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD3	4	0.19
(1,679)	1:78:A:GLU:HG2	1:79:A:ASN:HD22	10	0.19
(1,679)	1:78:A:GLU:HG3	1:79:A:ASN:HD22	10	0.19
(1,664)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	12	0.19
(1,664)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	12	0.19
(1,664)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	15	0.19
(1,664)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	15	0.19
(1,664)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	16	0.19
(1,664)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	16	0.19
(1,664)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	18	0.19
(1,664)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	18	0.19
(1,645)	1:101:A:ASN:HD22	1:101:A:ASN:H	6	0.19
(1,645)	1:101:A:ASN:HD22	1:101:A:ASN:H	18	0.19
(1,623)	1:30:A:ASP:HB2	1:12:A:ASN:HD22	8	0.19
(1,623)	1:30:A:ASP:HB3	1:12:A:ASN:HD22	8	0.19
(1,610)	1:14:A:GLN:HE22	1:29:A:GLU:H	19	0.19
(1,596)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	8	0.19
(1,596)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	8	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,591)	1:69:A:ASN:HB2	1:69:A:ASN:HD21	16	0.19
(1,591)	1:69:A:ASN:HB3	1:69:A:ASN:HD21	16	0.19
(1,569)	1:85:A:CYS:H	1:84:A:THR:H	1	0.19
(1,553)	1:115:A:ASP:HB2	1:104:A:CYS:H	9	0.19
(1,553)	1:115:A:ASP:HB3	1:104:A:CYS:H	9	0.19
(1,551)	1:104:A:CYS:HB2	1:104:A:CYS:H	18	0.19
(1,551)	1:104:A:CYS:HB3	1:104:A:CYS:H	18	0.19
(1,550)	1:104:A:CYS:HB2	1:104:A:CYS:H	18	0.19
(1,550)	1:104:A:CYS:HB3	1:104:A:CYS:H	18	0.19
(1,549)	1:115:A:ASP:HA	1:104:A:CYS:H	8	0.19
(1,516)	1:49:A:ILE:H	1:59:A:ILE:H	2	0.19
(1,510)	1:48:A:GLU:HB2	1:48:A:GLU:H	16	0.19
(1,510)	1:48:A:GLU:HB3	1:48:A:GLU:H	16	0.19
(1,501)	1:34:A:GLU:HB2	1:34:A:GLU:H	18	0.19
(1,501)	1:34:A:GLU:HB3	1:34:A:GLU:H	18	0.19
(1,499)	1:33:A:ASP:HB2	1:33:A:ASP:H	11	0.19
(1,499)	1:33:A:ASP:HB3	1:33:A:ASP:H	11	0.19
(1,499)	1:33:A:ASP:HB2	1:33:A:ASP:H	13	0.19
(1,499)	1:33:A:ASP:HB3	1:33:A:ASP:H	13	0.19
(1,475)	1:75:A:GLU:H	1:76:A:ASP:H	2	0.19
(1,462)	1:79:A:ASN:H	1:78:A:GLU:H	12	0.19
(1,454)	1:78:A:GLU:HG2	1:76:A:ASP:H	3	0.19
(1,454)	1:78:A:GLU:HG3	1:76:A:ASP:H	3	0.19
(1,454)	1:78:A:GLU:HG2	1:76:A:ASP:H	19	0.19
(1,454)	1:78:A:GLU:HG3	1:76:A:ASP:H	19	0.19
(1,451)	1:75:A:GLU:H	1:76:A:ASP:H	2	0.19
(1,447)	1:71:A:CYS:HA	1:74:A:GLY:H	20	0.19
(1,446)	1:73:A:SER:H	1:74:A:GLY:H	12	0.19
(1,446)	1:73:A:SER:H	1:74:A:GLY:H	15	0.19
(1,445)	1:75:A:GLU:H	1:74:A:GLY:H	18	0.19
(1,444)	1:76:A:ASP:H	1:74:A:GLY:H	13	0.19
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB2	1	0.19
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB3	1	0.19
(1,435)	1:72:A:ASP:HA	1:72:A:ASP:H	20	0.19
(1,433)	1:74:A:GLY:HA2	1:71:A:CYS:H	14	0.19
(1,433)	1:74:A:GLY:HA3	1:71:A:CYS:H	14	0.19
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB2	4	0.19
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB3	4	0.19
(1,390)	1:51:A:CYS:HB2	1:52:A:GLY:H	5	0.19
(1,390)	1:51:A:CYS:HB3	1:52:A:GLY:H	5	0.19
(1,374)	1:61:A:VAL:H	1:49:A:ILE:H	13	0.19
(1,372)	1:48:A:GLU:H	1:48:A:GLU:HA	1	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,372)	1:48:A:GLU:H	1:48:A:GLU:HA	11	0.19
(1,372)	1:48:A:GLU:H	1:48:A:GLU:HA	19	0.19
(1,351)	1:32:A:SER:H	1:33:A:ASP:H	16	0.19
(1,349)	1:32:A:SER:H	1:33:A:ASP:H	16	0.19
(1,343)	1:28:A:CYS:HB2	1:28:A:CYS:H	10	0.19
(1,343)	1:28:A:CYS:HB3	1:28:A:CYS:H	10	0.19
(1,343)	1:28:A:CYS:HB2	1:28:A:CYS:H	18	0.19
(1,343)	1:28:A:CYS:HB3	1:28:A:CYS:H	18	0.19
(1,335)	1:45:A:ARG:HD2	1:24:A:GLY:H	10	0.19
(1,335)	1:45:A:ARG:HD3	1:24:A:GLY:H	10	0.19
(1,313)	1:14:A:GLN:HG2	1:14:A:GLN:H	16	0.19
(1,313)	1:14:A:GLN:HG3	1:14:A:GLN:H	16	0.19
(1,298)	1:14:A:GLN:H	1:11:A:ASN:H	2	0.19
(1,290)	1:8:A:PHE:HA	1:9:A:VAL:H	7	0.19
(1,290)	1:8:A:PHE:HA	1:9:A:VAL:H	12	0.19
(1,283)	1:8:A:PHE:H	1:7:A:ASP:H	11	0.19
(1,279)	1:6:A:SER:HB2	1:6:A:SER:H	8	0.19
(1,279)	1:6:A:SER:HB3	1:6:A:SER:H	8	0.19
(1,277)	1:6:A:SER:HB2	1:6:A:SER:H	8	0.19
(1,277)	1:6:A:SER:HB3	1:6:A:SER:H	8	0.19
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD11	8	0.19
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD12	8	0.19
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD13	8	0.19
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD11	19	0.19
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD12	19	0.19
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD13	19	0.19
(1,228)	1:92:A:CYS:HB2	1:93:A:SER:H	11	0.19
(1,228)	1:92:A:CYS:HB3	1:93:A:SER:H	11	0.19
(1,226)	1:92:A:CYS:HB2	1:94:A:SER:H	4	0.19
(1,226)	1:92:A:CYS:HB3	1:94:A:SER:H	4	0.19
(1,215)	1:96:A:ARG:H	1:92:A:CYS:HB2	8	0.19
(1,215)	1:96:A:ARG:H	1:92:A:CYS:HB3	8	0.19
(1,203)	1:89:A:GLU:HB2	1:98:A:ILE:H	1	0.19
(1,203)	1:89:A:GLU:HB3	1:98:A:ILE:H	1	0.19
(1,187)	1:103:A:VAL:HG11	1:102:A:PHE:H	13	0.19
(1,187)	1:103:A:VAL:HG12	1:102:A:PHE:H	13	0.19
(1,187)	1:103:A:VAL:HG13	1:102:A:PHE:H	13	0.19
(1,187)	1:103:A:VAL:HG21	1:102:A:PHE:H	13	0.19
(1,187)	1:103:A:VAL:HG22	1:102:A:PHE:H	13	0.19
(1,187)	1:103:A:VAL:HG23	1:102:A:PHE:H	13	0.19
(1,180)	1:99:A:SER:HB2	1:102:A:PHE:H	4	0.19
(1,180)	1:99:A:SER:HB3	1:102:A:PHE:H	4	0.19

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,180)	1:99:A:SER:HB2	1:102:A:PHE:H	11	0.19
(1,180)	1:99:A:SER:HB3	1:102:A:PHE:H	11	0.19
(1,126)	1:117:A:LEU:HD11	1:114:A:SER:H	9	0.19
(1,126)	1:117:A:LEU:HD12	1:114:A:SER:H	9	0.19
(1,126)	1:117:A:LEU:HD13	1:114:A:SER:H	9	0.19
(1,126)	1:117:A:LEU:HD21	1:114:A:SER:H	9	0.19
(1,126)	1:117:A:LEU:HD22	1:114:A:SER:H	9	0.19
(1,126)	1:117:A:LEU:HD23	1:114:A:SER:H	9	0.19
(1,123)	1:115:A:ASP:HB2	1:115:A:ASP:H	11	0.19
(1,123)	1:115:A:ASP:HB3	1:115:A:ASP:H	11	0.19
(1,92)	1:7:A:ASP:HB2	1:8:A:PHE:H	4	0.19
(1,92)	1:7:A:ASP:HB3	1:8:A:PHE:H	4	0.19
(1,91)	1:14:A:GLN:HG2	1:15:A:CYS:H	1	0.19
(1,91)	1:14:A:GLN:HG3	1:15:A:CYS:H	1	0.19
(1,74)	1:65:A:CYS:H	1:65:A:CYS:HB2	1	0.19
(1,74)	1:65:A:CYS:H	1:65:A:CYS:HB3	1	0.19
(1,70)	1:77:A:GLU:HB2	1:78:A:GLU:H	13	0.19
(1,70)	1:77:A:GLU:HB3	1:78:A:GLU:H	13	0.19
(1,69)	1:78:A:GLU:HG2	1:78:A:GLU:H	20	0.19
(1,69)	1:78:A:GLU:HG3	1:78:A:GLU:H	20	0.19
(1,59)	1:65:A:CYS:H	1:66:A:ASP:H	12	0.19
(1,55)	1:71:A:CYS:H	1:70:A:ASP:H	17	0.19
(1,35)	1:115:A:ASP:H	1:116:A:GLU:H	16	0.19
(1,28)	1:118:A:ASP:H	1:117:A:LEU:H	17	0.19
(1,22)	1:91:A:THR:H	1:92:A:CYS:H	15	0.19
(1,14)	1:110:A:CYS:H	1:109:A:ASP:H	16	0.19
(1,6)	1:23:A:ASP:H	1:24:A:GLY:H	13	0.19
(4,7)	1:8:A:PHE:H	1:16:A:VAL:O	5	0.18
(3,7)	2:202:A:CA:CA	1:63:A:TRP:O	20	0.18
(2,394)	1:86:A:SER:HB2	1:86:A:SER:H	18	0.18
(2,382)	1:72:A:ASP:HB2	1:73:A:SER:H	12	0.18
(2,382)	1:72:A:ASP:HB3	1:73:A:SER:H	12	0.18
(2,370)	1:38:A:GLN:HG3	1:38:A:GLN:HE22	14	0.18
(2,370)	1:38:A:GLN:HG3	1:38:A:GLN:HE22	18	0.18
(2,331)	1:101:A:ASN:H	1:99:A:SER:H	8	0.18
(2,322)	1:69:A:ASN:HB2	1:71:A:CYS:H	15	0.18
(2,294)	1:61:A:VAL:HG13	1:48:A:GLU:H	15	0.18
(2,284)	1:117:A:LEU:HB3	1:117:A:LEU:H	17	0.18
(2,280)	1:92:A:CYS:H	1:91:A:THR:H	3	0.18
(2,280)	1:92:A:CYS:H	1:91:A:THR:H	12	0.18
(2,276)	1:56:A:THR:HB	1:57:A:GLN:H	10	0.18
(2,270)	1:111:A:SER:HA	1:110:A:CYS:H	14	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,246)	1:90:A:PHE:HB2	1:100:A:ARG:H	11	0.18
(2,246)	1:90:A:PHE:HB3	1:100:A:ARG:H	11	0.18
(2,226)	1:92:A:CYS:H	1:97:A:CYS:H	17	0.18
(2,218)	1:36:A:PRO:HD2	1:37:A:GLU:H	16	0.18
(2,218)	1:36:A:PRO:HD2	1:37:A:GLU:H	17	0.18
(2,188)	1:16:A:VAL:HG11	1:19:A:ARG:H	13	0.18
(2,188)	1:16:A:VAL:HG12	1:19:A:ARG:H	13	0.18
(2,188)	1:16:A:VAL:HG13	1:19:A:ARG:H	13	0.18
(2,188)	1:16:A:VAL:HG21	1:19:A:ARG:H	13	0.18
(2,188)	1:16:A:VAL:HG22	1:19:A:ARG:H	13	0.18
(2,188)	1:16:A:VAL:HG23	1:19:A:ARG:H	13	0.18
(2,182)	1:34:A:GLU:HG2	1:22:A:CYS:H	10	0.18
(2,181)	1:39:A:CYS:HB3	1:41:A:MET:H	4	0.18
(2,181)	1:39:A:CYS:HB3	1:41:A:MET:H	17	0.18
(2,173)	1:69:A:ASN:HD21	1:69:A:ASN:H	8	0.18
(2,164)	1:14:A:GLN:HB2	1:14:A:GLN:H	4	0.18
(2,164)	1:14:A:GLN:HB3	1:14:A:GLN:H	4	0.18
(2,90)	1:59:A:ILE:HD11	1:63:A:TRP:HE1	3	0.18
(2,89)	1:107:A:GLN:HB2	1:108:A:ASP:H	16	0.18
(2,89)	1:107:A:GLN:HB3	1:108:A:ASP:H	16	0.18
(2,80)	1:56:A:THR:HB	1:56:A:THR:H	7	0.18
(2,56)	1:114:A:SER:HA	1:117:A:LEU:H	3	0.18
(2,56)	1:114:A:SER:HA	1:117:A:LEU:H	7	0.18
(2,39)	1:117:A:LEU:HD13	1:115:A:ASP:H	18	0.18
(2,30)	1:14:A:GLN:H	1:10:A:CYS:H	1	0.18
(2,29)	1:28:A:CYS:HA	1:29:A:GLU:H	19	0.18
(2,22)	1:75:A:GLU:HA	1:78:A:GLU:H	13	0.18
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG21	4	0.18
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG22	4	0.18
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG23	4	0.18
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG21	19	0.18
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG22	19	0.18
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG23	19	0.18
(1,911)	1:57:A:GLN:HE21	1:71:A:CYS:H	3	0.18
(1,911)	1:57:A:GLN:HE21	1:71:A:CYS:H	6	0.18
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB2	4	0.18
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB3	4	0.18
(1,884)	1:50:A:SER:H	1:59:A:ILE:H	6	0.18
(1,884)	1:50:A:SER:H	1:59:A:ILE:H	8	0.18
(1,884)	1:50:A:SER:H	1:59:A:ILE:H	13	0.18
(1,884)	1:50:A:SER:H	1:59:A:ILE:H	19	0.18
(1,872)	1:32:A:SER:H	1:33:A:ASP:HB2	12	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,872)	1:32:A:SER:H	1:33:A:ASP:HB3	12	0.18
(1,869)	1:14:A:GLN:HE22	1:28:A:CYS:H	3	0.18
(1,867)	1:34:A:GLU:HG2	1:24:A:GLY:H	18	0.18
(1,867)	1:34:A:GLU:HG3	1:24:A:GLY:H	18	0.18
(1,864)	1:20:A:TRP:HA	1:20:A:TRP:HE1	8	0.18
(1,863)	1:17:A:PRO:HD2	1:20:A:TRP:HE1	19	0.18
(1,863)	1:17:A:PRO:HD3	1:20:A:TRP:HE1	19	0.18
(1,844)	1:79:A:ASN:HB2	1:92:A:CYS:H	15	0.18
(1,844)	1:79:A:ASN:HB3	1:92:A:CYS:H	15	0.18
(1,842)	1:80:A:CYS:HA	1:84:A:THR:H	2	0.18
(1,842)	1:80:A:CYS:HA	1:84:A:THR:H	13	0.18
(1,838)	1:58:A:CYS:HA	1:52:A:GLY:H	20	0.18
(1,837)	1:50:A:SER:H	1:45:A:ARG:HD2	2	0.18
(1,837)	1:50:A:SER:H	1:45:A:ARG:HD3	2	0.18
(1,837)	1:50:A:SER:H	1:45:A:ARG:HD2	16	0.18
(1,837)	1:50:A:SER:H	1:45:A:ARG:HD3	16	0.18
(1,832)	1:35:A:SER:H	1:38:A:GLN:H	3	0.18
(1,822)	1:113:A:GLY:HA2	1:116:A:GLU:H	7	0.18
(1,822)	1:113:A:GLY:HA3	1:116:A:GLU:H	7	0.18
(1,810)	1:101:A:ASN:HD21	1:105:A:ASN:HD22	4	0.18
(1,809)	1:106:A:GLY:H	1:104:A:CYS:H	1	0.18
(1,809)	1:106:A:GLY:H	1:104:A:CYS:H	8	0.18
(1,809)	1:106:A:GLY:H	1:104:A:CYS:H	20	0.18
(1,806)	1:101:A:ASN:HD21	1:102:A:PHE:H	11	0.18
(1,801)	1:102:A:PHE:HB2	1:98:A:ILE:H	7	0.18
(1,801)	1:102:A:PHE:HB3	1:98:A:ILE:H	7	0.18
(1,794)	1:82:A:ASN:HD22	1:94:A:SER:H	3	0.18
(1,791)	1:85:A:CYS:HB2	1:89:A:GLU:H	14	0.18
(1,791)	1:85:A:CYS:HB3	1:89:A:GLU:H	14	0.18
(1,788)	1:80:A:CYS:H	1:78:A:GLU:H	16	0.18
(1,788)	1:80:A:CYS:H	1:78:A:GLU:H	20	0.18
(1,784)	1:71:A:CYS:HB2	1:76:A:ASP:H	7	0.18
(1,784)	1:71:A:CYS:HB3	1:76:A:ASP:H	7	0.18
(1,772)	1:68:A:GLU:H	1:64:A:ARG:H	13	0.18
(1,766)	1:48:A:GLU:HB2	1:58:A:CYS:H	18	0.18
(1,766)	1:48:A:GLU:HB3	1:58:A:CYS:H	18	0.18
(1,759)	1:57:A:GLN:HE21	1:71:A:CYS:HA	3	0.18
(1,744)	1:48:A:GLU:H	1:47:A:HIS:H	2	0.18
(1,731)	1:28:A:CYS:HB2	1:32:A:SER:H	14	0.18
(1,731)	1:28:A:CYS:HB3	1:32:A:SER:H	14	0.18
(1,726)	1:34:A:GLU:HG2	1:27:A:ASP:H	3	0.18
(1,726)	1:34:A:GLU:HG3	1:27:A:ASP:H	3	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,726)	1:34:A:GLU:HG2	1:27:A:ASP:H	13	0.18
(1,726)	1:34:A:GLU:HG3	1:27:A:ASP:H	13	0.18
(1,724)	1:34:A:GLU:HB2	1:25:A:ASP:H	1	0.18
(1,724)	1:34:A:GLU:HB3	1:25:A:ASP:H	1	0.18
(1,724)	1:34:A:GLU:HB2	1:25:A:ASP:H	9	0.18
(1,724)	1:34:A:GLU:HB3	1:25:A:ASP:H	9	0.18
(1,718)	1:16:A:VAL:HB	1:20:A:TRP:HE1	8	0.18
(1,718)	1:16:A:VAL:HB	1:20:A:TRP:HE1	10	0.18
(1,689)	1:69:A:ASN:HD21	1:69:A:ASN:H	8	0.18
(1,683)	1:78:A:GLU:HG2	1:79:A:ASN:HD21	16	0.18
(1,683)	1:78:A:GLU:HG3	1:79:A:ASN:HD21	16	0.18
(1,680)	1:79:A:ASN:HD22	1:79:A:ASN:HB2	14	0.18
(1,680)	1:79:A:ASN:HD22	1:79:A:ASN:HB3	14	0.18
(1,680)	1:79:A:ASN:HD22	1:79:A:ASN:HB2	17	0.18
(1,680)	1:79:A:ASN:HD22	1:79:A:ASN:HB3	17	0.18
(1,679)	1:78:A:GLU:HG2	1:79:A:ASN:HD22	6	0.18
(1,679)	1:78:A:GLU:HG3	1:79:A:ASN:HD22	6	0.18
(1,664)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	1	0.18
(1,664)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	1	0.18
(1,664)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	5	0.18
(1,664)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	5	0.18
(1,664)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	8	0.18
(1,664)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	8	0.18
(1,664)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	9	0.18
(1,664)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	9	0.18
(1,664)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	10	0.18
(1,664)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	10	0.18
(1,664)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	13	0.18
(1,664)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	13	0.18
(1,664)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	20	0.18
(1,664)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	20	0.18
(1,636)	1:78:A:GLU:HB2	1:79:A:ASN:HD22	2	0.18
(1,636)	1:78:A:GLU:HB2	1:79:A:ASN:HD22	2	0.18
(1,636)	1:78:A:GLU:HB3	1:79:A:ASN:HD22	2	0.18
(1,636)	1:78:A:GLU:HB3	1:79:A:ASN:HD22	2	0.18
(1,628)	1:71:A:CYS:HB2	1:57:A:GLN:HE22	9	0.18
(1,628)	1:71:A:CYS:HB3	1:57:A:GLN:HE22	9	0.18
(1,626)	1:71:A:CYS:HA	1:57:A:GLN:HE22	4	0.18
(1,623)	1:30:A:ASP:HB2	1:12:A:ASN:HD22	6	0.18
(1,623)	1:30:A:ASP:HB3	1:12:A:ASN:HD22	6	0.18
(1,612)	1:15:A:CYS:H	1:14:A:GLN:HE22	19	0.18
(1,607)	1:11:A:ASN:HB2	1:11:A:ASN:HD21	11	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,607)	1:11:A:ASN:HB3	1:11:A:ASN:HD21	11	0.18
(1,607)	1:11:A:ASN:HB2	1:11:A:ASN:HD21	16	0.18
(1,607)	1:11:A:ASN:HB3	1:11:A:ASN:HD21	16	0.18
(1,607)	1:11:A:ASN:HB2	1:11:A:ASN:HD21	19	0.18
(1,607)	1:11:A:ASN:HB3	1:11:A:ASN:HD21	19	0.18
(1,591)	1:69:A:ASN:HB2	1:69:A:ASN:HD21	3	0.18
(1,591)	1:69:A:ASN:HB3	1:69:A:ASN:HD21	3	0.18
(1,586)	1:69:A:ASN:HA	1:64:A:ARG:H	10	0.18
(1,585)	1:28:A:CYS:H	1:27:A:ASP:H	1	0.18
(1,580)	1:48:A:GLU:HG2	1:49:A:ILE:H	7	0.18
(1,580)	1:48:A:GLU:HG3	1:49:A:ILE:H	7	0.18
(1,578)	1:52:A:GLY:H	1:50:A:SER:HB2	10	0.18
(1,578)	1:52:A:GLY:H	1:50:A:SER:HB3	10	0.18
(1,569)	1:85:A:CYS:H	1:84:A:THR:H	8	0.18
(1,543)	1:112:A:ASP:HB2	1:114:A:SER:H	13	0.18
(1,543)	1:112:A:ASP:HB3	1:114:A:SER:H	13	0.18
(1,541)	1:115:A:ASP:HB2	1:116:A:GLU:H	3	0.18
(1,541)	1:115:A:ASP:HB3	1:116:A:GLU:H	3	0.18
(1,516)	1:49:A:ILE:H	1:59:A:ILE:H	20	0.18
(1,504)	1:39:A:CYS:HB2	1:39:A:CYS:H	12	0.18
(1,504)	1:39:A:CYS:HB3	1:39:A:CYS:H	12	0.18
(1,499)	1:33:A:ASP:HB2	1:33:A:ASP:H	16	0.18
(1,499)	1:33:A:ASP:HB3	1:33:A:ASP:H	16	0.18
(1,483)	1:10:A:CYS:HB2	1:14:A:GLN:H	15	0.18
(1,483)	1:10:A:CYS:HB3	1:14:A:GLN:H	15	0.18
(1,482)	1:11:A:ASN:HD21	1:11:A:ASN:H	16	0.18
(1,476)	1:7:A:ASP:H	1:3:A:CYS:HB2	2	0.18
(1,476)	1:7:A:ASP:H	1:3:A:CYS:HB3	2	0.18
(1,475)	1:75:A:GLU:H	1:76:A:ASP:H	1	0.18
(1,475)	1:75:A:GLU:H	1:76:A:ASP:H	12	0.18
(1,475)	1:75:A:GLU:H	1:76:A:ASP:H	20	0.18
(1,473)	1:85:A:CYS:H	1:86:A:SER:H	2	0.18
(1,468)	1:78:A:GLU:HG2	1:79:A:ASN:H	2	0.18
(1,468)	1:78:A:GLU:HG3	1:79:A:ASN:H	2	0.18
(1,468)	1:78:A:GLU:HG2	1:79:A:ASN:H	11	0.18
(1,468)	1:78:A:GLU:HG3	1:79:A:ASN:H	11	0.18
(1,466)	1:80:A:CYS:HA	1:79:A:ASN:H	1	0.18
(1,466)	1:80:A:CYS:HA	1:79:A:ASN:H	5	0.18
(1,466)	1:80:A:CYS:HA	1:79:A:ASN:H	9	0.18
(1,462)	1:79:A:ASN:H	1:78:A:GLU:H	15	0.18
(1,460)	1:74:A:GLY:HA2	1:77:A:GLU:H	2	0.18
(1,460)	1:74:A:GLY:HA3	1:77:A:GLU:H	2	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,451)	1:75:A:GLU:H	1:76:A:ASP:H	1	0.18
(1,451)	1:75:A:GLU:H	1:76:A:ASP:H	12	0.18
(1,451)	1:75:A:GLU:H	1:76:A:ASP:H	20	0.18
(1,445)	1:75:A:GLU:H	1:74:A:GLY:H	12	0.18
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB2	12	0.18
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB3	12	0.18
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB2	14	0.18
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB3	14	0.18
(1,419)	1:65:A:CYS:HB2	1:66:A:ASP:H	13	0.18
(1,419)	1:65:A:CYS:HB3	1:66:A:ASP:H	13	0.18
(1,415)	1:64:A:ARG:HA	1:65:A:CYS:H	6	0.18
(1,409)	1:60:A:PRO:HA	1:61:A:VAL:H	1	0.18
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB1	1	0.18
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB2	1	0.18
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB3	1	0.18
(1,390)	1:51:A:CYS:HB2	1:52:A:GLY:H	8	0.18
(1,390)	1:51:A:CYS:HB3	1:52:A:GLY:H	8	0.18
(1,390)	1:51:A:CYS:HB2	1:52:A:GLY:H	13	0.18
(1,390)	1:51:A:CYS:HB3	1:52:A:GLY:H	13	0.18
(1,390)	1:51:A:CYS:HB2	1:52:A:GLY:H	16	0.18
(1,390)	1:51:A:CYS:HB3	1:52:A:GLY:H	16	0.18
(1,378)	1:48:A:GLU:HG2	1:49:A:ILE:H	7	0.18
(1,378)	1:48:A:GLU:HG3	1:49:A:ILE:H	7	0.18
(1,372)	1:48:A:GLU:H	1:48:A:GLU:HA	8	0.18
(1,369)	1:43:A:THR:HB	1:44:A:CYS:H	1	0.18
(1,369)	1:43:A:THR:HB	1:44:A:CYS:H	14	0.18
(1,369)	1:43:A:THR:HB	1:44:A:CYS:H	17	0.18
(1,367)	1:42:A:ARG:HG2	1:43:A:THR:H	9	0.18
(1,367)	1:42:A:ARG:HG2	1:43:A:THR:H	9	0.18
(1,367)	1:42:A:ARG:HG3	1:43:A:THR:H	9	0.18
(1,367)	1:42:A:ARG:HG3	1:43:A:THR:H	9	0.18
(1,351)	1:32:A:SER:H	1:33:A:ASP:H	1	0.18
(1,351)	1:32:A:SER:H	1:33:A:ASP:H	2	0.18
(1,351)	1:32:A:SER:H	1:33:A:ASP:H	13	0.18
(1,351)	1:32:A:SER:H	1:33:A:ASP:H	20	0.18
(1,349)	1:32:A:SER:H	1:33:A:ASP:H	1	0.18
(1,349)	1:32:A:SER:H	1:33:A:ASP:H	2	0.18
(1,349)	1:32:A:SER:H	1:33:A:ASP:H	13	0.18
(1,349)	1:32:A:SER:H	1:33:A:ASP:H	20	0.18
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB2	7	0.18
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB3	7	0.18
(1,328)	1:22:A:CYS:HB2	1:22:A:CYS:H	8	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,328)	1:22:A:CYS:HB3	1:22:A:CYS:H	8	0.18
(1,328)	1:22:A:CYS:HB2	1:22:A:CYS:H	9	0.18
(1,328)	1:22:A:CYS:HB3	1:22:A:CYS:H	9	0.18
(1,312)	1:14:A:GLN:HG2	1:14:A:GLN:H	15	0.18
(1,312)	1:14:A:GLN:HG3	1:14:A:GLN:H	15	0.18
(1,312)	1:14:A:GLN:HG2	1:14:A:GLN:H	20	0.18
(1,312)	1:14:A:GLN:HG3	1:14:A:GLN:H	20	0.18
(1,308)	1:13:A:GLY:H	1:14:A:GLN:H	15	0.18
(1,302)	1:14:A:GLN:H	1:12:A:ASN:H	15	0.18
(1,299)	1:11:A:ASN:H	1:12:A:ASN:H	1	0.18
(1,290)	1:8:A:PHE:HA	1:9:A:VAL:H	4	0.18
(1,290)	1:8:A:PHE:HA	1:9:A:VAL:H	11	0.18
(1,269)	1:7:A:ASP:H	1:4:A:ALA:H	6	0.18
(1,248)	1:83:A:ILE:HB	1:84:A:THR:H	1	0.18
(1,248)	1:83:A:ILE:HB	1:84:A:THR:H	11	0.18
(1,241)	1:86:A:SER:H	1:89:A:GLU:H	17	0.18
(1,228)	1:92:A:CYS:HB2	1:93:A:SER:H	4	0.18
(1,228)	1:92:A:CYS:HB3	1:93:A:SER:H	4	0.18
(1,228)	1:92:A:CYS:HB2	1:93:A:SER:H	14	0.18
(1,228)	1:92:A:CYS:HB3	1:93:A:SER:H	14	0.18
(1,226)	1:92:A:CYS:HB2	1:94:A:SER:H	20	0.18
(1,226)	1:92:A:CYS:HB3	1:94:A:SER:H	20	0.18
(1,215)	1:96:A:ARG:H	1:92:A:CYS:HB2	2	0.18
(1,215)	1:96:A:ARG:H	1:92:A:CYS:HB3	2	0.18
(1,205)	1:98:A:ILE:HG12	1:98:A:ILE:H	15	0.18
(1,205)	1:98:A:ILE:HG13	1:98:A:ILE:H	15	0.18
(1,204)	1:98:A:ILE:HG12	1:98:A:ILE:H	8	0.18
(1,204)	1:98:A:ILE:HG13	1:98:A:ILE:H	8	0.18
(1,204)	1:98:A:ILE:HG12	1:98:A:ILE:H	14	0.18
(1,204)	1:98:A:ILE:HG13	1:98:A:ILE:H	14	0.18
(1,184)	1:103:A:VAL:HB	1:102:A:PHE:H	15	0.18
(1,174)	1:103:A:VAL:H	1:101:A:ASN:HB2	18	0.18
(1,174)	1:103:A:VAL:H	1:101:A:ASN:HB3	18	0.18
(1,137)	1:109:A:ASP:H	1:113:A:GLY:HA2	5	0.18
(1,137)	1:109:A:ASP:H	1:113:A:GLY:HA3	5	0.18
(1,123)	1:115:A:ASP:HB2	1:115:A:ASP:H	3	0.18
(1,123)	1:115:A:ASP:HB3	1:115:A:ASP:H	3	0.18
(1,123)	1:115:A:ASP:HB2	1:115:A:ASP:H	19	0.18
(1,123)	1:115:A:ASP:HB3	1:115:A:ASP:H	19	0.18
(1,69)	1:78:A:GLU:HG2	1:78:A:GLU:H	1	0.18
(1,69)	1:78:A:GLU:HG3	1:78:A:GLU:H	1	0.18
(1,59)	1:65:A:CYS:H	1:66:A:ASP:H	19	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,42)	1:96:A:ARG:H	1:97:A:CYS:H	2	0.18
(1,41)	1:96:A:ARG:H	1:97:A:CYS:H	2	0.18
(1,33)	1:115:A:ASP:H	1:114:A:SER:H	2	0.18
(1,33)	1:115:A:ASP:H	1:114:A:SER:H	8	0.18
(1,28)	1:118:A:ASP:H	1:117:A:LEU:H	5	0.18
(1,28)	1:118:A:ASP:H	1:117:A:LEU:H	14	0.18
(1,24)	1:104:A:CYS:H	1:105:A:ASN:H	6	0.18
(1,24)	1:104:A:CYS:H	1:105:A:ASN:H	7	0.18
(1,23)	1:104:A:CYS:H	1:105:A:ASN:H	6	0.18
(1,23)	1:104:A:CYS:H	1:105:A:ASN:H	7	0.18
(1,22)	1:91:A:THR:H	1:92:A:CYS:H	3	0.18
(1,22)	1:91:A:THR:H	1:92:A:CYS:H	12	0.18
(1,18)	1:81:A:GLY:H	1:82:A:ASN:H	17	0.18
(1,17)	1:81:A:GLY:H	1:80:A:CYS:H	20	0.18
(1,6)	1:23:A:ASP:H	1:24:A:GLY:H	6	0.18
(1,6)	1:23:A:ASP:H	1:24:A:GLY:H	7	0.18
(4,5)	1:49:A:ILE:O	1:59:A:ILE:H	7	0.17
(4,5)	1:49:A:ILE:O	1:59:A:ILE:H	11	0.17
(4,2)	1:90:A:PHE:O	1:98:A:ILE:H	18	0.17
(3,7)	2:202:A:CA:CA	1:63:A:TRP:O	3	0.17
(3,7)	2:202:A:CA:CA	1:63:A:TRP:O	11	0.17
(3,7)	2:202:A:CA:CA	1:63:A:TRP:O	16	0.17
(2,381)	1:100:A:ARG:HD3	1:90:A:PHE:H	15	0.17
(2,366)	1:107:A:GLN:HA	1:106:A:GLY:H	4	0.17
(2,353)	1:99:A:SER:HG	1:101:A:ASN:HD22	12	0.17
(2,298)	1:28:A:CYS:HB3	1:14:A:GLN:HE22	12	0.17
(2,298)	1:28:A:CYS:HB2	1:14:A:GLN:HE22	15	0.17
(2,280)	1:92:A:CYS:H	1:91:A:THR:H	4	0.17
(2,280)	1:92:A:CYS:H	1:91:A:THR:H	11	0.17
(2,280)	1:92:A:CYS:H	1:91:A:THR:H	14	0.17
(2,276)	1:43:A:THR:HA	1:57:A:GLN:H	11	0.17
(2,263)	1:63:A:TRP:HB2	1:63:A:TRP:H	11	0.17
(2,245)	1:36:A:PRO:HA	1:39:A:CYS:H	16	0.17
(2,235)	1:80:A:CYS:HA	1:85:A:CYS:H	11	0.17
(2,226)	1:92:A:CYS:H	1:97:A:CYS:H	7	0.17
(2,226)	1:98:A:ILE:H	1:97:A:CYS:H	16	0.17
(2,218)	1:36:A:PRO:HD2	1:37:A:GLU:H	20	0.17
(2,196)	1:40:A:HIS:HA	1:42:A:ARG:H	15	0.17
(2,188)	1:16:A:VAL:HG11	1:19:A:ARG:H	3	0.17
(2,188)	1:16:A:VAL:HG12	1:19:A:ARG:H	3	0.17
(2,188)	1:16:A:VAL:HG13	1:19:A:ARG:H	3	0.17
(2,188)	1:16:A:VAL:HG21	1:19:A:ARG:H	3	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,188)	1:16:A:VAL:HG22	1:19:A:ARG:H	3	0.17
(2,188)	1:16:A:VAL:HG23	1:19:A:ARG:H	3	0.17
(2,181)	1:39:A:CYS:HB3	1:41:A:MET:H	9	0.17
(2,181)	1:39:A:CYS:HB3	1:41:A:MET:H	11	0.17
(2,174)	1:117:A:LEU:HB2	1:116:A:GLU:H	10	0.17
(2,168)	1:38:A:GLN:HG3	1:38:A:GLN:H	3	0.17
(2,164)	1:14:A:GLN:HB2	1:14:A:GLN:H	13	0.17
(2,164)	1:14:A:GLN:HB3	1:14:A:GLN:H	13	0.17
(2,164)	1:14:A:GLN:HB2	1:14:A:GLN:H	14	0.17
(2,164)	1:14:A:GLN:HB3	1:14:A:GLN:H	14	0.17
(2,82)	1:94:A:SER:HB3	1:94:A:SER:H	15	0.17
(2,52)	1:60:A:PRO:HD2	1:63:A:TRP:HE1	8	0.17
(2,38)	1:96:A:ARG:HB3	1:97:A:CYS:H	11	0.17
(2,11)	1:110:A:CYS:HA	1:113:A:GLY:H	3	0.17
(1,930)	1:102:A:PHE:HE2	1:107:A:GLN:HG2	9	0.17
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG21	11	0.17
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG22	11	0.17
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG23	11	0.17
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG21	16	0.17
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG22	16	0.17
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG23	16	0.17
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG11	5	0.17
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG12	5	0.17
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG13	5	0.17
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG21	5	0.17
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG22	5	0.17
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG23	5	0.17
(1,911)	1:57:A:GLN:HE21	1:71:A:CYS:H	13	0.17
(1,902)	1:94:A:SER:HB2	1:82:A:ASN:HD21	14	0.17
(1,902)	1:94:A:SER:HB3	1:82:A:ASN:HD21	14	0.17
(1,898)	1:57:A:GLN:HE22	1:71:A:CYS:H	4	0.17
(1,886)	1:51:A:CYS:H	1:58:A:CYS:H	2	0.17
(1,886)	1:51:A:CYS:H	1:58:A:CYS:H	14	0.17
(1,886)	1:51:A:CYS:H	1:58:A:CYS:H	17	0.17
(1,876)	1:39:A:CYS:HB2	1:43:A:THR:H	7	0.17
(1,876)	1:39:A:CYS:HB3	1:43:A:THR:H	7	0.17
(1,876)	1:39:A:CYS:HB2	1:43:A:THR:H	8	0.17
(1,876)	1:39:A:CYS:HB3	1:43:A:THR:H	8	0.17
(1,869)	1:14:A:GLN:HE22	1:28:A:CYS:H	6	0.17
(1,864)	1:20:A:TRP:HA	1:20:A:TRP:HE1	14	0.17
(1,864)	1:20:A:TRP:HA	1:20:A:TRP:HE1	20	0.17
(1,863)	1:17:A:PRO:HD2	1:20:A:TRP:HE1	1	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,863)	1:17:A:PRO:HD3	1:20:A:TRP:HE1	1	0.17
(1,860)	1:16:A:VAL:HB	1:19:A:ARG:H	20	0.17
(1,859)	1:3:A:CYS:HB2	1:18:A:SER:H	1	0.17
(1,859)	1:3:A:CYS:HB3	1:18:A:SER:H	1	0.17
(1,842)	1:80:A:CYS:HA	1:84:A:THR:H	15	0.17
(1,838)	1:58:A:CYS:HA	1:52:A:GLY:H	10	0.17
(1,837)	1:50:A:SER:H	1:45:A:ARG:HD2	6	0.17
(1,837)	1:50:A:SER:H	1:45:A:ARG:HD3	6	0.17
(1,820)	1:110:A:CYS:H	1:115:A:ASP:H	19	0.17
(1,816)	1:109:A:ASP:H	1:116:A:GLU:HG2	15	0.17
(1,816)	1:109:A:ASP:H	1:116:A:GLU:HG3	15	0.17
(1,811)	1:107:A:GLN:H	1:105:A:ASN:HD21	13	0.17
(1,809)	1:106:A:GLY:H	1:104:A:CYS:H	11	0.17
(1,803)	1:101:A:ASN:HD21	1:99:A:SER:H	16	0.17
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG21	18	0.17
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG22	18	0.17
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG23	18	0.17
(1,792)	1:97:A:CYS:HB2	1:91:A:THR:H	3	0.17
(1,792)	1:97:A:CYS:HB3	1:91:A:THR:H	3	0.17
(1,791)	1:85:A:CYS:HB2	1:89:A:GLU:H	20	0.17
(1,791)	1:85:A:CYS:HB3	1:89:A:GLU:H	20	0.17
(1,786)	1:71:A:CYS:H	1:76:A:ASP:H	4	0.17
(1,781)	1:73:A:SER:H	1:71:A:CYS:HB2	13	0.17
(1,781)	1:73:A:SER:H	1:71:A:CYS:HB3	13	0.17
(1,781)	1:73:A:SER:H	1:71:A:CYS:HB2	17	0.17
(1,781)	1:73:A:SER:H	1:71:A:CYS:HB3	17	0.17
(1,768)	1:58:A:CYS:HA	1:59:A:ILE:H	10	0.17
(1,763)	1:58:A:CYS:HB2	1:58:A:CYS:H	10	0.17
(1,763)	1:58:A:CYS:HB3	1:58:A:CYS:H	10	0.17
(1,744)	1:48:A:GLU:H	1:47:A:HIS:H	7	0.17
(1,744)	1:48:A:GLU:H	1:47:A:HIS:H	13	0.17
(1,744)	1:48:A:GLU:H	1:47:A:HIS:H	19	0.17
(1,735)	1:28:A:CYS:HB2	1:33:A:ASP:H	7	0.17
(1,735)	1:28:A:CYS:HB3	1:33:A:ASP:H	7	0.17
(1,731)	1:28:A:CYS:HB2	1:32:A:SER:H	17	0.17
(1,731)	1:28:A:CYS:HB3	1:32:A:SER:H	17	0.17
(1,726)	1:34:A:GLU:HG2	1:27:A:ASP:H	16	0.17
(1,726)	1:34:A:GLU:HG3	1:27:A:ASP:H	16	0.17
(1,718)	1:16:A:VAL:HB	1:20:A:TRP:HE1	11	0.17
(1,718)	1:16:A:VAL:HB	1:20:A:TRP:HE1	13	0.17
(1,696)	1:44:A:CYS:HB2	1:34:A:GLU:H	9	0.17
(1,696)	1:44:A:CYS:HB3	1:34:A:GLU:H	9	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD2	16	0.17
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD3	16	0.17
(1,664)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	6	0.17
(1,664)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	6	0.17
(1,664)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	11	0.17
(1,664)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	11	0.17
(1,664)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	19	0.17
(1,664)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	19	0.17
(1,612)	1:15:A:CYS:H	1:14:A:GLN:HE22	5	0.17
(1,612)	1:15:A:CYS:H	1:14:A:GLN:HE22	11	0.17
(1,607)	1:11:A:ASN:HB2	1:11:A:ASN:HD21	13	0.17
(1,607)	1:11:A:ASN:HB3	1:11:A:ASN:HD21	13	0.17
(1,607)	1:11:A:ASN:HB2	1:11:A:ASN:HD21	20	0.17
(1,607)	1:11:A:ASN:HB3	1:11:A:ASN:HD21	20	0.17
(1,603)	1:32:A:SER:HB2	1:11:A:ASN:HD22	2	0.17
(1,603)	1:32:A:SER:HB3	1:11:A:ASN:HD22	2	0.17
(1,598)	1:74:A:GLY:HA2	1:69:A:ASN:HD22	8	0.17
(1,598)	1:74:A:GLY:HA3	1:69:A:ASN:HD22	8	0.17
(1,597)	1:74:A:GLY:HA2	1:69:A:ASN:HD22	8	0.17
(1,597)	1:74:A:GLY:HA3	1:69:A:ASN:HD22	8	0.17
(1,592)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	20	0.17
(1,592)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	20	0.17
(1,591)	1:69:A:ASN:HB2	1:69:A:ASN:HD21	1	0.17
(1,591)	1:69:A:ASN:HB3	1:69:A:ASN:HD21	1	0.17
(1,591)	1:69:A:ASN:HB2	1:69:A:ASN:HD21	8	0.17
(1,591)	1:69:A:ASN:HB3	1:69:A:ASN:HD21	8	0.17
(1,591)	1:69:A:ASN:HB2	1:69:A:ASN:HD21	11	0.17
(1,591)	1:69:A:ASN:HB3	1:69:A:ASN:HD21	11	0.17
(1,582)	1:46:A:ILE:H	1:45:A:ARG:H	14	0.17
(1,560)	1:90:A:PHE:H	1:99:A:SER:H	16	0.17
(1,556)	1:101:A:ASN:HD21	1:101:A:ASN:H	9	0.17
(1,542)	1:112:A:ASP:H	1:114:A:SER:H	8	0.17
(1,541)	1:115:A:ASP:HB2	1:116:A:GLU:H	6	0.17
(1,541)	1:115:A:ASP:HB3	1:116:A:GLU:H	6	0.17
(1,516)	1:49:A:ILE:H	1:59:A:ILE:H	9	0.17
(1,516)	1:49:A:ILE:H	1:59:A:ILE:H	16	0.17
(1,510)	1:48:A:GLU:HB2	1:48:A:GLU:H	18	0.17
(1,510)	1:48:A:GLU:HB3	1:48:A:GLU:H	18	0.17
(1,509)	1:46:A:ILE:HA	1:46:A:ILE:H	4	0.17
(1,504)	1:39:A:CYS:HB2	1:39:A:CYS:H	8	0.17
(1,504)	1:39:A:CYS:HB3	1:39:A:CYS:H	8	0.17
(1,501)	1:34:A:GLU:HB2	1:34:A:GLU:H	20	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,501)	1:34:A:GLU:HB3	1:34:A:GLU:H	20	0.17
(1,499)	1:33:A:ASP:HB2	1:33:A:ASP:H	17	0.17
(1,499)	1:33:A:ASP:HB3	1:33:A:ASP:H	17	0.17
(1,483)	1:10:A:CYS:HB2	1:14:A:GLN:H	4	0.17
(1,483)	1:10:A:CYS:HB3	1:14:A:GLN:H	4	0.17
(1,483)	1:10:A:CYS:HB2	1:14:A:GLN:H	20	0.17
(1,483)	1:10:A:CYS:HB3	1:14:A:GLN:H	20	0.17
(1,475)	1:75:A:GLU:H	1:76:A:ASP:H	16	0.17
(1,475)	1:75:A:GLU:H	1:76:A:ASP:H	18	0.17
(1,475)	1:75:A:GLU:H	1:76:A:ASP:H	19	0.17
(1,473)	1:85:A:CYS:H	1:86:A:SER:H	1	0.17
(1,473)	1:85:A:CYS:H	1:86:A:SER:H	20	0.17
(1,468)	1:78:A:GLU:HG2	1:79:A:ASN:H	3	0.17
(1,468)	1:78:A:GLU:HG3	1:79:A:ASN:H	3	0.17
(1,454)	1:78:A:GLU:HG2	1:76:A:ASP:H	12	0.17
(1,454)	1:78:A:GLU:HG3	1:76:A:ASP:H	12	0.17
(1,451)	1:75:A:GLU:H	1:76:A:ASP:H	16	0.17
(1,451)	1:75:A:GLU:H	1:76:A:ASP:H	18	0.17
(1,451)	1:75:A:GLU:H	1:76:A:ASP:H	19	0.17
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB2	15	0.17
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB3	15	0.17
(1,438)	1:72:A:ASP:H	1:73:A:SER:H	10	0.17
(1,435)	1:72:A:ASP:HA	1:72:A:ASP:H	5	0.17
(1,419)	1:65:A:CYS:HB2	1:66:A:ASP:H	2	0.17
(1,419)	1:65:A:CYS:HB3	1:66:A:ASP:H	2	0.17
(1,418)	1:64:A:ARG:HA	1:66:A:ASP:H	1	0.17
(1,418)	1:64:A:ARG:HA	1:66:A:ASP:H	15	0.17
(1,415)	1:64:A:ARG:HA	1:65:A:CYS:H	15	0.17
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB2	1	0.17
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB3	1	0.17
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB2	14	0.17
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB3	14	0.17
(1,409)	1:60:A:PRO:HA	1:61:A:VAL:H	13	0.17
(1,409)	1:60:A:PRO:HA	1:61:A:VAL:H	17	0.17
(1,383)	1:51:A:CYS:H	1:50:A:SER:HA	18	0.17
(1,377)	1:60:A:PRO:HA	1:49:A:ILE:H	3	0.17
(1,375)	1:48:A:GLU:HA	1:49:A:ILE:H	6	0.17
(1,374)	1:61:A:VAL:H	1:49:A:ILE:H	19	0.17
(1,369)	1:43:A:THR:HB	1:44:A:CYS:H	7	0.17
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB2	17	0.17
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB3	17	0.17
(1,348)	1:30:A:ASP:HB2	1:31:A:GLY:H	7	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,348)	1:30:A:ASP:HB3	1:31:A:GLY:H	7	0.17
(1,346)	1:32:A:SER:H	1:31:A:GLY:H	8	0.17
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB2	2	0.17
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB3	2	0.17
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB2	9	0.17
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB3	9	0.17
(1,313)	1:14:A:GLN:HG2	1:14:A:GLN:H	3	0.17
(1,313)	1:14:A:GLN:HG3	1:14:A:GLN:H	3	0.17
(1,312)	1:14:A:GLN:HG2	1:14:A:GLN:H	4	0.17
(1,312)	1:14:A:GLN:HG3	1:14:A:GLN:H	4	0.17
(1,312)	1:14:A:GLN:HG2	1:14:A:GLN:H	14	0.17
(1,312)	1:14:A:GLN:HG3	1:14:A:GLN:H	14	0.17
(1,308)	1:13:A:GLY:H	1:14:A:GLN:H	6	0.17
(1,308)	1:13:A:GLY:H	1:14:A:GLN:H	10	0.17
(1,302)	1:14:A:GLN:H	1:12:A:ASN:H	14	0.17
(1,293)	1:8:A:PHE:HB2	1:9:A:VAL:H	16	0.17
(1,293)	1:8:A:PHE:HB3	1:9:A:VAL:H	16	0.17
(1,290)	1:8:A:PHE:HA	1:9:A:VAL:H	1	0.17
(1,290)	1:8:A:PHE:HA	1:9:A:VAL:H	6	0.17
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	6	0.17
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	6	0.17
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	6	0.17
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	6	0.17
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	18	0.17
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	18	0.17
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	18	0.17
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	18	0.17
(1,241)	1:86:A:SER:H	1:89:A:GLU:H	10	0.17
(1,226)	1:92:A:CYS:HB2	1:94:A:SER:H	12	0.17
(1,226)	1:92:A:CYS:HB3	1:94:A:SER:H	12	0.17
(1,226)	1:92:A:CYS:HB2	1:94:A:SER:H	15	0.17
(1,226)	1:92:A:CYS:HB3	1:94:A:SER:H	15	0.17
(1,205)	1:98:A:ILE:HG12	1:98:A:ILE:H	20	0.17
(1,205)	1:98:A:ILE:HG13	1:98:A:ILE:H	20	0.17
(1,196)	1:98:A:ILE:HA	1:99:A:SER:H	3	0.17
(1,187)	1:103:A:VAL:HG11	1:102:A:PHE:H	20	0.17
(1,187)	1:103:A:VAL:HG12	1:102:A:PHE:H	20	0.17
(1,187)	1:103:A:VAL:HG13	1:102:A:PHE:H	20	0.17
(1,187)	1:103:A:VAL:HG21	1:102:A:PHE:H	20	0.17
(1,187)	1:103:A:VAL:HG22	1:102:A:PHE:H	20	0.17
(1,187)	1:103:A:VAL:HG23	1:102:A:PHE:H	20	0.17
(1,184)	1:103:A:VAL:HB	1:102:A:PHE:H	14	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,143)	1:106:A:GLY:H	1:107:A:GLN:H	10	0.17
(1,130)	1:115:A:ASP:HB2	1:113:A:GLY:H	20	0.17
(1,130)	1:115:A:ASP:HB3	1:113:A:GLY:H	20	0.17
(1,128)	1:114:A:SER:HA	1:114:A:SER:H	11	0.17
(1,127)	1:114:A:SER:H	1:114:A:SER:HB2	18	0.17
(1,127)	1:114:A:SER:H	1:114:A:SER:HB3	18	0.17
(1,123)	1:115:A:ASP:HB2	1:115:A:ASP:H	10	0.17
(1,123)	1:115:A:ASP:HB3	1:115:A:ASP:H	10	0.17
(1,123)	1:115:A:ASP:HB2	1:115:A:ASP:H	15	0.17
(1,123)	1:115:A:ASP:HB3	1:115:A:ASP:H	15	0.17
(1,123)	1:115:A:ASP:HB2	1:115:A:ASP:H	16	0.17
(1,123)	1:115:A:ASP:HB3	1:115:A:ASP:H	16	0.17
(1,116)	1:116:A:GLU:HG2	1:116:A:GLU:H	19	0.17
(1,116)	1:116:A:GLU:HG3	1:116:A:GLU:H	19	0.17
(1,84)	1:14:A:GLN:HG2	1:29:A:GLU:H	19	0.17
(1,84)	1:14:A:GLN:HG3	1:29:A:GLU:H	19	0.17
(1,84)	1:14:A:GLN:HG2	1:29:A:GLU:H	20	0.17
(1,84)	1:14:A:GLN:HG3	1:29:A:GLU:H	20	0.17
(1,74)	1:65:A:CYS:H	1:65:A:CYS:HB2	11	0.17
(1,74)	1:65:A:CYS:H	1:65:A:CYS:HB3	11	0.17
(1,53)	1:77:A:GLU:H	1:76:A:ASP:H	12	0.17
(1,52)	1:76:A:ASP:H	1:77:A:GLU:H	12	0.17
(1,49)	1:94:A:SER:H	1:93:A:SER:H	7	0.17
(1,28)	1:118:A:ASP:H	1:117:A:LEU:H	18	0.17
(1,24)	1:104:A:CYS:H	1:105:A:ASN:H	4	0.17
(1,23)	1:104:A:CYS:H	1:105:A:ASN:H	4	0.17
(1,22)	1:91:A:THR:H	1:92:A:CYS:H	4	0.17
(1,22)	1:91:A:THR:H	1:92:A:CYS:H	11	0.17
(1,22)	1:91:A:THR:H	1:92:A:CYS:H	14	0.17
(1,18)	1:81:A:GLY:H	1:82:A:ASN:H	8	0.17
(1,17)	1:81:A:GLY:H	1:80:A:CYS:H	14	0.17
(1,6)	1:23:A:ASP:H	1:24:A:GLY:H	1	0.17
(1,6)	1:23:A:ASP:H	1:24:A:GLY:H	2	0.17
(1,6)	1:23:A:ASP:H	1:24:A:GLY:H	10	0.17
(1,6)	1:23:A:ASP:H	1:24:A:GLY:H	16	0.17
(4,5)	1:49:A:ILE:O	1:59:A:ILE:H	10	0.16
(3,7)	2:202:A:CA:CA	1:63:A:TRP:O	2	0.16
(3,7)	2:202:A:CA:CA	1:63:A:TRP:O	13	0.16
(3,7)	2:202:A:CA:CA	1:63:A:TRP:O	15	0.16
(2,366)	1:107:A:GLN:HA	1:106:A:GLY:H	3	0.16
(2,363)	1:49:A:ILE:HB	1:49:A:ILE:H	4	0.16
(2,331)	1:101:A:ASN:H	1:99:A:SER:H	7	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,323)	1:64:A:ARG:HG2	1:68:A:GLU:H	14	0.16
(2,311)	1:97:A:CYS:HB2	1:91:A:THR:H	4	0.16
(2,307)	1:59:A:ILE:HD13	1:63:A:TRP:H	16	0.16
(2,301)	1:11:A:ASN:HD22	1:32:A:SER:H	18	0.16
(2,246)	1:90:A:PHE:HB2	1:100:A:ARG:H	9	0.16
(2,246)	1:90:A:PHE:HB3	1:100:A:ARG:H	9	0.16
(2,246)	1:90:A:PHE:HB2	1:100:A:ARG:H	14	0.16
(2,246)	1:90:A:PHE:HB3	1:100:A:ARG:H	14	0.16
(2,236)	1:21:A:LYS:HB2	1:21:A:LYS:H	1	0.16
(2,226)	1:98:A:ILE:H	1:97:A:CYS:H	9	0.16
(2,187)	1:118:A:ASP:HA	1:119:A:CYS:H	5	0.16
(2,164)	1:14:A:GLN:HB2	1:14:A:GLN:H	3	0.16
(2,164)	1:14:A:GLN:HB3	1:14:A:GLN:H	3	0.16
(2,104)	1:80:A:CYS:HB3	1:80:A:CYS:H	15	0.16
(2,89)	1:107:A:GLN:HB2	1:108:A:ASP:H	19	0.16
(2,89)	1:107:A:GLN:HB3	1:108:A:ASP:H	19	0.16
(2,83)	1:35:A:SER:HB3	1:38:A:GLN:H	1	0.16
(2,83)	1:35:A:SER:HB3	1:38:A:GLN:H	15	0.16
(2,52)	1:80:A:CYS:HB3	1:63:A:TRP:HE1	6	0.16
(2,12)	1:10:A:CYS:HB3	1:13:A:GLY:H	18	0.16
(1,930)	1:102:A:PHE:HE2	1:107:A:GLN:HG2	20	0.16
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG21	10	0.16
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG22	10	0.16
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG23	10	0.16
(1,917)	1:28:A:CYS:H	1:14:A:GLN:HG2	2	0.16
(1,915)	1:51:A:CYS:HA	1:71:A:CYS:H	13	0.16
(1,905)	1:101:A:ASN:HD21	1:105:A:ASN:HD21	2	0.16
(1,884)	1:50:A:SER:H	1:59:A:ILE:H	12	0.16
(1,882)	1:58:A:CYS:HA	1:50:A:SER:H	1	0.16
(1,873)	1:34:A:GLU:HB2	1:33:A:ASP:H	4	0.16
(1,873)	1:34:A:GLU:HB3	1:33:A:ASP:H	4	0.16
(1,872)	1:32:A:SER:H	1:33:A:ASP:HB2	16	0.16
(1,872)	1:32:A:SER:H	1:33:A:ASP:HB3	16	0.16
(1,864)	1:20:A:TRP:HA	1:20:A:TRP:HE1	3	0.16
(1,864)	1:20:A:TRP:HA	1:20:A:TRP:HE1	18	0.16
(1,863)	1:17:A:PRO:HD2	1:20:A:TRP:HE1	5	0.16
(1,863)	1:17:A:PRO:HD3	1:20:A:TRP:HE1	5	0.16
(1,851)	1:32:A:SER:H	1:11:A:ASN:HD22	18	0.16
(1,849)	1:33:A:ASP:H	1:11:A:ASN:H	1	0.16
(1,844)	1:79:A:ASN:HB2	1:92:A:CYS:H	6	0.16
(1,844)	1:79:A:ASN:HB3	1:92:A:CYS:H	6	0.16
(1,839)	1:55:A:SER:H	1:57:A:GLN:H	18	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,832)	1:35:A:SER:H	1:38:A:GLN:H	17	0.16
(1,820)	1:110:A:CYS:H	1:115:A:ASP:H	17	0.16
(1,816)	1:109:A:ASP:H	1:116:A:GLU:HG2	12	0.16
(1,816)	1:109:A:ASP:H	1:116:A:GLU:HG3	12	0.16
(1,810)	1:101:A:ASN:HD21	1:105:A:ASN:HD22	14	0.16
(1,810)	1:101:A:ASN:HD21	1:105:A:ASN:HD22	17	0.16
(1,809)	1:106:A:GLY:H	1:104:A:CYS:H	15	0.16
(1,808)	1:116:A:GLU:HB2	1:104:A:CYS:H	17	0.16
(1,808)	1:116:A:GLU:HB3	1:104:A:CYS:H	17	0.16
(1,806)	1:101:A:ASN:HD21	1:102:A:PHE:H	14	0.16
(1,800)	1:85:A:CYS:HB2	1:98:A:ILE:H	2	0.16
(1,800)	1:85:A:CYS:HB3	1:98:A:ILE:H	2	0.16
(1,799)	1:85:A:CYS:HA	1:97:A:CYS:H	14	0.16
(1,798)	1:85:A:CYS:HB2	1:97:A:CYS:H	6	0.16
(1,798)	1:85:A:CYS:HB3	1:97:A:CYS:H	6	0.16
(1,797)	1:91:A:THR:HG1	1:96:A:ARG:H	12	0.16
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG21	14	0.16
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG22	14	0.16
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG23	14	0.16
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG21	17	0.16
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG22	17	0.16
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG23	17	0.16
(1,792)	1:97:A:CYS:HB2	1:91:A:THR:H	4	0.16
(1,792)	1:97:A:CYS:HB3	1:91:A:THR:H	4	0.16
(1,791)	1:85:A:CYS:HB2	1:89:A:GLU:H	4	0.16
(1,791)	1:85:A:CYS:HB3	1:89:A:GLU:H	4	0.16
(1,788)	1:80:A:CYS:H	1:78:A:GLU:H	3	0.16
(1,784)	1:71:A:CYS:HB2	1:76:A:ASP:H	1	0.16
(1,784)	1:71:A:CYS:HB3	1:76:A:ASP:H	1	0.16
(1,784)	1:71:A:CYS:HB2	1:76:A:ASP:H	4	0.16
(1,784)	1:71:A:CYS:HB3	1:76:A:ASP:H	4	0.16
(1,741)	1:9:A:VAL:HG11	1:38:A:GLN:HE21	7	0.16
(1,741)	1:9:A:VAL:HG12	1:38:A:GLN:HE21	7	0.16
(1,741)	1:9:A:VAL:HG13	1:38:A:GLN:HE21	7	0.16
(1,741)	1:9:A:VAL:HG21	1:38:A:GLN:HE21	7	0.16
(1,741)	1:9:A:VAL:HG22	1:38:A:GLN:HE21	7	0.16
(1,741)	1:9:A:VAL:HG23	1:38:A:GLN:HE21	7	0.16
(1,735)	1:28:A:CYS:HB2	1:33:A:ASP:H	9	0.16
(1,735)	1:28:A:CYS:HB3	1:33:A:ASP:H	9	0.16
(1,731)	1:28:A:CYS:HB2	1:32:A:SER:H	5	0.16
(1,731)	1:28:A:CYS:HB3	1:32:A:SER:H	5	0.16
(1,731)	1:28:A:CYS:HB2	1:32:A:SER:H	9	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,731)	1:28:A:CYS:HB3	1:32:A:SER:H	9	0.16
(1,724)	1:34:A:GLU:HB2	1:25:A:ASP:H	20	0.16
(1,724)	1:34:A:GLU:HB3	1:25:A:ASP:H	20	0.16
(1,718)	1:16:A:VAL:HB	1:20:A:TRP:HE1	3	0.16
(1,717)	1:20:A:TRP:HE1	1:20:A:TRP:H	12	0.16
(1,716)	1:28:A:CYS:HB2	1:14:A:GLN:HE22	17	0.16
(1,716)	1:28:A:CYS:HB3	1:14:A:GLN:HE22	17	0.16
(1,711)	1:10:A:CYS:HB2	1:11:A:ASN:H	1	0.16
(1,711)	1:10:A:CYS:HB3	1:11:A:ASN:H	1	0.16
(1,705)	1:100:A:ARG:H	1:100:A:ARG:HD2	14	0.16
(1,705)	1:100:A:ARG:H	1:100:A:ARG:HD3	14	0.16
(1,680)	1:79:A:ASN:HD22	1:79:A:ASN:HB2	15	0.16
(1,680)	1:79:A:ASN:HD22	1:79:A:ASN:HB3	15	0.16
(1,664)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	2	0.16
(1,664)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	2	0.16
(1,664)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	3	0.16
(1,664)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	3	0.16
(1,664)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	7	0.16
(1,664)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	7	0.16
(1,664)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	17	0.16
(1,664)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	17	0.16
(1,648)	1:101:A:ASN:HD22	1:101:A:ASN:HA	2	0.16
(1,645)	1:101:A:ASN:HD22	1:101:A:ASN:H	7	0.16
(1,626)	1:71:A:CYS:HA	1:57:A:GLN:HE22	18	0.16
(1,623)	1:30:A:ASP:HB2	1:12:A:ASN:HD22	9	0.16
(1,623)	1:30:A:ASP:HB3	1:12:A:ASN:HD22	9	0.16
(1,610)	1:14:A:GLN:HE22	1:29:A:GLU:H	16	0.16
(1,607)	1:11:A:ASN:HB2	1:11:A:ASN:HD21	7	0.16
(1,607)	1:11:A:ASN:HB3	1:11:A:ASN:HD21	7	0.16
(1,596)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	12	0.16
(1,596)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	12	0.16
(1,591)	1:69:A:ASN:HB2	1:69:A:ASN:HD21	7	0.16
(1,591)	1:69:A:ASN:HB3	1:69:A:ASN:HD21	7	0.16
(1,580)	1:48:A:GLU:HG2	1:49:A:ILE:H	13	0.16
(1,580)	1:48:A:GLU:HG3	1:49:A:ILE:H	13	0.16
(1,562)	1:102:A:PHE:HB2	1:99:A:SER:H	14	0.16
(1,562)	1:102:A:PHE:HB3	1:99:A:SER:H	14	0.16
(1,560)	1:90:A:PHE:H	1:99:A:SER:H	10	0.16
(1,551)	1:104:A:CYS:HB2	1:104:A:CYS:H	6	0.16
(1,551)	1:104:A:CYS:HB3	1:104:A:CYS:H	6	0.16
(1,551)	1:104:A:CYS:HB2	1:104:A:CYS:H	13	0.16
(1,551)	1:104:A:CYS:HB3	1:104:A:CYS:H	13	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,550)	1:104:A:CYS:HB2	1:104:A:CYS:H	6	0.16
(1,550)	1:104:A:CYS:HB3	1:104:A:CYS:H	6	0.16
(1,550)	1:104:A:CYS:HB2	1:104:A:CYS:H	13	0.16
(1,550)	1:104:A:CYS:HB3	1:104:A:CYS:H	13	0.16
(1,541)	1:115:A:ASP:HB2	1:116:A:GLU:H	9	0.16
(1,541)	1:115:A:ASP:HB3	1:116:A:GLU:H	9	0.16
(1,536)	1:89:A:GLU:HB2	1:86:A:SER:H	5	0.16
(1,536)	1:89:A:GLU:HB3	1:86:A:SER:H	5	0.16
(1,518)	1:49:A:ILE:H	1:61:A:VAL:H	3	0.16
(1,518)	1:49:A:ILE:H	1:61:A:VAL:H	6	0.16
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	1	0.16
(1,517)	1:59:A:ILE:HG12	1:59:A:ILE:H	1	0.16
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	1	0.16
(1,517)	1:59:A:ILE:HG13	1:59:A:ILE:H	1	0.16
(1,516)	1:49:A:ILE:H	1:59:A:ILE:H	7	0.16
(1,516)	1:49:A:ILE:H	1:59:A:ILE:H	10	0.16
(1,512)	1:59:A:ILE:H	1:49:A:ILE:H	8	0.16
(1,510)	1:48:A:GLU:HB2	1:48:A:GLU:H	14	0.16
(1,510)	1:48:A:GLU:HB3	1:48:A:GLU:H	14	0.16
(1,501)	1:34:A:GLU:HB2	1:34:A:GLU:H	7	0.16
(1,501)	1:34:A:GLU:HB3	1:34:A:GLU:H	7	0.16
(1,501)	1:34:A:GLU:HB2	1:34:A:GLU:H	13	0.16
(1,501)	1:34:A:GLU:HB3	1:34:A:GLU:H	13	0.16
(1,499)	1:33:A:ASP:HB2	1:33:A:ASP:H	2	0.16
(1,499)	1:33:A:ASP:HB3	1:33:A:ASP:H	2	0.16
(1,499)	1:33:A:ASP:HB2	1:33:A:ASP:H	3	0.16
(1,499)	1:33:A:ASP:HB3	1:33:A:ASP:H	3	0.16
(1,499)	1:33:A:ASP:HB2	1:33:A:ASP:H	18	0.16
(1,499)	1:33:A:ASP:HB3	1:33:A:ASP:H	18	0.16
(1,495)	1:31:A:GLY:H	1:29:A:GLU:H	16	0.16
(1,485)	1:8:A:PHE:H	1:18:A:SER:H	9	0.16
(1,483)	1:10:A:CYS:HB2	1:14:A:GLN:H	13	0.16
(1,483)	1:10:A:CYS:HB3	1:14:A:GLN:H	13	0.16
(1,477)	1:9:A:VAL:HA	1:9:A:VAL:H	18	0.16
(1,476)	1:7:A:ASP:H	1:3:A:CYS:HB2	16	0.16
(1,476)	1:7:A:ASP:H	1:3:A:CYS:HB3	16	0.16
(1,473)	1:85:A:CYS:H	1:86:A:SER:H	6	0.16
(1,473)	1:85:A:CYS:H	1:86:A:SER:H	9	0.16
(1,469)	1:78:A:GLU:HB2	1:79:A:ASN:H	18	0.16
(1,469)	1:78:A:GLU:HB2	1:79:A:ASN:H	18	0.16
(1,469)	1:78:A:GLU:HB3	1:79:A:ASN:H	18	0.16
(1,469)	1:78:A:GLU:HB3	1:79:A:ASN:H	18	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,466)	1:80:A:CYS:HA	1:79:A:ASN:H	7	0.16
(1,462)	1:79:A:ASN:H	1:78:A:GLU:H	4	0.16
(1,462)	1:79:A:ASN:H	1:78:A:GLU:H	5	0.16
(1,462)	1:79:A:ASN:H	1:78:A:GLU:H	8	0.16
(1,446)	1:73:A:SER:H	1:74:A:GLY:H	4	0.16
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB2	20	0.16
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB3	20	0.16
(1,439)	1:75:A:GLU:H	1:73:A:SER:H	4	0.16
(1,439)	1:75:A:GLU:H	1:73:A:SER:H	18	0.16
(1,435)	1:72:A:ASP:HA	1:72:A:ASP:H	7	0.16
(1,435)	1:72:A:ASP:HA	1:72:A:ASP:H	9	0.16
(1,435)	1:72:A:ASP:HA	1:72:A:ASP:H	17	0.16
(1,415)	1:64:A:ARG:HA	1:65:A:CYS:H	7	0.16
(1,415)	1:64:A:ARG:HA	1:65:A:CYS:H	17	0.16
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB2	5	0.16
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB3	5	0.16
(1,409)	1:60:A:PRO:HA	1:61:A:VAL:H	5	0.16
(1,409)	1:60:A:PRO:HA	1:61:A:VAL:H	9	0.16
(1,409)	1:60:A:PRO:HA	1:61:A:VAL:H	11	0.16
(1,409)	1:60:A:PRO:HA	1:61:A:VAL:H	20	0.16
(1,390)	1:51:A:CYS:HB2	1:52:A:GLY:H	11	0.16
(1,390)	1:51:A:CYS:HB3	1:52:A:GLY:H	11	0.16
(1,386)	1:51:A:CYS:HB2	1:51:A:CYS:H	12	0.16
(1,386)	1:51:A:CYS:HB3	1:51:A:CYS:H	12	0.16
(1,378)	1:48:A:GLU:HG2	1:49:A:ILE:H	13	0.16
(1,378)	1:48:A:GLU:HG3	1:49:A:ILE:H	13	0.16
(1,374)	1:61:A:VAL:H	1:49:A:ILE:H	2	0.16
(1,374)	1:61:A:VAL:H	1:49:A:ILE:H	7	0.16
(1,372)	1:48:A:GLU:H	1:48:A:GLU:HA	17	0.16
(1,370)	1:44:A:CYS:HB2	1:44:A:CYS:H	19	0.16
(1,370)	1:44:A:CYS:HB3	1:44:A:CYS:H	19	0.16
(1,369)	1:43:A:THR:HB	1:44:A:CYS:H	2	0.16
(1,365)	1:43:A:THR:HB	1:43:A:THR:H	19	0.16
(1,351)	1:32:A:SER:H	1:33:A:ASP:H	12	0.16
(1,349)	1:32:A:SER:H	1:33:A:ASP:H	12	0.16
(1,348)	1:30:A:ASP:HB2	1:31:A:GLY:H	16	0.16
(1,348)	1:30:A:ASP:HB3	1:31:A:GLY:H	16	0.16
(1,343)	1:28:A:CYS:HB2	1:28:A:CYS:H	5	0.16
(1,343)	1:28:A:CYS:HB3	1:28:A:CYS:H	5	0.16
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB2	11	0.16
(1,339)	1:25:A:ASP:H	1:20:A:TRP:HB3	11	0.16
(1,328)	1:22:A:CYS:HB2	1:22:A:CYS:H	10	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,328)	1:22:A:CYS:HB3	1:22:A:CYS:H	10	0.16
(1,320)	1:7:A:ASP:HA	1:18:A:SER:H	14	0.16
(1,312)	1:14:A:GLN:HG2	1:14:A:GLN:H	8	0.16
(1,312)	1:14:A:GLN:HG3	1:14:A:GLN:H	8	0.16
(1,308)	1:13:A:GLY:H	1:14:A:GLN:H	7	0.16
(1,308)	1:13:A:GLY:H	1:14:A:GLN:H	13	0.16
(1,299)	1:11:A:ASN:H	1:12:A:ASN:H	2	0.16
(1,290)	1:8:A:PHE:HA	1:9:A:VAL:H	8	0.16
(1,290)	1:8:A:PHE:HA	1:9:A:VAL:H	15	0.16
(1,290)	1:8:A:PHE:HA	1:9:A:VAL:H	17	0.16
(1,290)	1:8:A:PHE:HA	1:9:A:VAL:H	20	0.16
(1,286)	1:7:A:ASP:HB2	1:7:A:ASP:H	3	0.16
(1,286)	1:7:A:ASP:HB3	1:7:A:ASP:H	3	0.16
(1,286)	1:7:A:ASP:HB2	1:7:A:ASP:H	18	0.16
(1,286)	1:7:A:ASP:HB3	1:7:A:ASP:H	18	0.16
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	5	0.16
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	5	0.16
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	5	0.16
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	5	0.16
(1,241)	1:86:A:SER:H	1:89:A:GLU:H	15	0.16
(1,204)	1:98:A:ILE:HG12	1:98:A:ILE:H	6	0.16
(1,204)	1:98:A:ILE:HG13	1:98:A:ILE:H	6	0.16
(1,204)	1:98:A:ILE:HG12	1:98:A:ILE:H	11	0.16
(1,204)	1:98:A:ILE:HG13	1:98:A:ILE:H	11	0.16
(1,204)	1:98:A:ILE:HG12	1:98:A:ILE:H	13	0.16
(1,204)	1:98:A:ILE:HG13	1:98:A:ILE:H	13	0.16
(1,190)	1:101:A:ASN:HB2	1:101:A:ASN:H	6	0.16
(1,190)	1:101:A:ASN:HB3	1:101:A:ASN:H	6	0.16
(1,190)	1:101:A:ASN:HB2	1:101:A:ASN:H	18	0.16
(1,190)	1:101:A:ASN:HB3	1:101:A:ASN:H	18	0.16
(1,180)	1:99:A:SER:HB2	1:102:A:PHE:H	1	0.16
(1,180)	1:99:A:SER:HB3	1:102:A:PHE:H	1	0.16
(1,174)	1:103:A:VAL:H	1:101:A:ASN:HB2	9	0.16
(1,174)	1:103:A:VAL:H	1:101:A:ASN:HB3	9	0.16
(1,143)	1:106:A:GLY:H	1:107:A:GLN:H	3	0.16
(1,130)	1:115:A:ASP:HB2	1:113:A:GLY:H	12	0.16
(1,130)	1:115:A:ASP:HB3	1:113:A:GLY:H	12	0.16
(1,128)	1:114:A:SER:HA	1:114:A:SER:H	3	0.16
(1,128)	1:114:A:SER:HA	1:114:A:SER:H	4	0.16
(1,125)	1:114:A:SER:H	1:113:A:GLY:HA2	18	0.16
(1,125)	1:114:A:SER:H	1:113:A:GLY:HA3	18	0.16
(1,123)	1:115:A:ASP:HB2	1:115:A:ASP:H	9	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,123)	1:115:A:ASP:HB3	1:115:A:ASP:H	9	0.16
(1,123)	1:115:A:ASP:HB2	1:115:A:ASP:H	13	0.16
(1,123)	1:115:A:ASP:HB3	1:115:A:ASP:H	13	0.16
(1,122)	1:115:A:ASP:HB2	1:115:A:ASP:H	12	0.16
(1,122)	1:115:A:ASP:HB3	1:115:A:ASP:H	12	0.16
(1,114)	1:117:A:LEU:HD11	1:117:A:LEU:H	16	0.16
(1,114)	1:117:A:LEU:HD12	1:117:A:LEU:H	16	0.16
(1,114)	1:117:A:LEU:HD13	1:117:A:LEU:H	16	0.16
(1,114)	1:117:A:LEU:HD21	1:117:A:LEU:H	16	0.16
(1,114)	1:117:A:LEU:HD22	1:117:A:LEU:H	16	0.16
(1,114)	1:117:A:LEU:HD23	1:117:A:LEU:H	16	0.16
(1,109)	1:119:A:CYS:H	1:117:A:LEU:HG	15	0.16
(1,80)	1:44:A:CYS:HB2	1:45:A:ARG:H	8	0.16
(1,80)	1:44:A:CYS:HB3	1:45:A:ARG:H	8	0.16
(1,74)	1:65:A:CYS:H	1:65:A:CYS:HB2	10	0.16
(1,74)	1:65:A:CYS:H	1:65:A:CYS:HB3	10	0.16
(1,63)	1:39:A:CYS:H	1:40:A:HIS:H	8	0.16
(1,59)	1:65:A:CYS:H	1:66:A:ASP:H	3	0.16
(1,59)	1:65:A:CYS:H	1:66:A:ASP:H	4	0.16
(1,59)	1:65:A:CYS:H	1:66:A:ASP:H	16	0.16
(1,59)	1:65:A:CYS:H	1:66:A:ASP:H	20	0.16
(1,56)	1:70:A:ASP:H	1:71:A:CYS:H	2	0.16
(1,49)	1:94:A:SER:H	1:93:A:SER:H	8	0.16
(1,42)	1:96:A:ARG:H	1:97:A:CYS:H	1	0.16
(1,41)	1:96:A:ARG:H	1:97:A:CYS:H	1	0.16
(1,35)	1:115:A:ASP:H	1:116:A:GLU:H	9	0.16
(1,28)	1:118:A:ASP:H	1:117:A:LEU:H	11	0.16
(1,12)	1:34:A:GLU:H	1:33:A:ASP:H	15	0.16
(1,9)	1:12:A:ASN:H	1:11:A:ASN:H	15	0.16
(1,7)	1:22:A:CYS:H	1:23:A:ASP:H	10	0.16
(1,6)	1:23:A:ASP:H	1:24:A:GLY:H	5	0.16
(4,5)	1:49:A:ILE:O	1:59:A:ILE:H	5	0.15
(4,2)	1:90:A:PHE:O	1:98:A:ILE:H	6	0.15
(3,10)	2:202:A:CA:CA	1:70:A:ASP:OD2	7	0.15
(3,7)	2:202:A:CA:CA	1:63:A:TRP:O	19	0.15
(2,391)	1:17:A:PRO:HD2	1:16:A:VAL:H	3	0.15
(2,391)	1:17:A:PRO:HD2	1:16:A:VAL:H	18	0.15
(2,382)	1:72:A:ASP:HB2	1:73:A:SER:H	9	0.15
(2,382)	1:72:A:ASP:HB3	1:73:A:SER:H	9	0.15
(2,370)	1:38:A:GLN:HG2	1:38:A:GLN:HE22	8	0.15
(2,366)	1:107:A:GLN:HA	1:106:A:GLY:H	19	0.15
(2,362)	1:14:A:GLN:HB2	1:10:A:CYS:H	5	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,362)	1:14:A:GLN:HB3	1:10:A:CYS:H	5	0.15
(2,361)	1:61:A:VAL:HG11	1:64:A:ARG:H	1	0.15
(2,361)	1:61:A:VAL:HG11	1:64:A:ARG:H	4	0.15
(2,353)	1:99:A:SER:HG	1:101:A:ASN:HD22	3	0.15
(2,353)	1:99:A:SER:HG	1:101:A:ASN:HD22	7	0.15
(2,339)	1:9:A:VAL:HG11	1:13:A:GLY:H	12	0.15
(2,339)	1:9:A:VAL:HG12	1:13:A:GLY:H	12	0.15
(2,339)	1:9:A:VAL:HG13	1:13:A:GLY:H	12	0.15
(2,339)	1:9:A:VAL:HG21	1:13:A:GLY:H	12	0.15
(2,339)	1:9:A:VAL:HG22	1:13:A:GLY:H	12	0.15
(2,339)	1:9:A:VAL:HG23	1:13:A:GLY:H	12	0.15
(2,331)	1:101:A:ASN:H	1:99:A:SER:H	16	0.15
(2,329)	1:90:A:PHE:HA	1:98:A:ILE:H	9	0.15
(2,311)	1:97:A:CYS:HB3	1:91:A:THR:H	7	0.15
(2,301)	1:11:A:ASN:HD22	1:32:A:SER:H	2	0.15
(2,301)	1:11:A:ASN:HD22	1:32:A:SER:H	3	0.15
(2,288)	1:75:A:GLU:HB2	1:75:A:GLU:H	8	0.15
(2,288)	1:75:A:GLU:HB3	1:75:A:GLU:H	8	0.15
(2,276)	1:43:A:THR:HA	1:57:A:GLN:H	8	0.15
(2,246)	1:90:A:PHE:HB2	1:100:A:ARG:H	13	0.15
(2,246)	1:90:A:PHE:HB3	1:100:A:ARG:H	13	0.15
(2,246)	1:90:A:PHE:HB2	1:100:A:ARG:H	18	0.15
(2,246)	1:90:A:PHE:HB3	1:100:A:ARG:H	18	0.15
(2,235)	1:86:A:SER:HA	1:85:A:CYS:H	19	0.15
(2,221)	1:2:A:THR:HG1	1:2:A:THR:H	14	0.15
(2,218)	1:36:A:PRO:HD2	1:37:A:GLU:H	7	0.15
(2,218)	1:36:A:PRO:HD2	1:37:A:GLU:H	12	0.15
(2,210)	1:33:A:ASP:HA	1:38:A:GLN:HE21	17	0.15
(2,206)	1:34:A:GLU:HB3	1:22:A:CYS:H	18	0.15
(2,188)	1:16:A:VAL:HG11	1:19:A:ARG:H	4	0.15
(2,188)	1:16:A:VAL:HG12	1:19:A:ARG:H	4	0.15
(2,188)	1:16:A:VAL:HG13	1:19:A:ARG:H	4	0.15
(2,188)	1:16:A:VAL:HG21	1:19:A:ARG:H	4	0.15
(2,188)	1:16:A:VAL:HG22	1:19:A:ARG:H	4	0.15
(2,188)	1:16:A:VAL:HG23	1:19:A:ARG:H	4	0.15
(2,187)	1:116:A:GLU:HA	1:119:A:CYS:H	20	0.15
(2,181)	1:39:A:CYS:HB3	1:41:A:MET:H	13	0.15
(2,179)	1:9:A:VAL:HG11	1:10:A:CYS:H	3	0.15
(2,179)	1:9:A:VAL:HG12	1:10:A:CYS:H	3	0.15
(2,179)	1:9:A:VAL:HG13	1:10:A:CYS:H	3	0.15
(2,179)	1:9:A:VAL:HG21	1:10:A:CYS:H	3	0.15
(2,179)	1:9:A:VAL:HG22	1:10:A:CYS:H	3	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,179)	1:9:A:VAL:HG23	1:10:A:CYS:H	3	0.15
(2,164)	1:14:A:GLN:HB2	1:14:A:GLN:H	16	0.15
(2,164)	1:14:A:GLN:HB3	1:14:A:GLN:H	16	0.15
(2,117)	1:14:A:GLN:HB2	1:12:A:ASN:HD21	5	0.15
(2,117)	1:14:A:GLN:HB3	1:12:A:ASN:HD21	5	0.15
(2,115)	1:80:A:CYS:H	1:81:A:GLY:H	9	0.15
(2,115)	1:80:A:CYS:H	1:81:A:GLY:H	19	0.15
(2,89)	1:107:A:GLN:HB2	1:108:A:ASP:H	11	0.15
(2,89)	1:107:A:GLN:HB3	1:108:A:ASP:H	11	0.15
(2,83)	1:35:A:SER:HB3	1:38:A:GLN:H	12	0.15
(2,80)	1:56:A:THR:HB	1:56:A:THR:H	10	0.15
(2,75)	1:108:A:ASP:HA	1:108:A:ASP:H	14	0.15
(2,74)	1:46:A:ILE:HB	1:46:A:ILE:H	7	0.15
(2,74)	1:46:A:ILE:HB	1:46:A:ILE:H	19	0.15
(2,52)	1:60:A:PRO:HD2	1:63:A:TRP:HE1	10	0.15
(2,49)	1:35:A:SER:HB3	1:39:A:CYS:H	3	0.15
(2,22)	1:75:A:GLU:HA	1:78:A:GLU:H	2	0.15
(2,11)	1:110:A:CYS:HA	1:113:A:GLY:H	4	0.15
(2,2)	1:32:A:SER:HA	1:35:A:SER:H	3	0.15
(1,928)	1:102:A:PHE:HA	1:103:A:VAL:HG11	16	0.15
(1,928)	1:102:A:PHE:HA	1:103:A:VAL:HG12	16	0.15
(1,928)	1:102:A:PHE:HA	1:103:A:VAL:HG13	16	0.15
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG21	7	0.15
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG22	7	0.15
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG23	7	0.15
(1,917)	1:28:A:CYS:H	1:14:A:GLN:HG2	5	0.15
(1,911)	1:57:A:GLN:HE21	1:71:A:CYS:H	19	0.15
(1,906)	1:13:A:GLY:HA2	1:12:A:ASN:HD22	9	0.15
(1,906)	1:13:A:GLY:HA3	1:12:A:ASN:HD22	9	0.15
(1,900)	1:83:A:ILE:HG12	1:82:A:ASN:H	10	0.15
(1,900)	1:83:A:ILE:HG13	1:82:A:ASN:H	10	0.15
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB2	17	0.15
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB3	17	0.15
(1,886)	1:51:A:CYS:H	1:58:A:CYS:H	7	0.15
(1,884)	1:50:A:SER:H	1:59:A:ILE:H	7	0.15
(1,876)	1:39:A:CYS:HB2	1:43:A:THR:H	20	0.15
(1,876)	1:39:A:CYS:HB3	1:43:A:THR:H	20	0.15
(1,872)	1:32:A:SER:H	1:33:A:ASP:HB2	13	0.15
(1,872)	1:32:A:SER:H	1:33:A:ASP:HB3	13	0.15
(1,871)	1:30:A:ASP:HB2	1:32:A:SER:H	1	0.15
(1,871)	1:30:A:ASP:HB3	1:32:A:SER:H	1	0.15
(1,853)	1:10:A:CYS:HB2	1:12:A:ASN:H	15	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,853)	1:10:A:CYS:HB3	1:12:A:ASN:H	15	0.15
(1,851)	1:32:A:SER:H	1:11:A:ASN:HD22	2	0.15
(1,851)	1:32:A:SER:H	1:11:A:ASN:HD22	3	0.15
(1,851)	1:32:A:SER:H	1:11:A:ASN:HD22	12	0.15
(1,838)	1:58:A:CYS:HA	1:52:A:GLY:H	15	0.15
(1,838)	1:58:A:CYS:HA	1:52:A:GLY:H	17	0.15
(1,835)	1:45:A:ARG:HB2	1:46:A:ILE:H	8	0.15
(1,835)	1:45:A:ARG:HB3	1:46:A:ILE:H	8	0.15
(1,831)	1:73:A:SER:H	1:75:A:GLU:H	2	0.15
(1,828)	1:85:A:CYS:HA	1:86:A:SER:H	4	0.15
(1,828)	1:85:A:CYS:HA	1:86:A:SER:H	16	0.15
(1,822)	1:113:A:GLY:HA2	1:116:A:GLU:H	6	0.15
(1,822)	1:113:A:GLY:HA3	1:116:A:GLU:H	6	0.15
(1,816)	1:109:A:ASP:H	1:116:A:GLU:HG2	13	0.15
(1,816)	1:109:A:ASP:H	1:116:A:GLU:HG3	13	0.15
(1,816)	1:109:A:ASP:H	1:116:A:GLU:HG2	20	0.15
(1,816)	1:109:A:ASP:H	1:116:A:GLU:HG3	20	0.15
(1,811)	1:107:A:GLN:H	1:105:A:ASN:HD21	18	0.15
(1,809)	1:106:A:GLY:H	1:104:A:CYS:H	14	0.15
(1,800)	1:85:A:CYS:HB2	1:98:A:ILE:H	19	0.15
(1,800)	1:85:A:CYS:HB3	1:98:A:ILE:H	19	0.15
(1,797)	1:91:A:THR:HG23	1:96:A:ARG:H	19	0.15
(1,792)	1:97:A:CYS:HB2	1:91:A:THR:H	19	0.15
(1,792)	1:97:A:CYS:HB3	1:91:A:THR:H	19	0.15
(1,791)	1:85:A:CYS:HB2	1:89:A:GLU:H	12	0.15
(1,791)	1:85:A:CYS:HB3	1:89:A:GLU:H	12	0.15
(1,787)	1:73:A:SER:H	1:76:A:ASP:H	13	0.15
(1,784)	1:71:A:CYS:HB2	1:76:A:ASP:H	14	0.15
(1,784)	1:71:A:CYS:HB3	1:76:A:ASP:H	14	0.15
(1,781)	1:73:A:SER:H	1:71:A:CYS:HB2	11	0.15
(1,781)	1:73:A:SER:H	1:71:A:CYS:HB3	11	0.15
(1,766)	1:48:A:GLU:HB2	1:58:A:CYS:H	14	0.15
(1,766)	1:48:A:GLU:HB3	1:58:A:CYS:H	14	0.15
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	6	0.15
(1,756)	1:57:A:GLN:HB2	1:57:A:GLN:HE21	6	0.15
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	6	0.15
(1,756)	1:57:A:GLN:HB3	1:57:A:GLN:HE21	6	0.15
(1,734)	1:32:A:SER:H	1:11:A:ASN:H	6	0.15
(1,726)	1:34:A:GLU:HG2	1:27:A:ASP:H	12	0.15
(1,726)	1:34:A:GLU:HG3	1:27:A:ASP:H	12	0.15
(1,718)	1:16:A:VAL:HB	1:20:A:TRP:HE1	6	0.15
(1,712)	1:32:A:SER:H	1:11:A:ASN:H	6	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,705)	1:100:A:ARG:H	1:100:A:ARG:HD2	6	0.15
(1,705)	1:100:A:ARG:H	1:100:A:ARG:HD3	6	0.15
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG2	8	0.15
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG3	8	0.15
(1,683)	1:78:A:GLU:HG2	1:79:A:ASN:HD21	12	0.15
(1,683)	1:78:A:GLU:HG3	1:79:A:ASN:HD21	12	0.15
(1,683)	1:78:A:GLU:HG2	1:79:A:ASN:HD21	20	0.15
(1,683)	1:78:A:GLU:HG3	1:79:A:ASN:HD21	20	0.15
(1,664)	1:105:A:ASN:HB2	1:105:A:ASN:HD21	4	0.15
(1,664)	1:105:A:ASN:HB3	1:105:A:ASN:HD21	4	0.15
(1,662)	1:102:A:PHE:HB2	1:105:A:ASN:HD21	7	0.15
(1,662)	1:102:A:PHE:HB3	1:105:A:ASN:HD21	7	0.15
(1,658)	1:102:A:PHE:HA	1:105:A:ASN:HD22	8	0.15
(1,658)	1:102:A:PHE:HA	1:105:A:ASN:HD22	16	0.15
(1,645)	1:101:A:ASN:HD22	1:101:A:ASN:H	3	0.15
(1,627)	1:72:A:ASP:HA	1:57:A:GLN:HE22	15	0.15
(1,623)	1:30:A:ASP:HB2	1:12:A:ASN:HD22	3	0.15
(1,623)	1:30:A:ASP:HB3	1:12:A:ASN:HD22	3	0.15
(1,612)	1:15:A:CYS:H	1:14:A:GLN:HE22	1	0.15
(1,610)	1:14:A:GLN:HE22	1:29:A:GLU:H	11	0.15
(1,607)	1:11:A:ASN:HB2	1:11:A:ASN:HD21	17	0.15
(1,607)	1:11:A:ASN:HB3	1:11:A:ASN:HD21	17	0.15
(1,601)	1:11:A:ASN:H	1:11:A:ASN:HD22	17	0.15
(1,586)	1:69:A:ASN:HA	1:64:A:ARG:H	13	0.15
(1,580)	1:48:A:GLU:HG2	1:49:A:ILE:H	5	0.15
(1,580)	1:48:A:GLU:HG3	1:49:A:ILE:H	5	0.15
(1,578)	1:52:A:GLY:H	1:50:A:SER:HB2	18	0.15
(1,578)	1:52:A:GLY:H	1:50:A:SER:HB3	18	0.15
(1,574)	1:64:A:ARG:H	1:65:A:CYS:H	20	0.15
(1,560)	1:90:A:PHE:H	1:99:A:SER:H	11	0.15
(1,560)	1:90:A:PHE:H	1:99:A:SER:H	13	0.15
(1,551)	1:104:A:CYS:HB2	1:104:A:CYS:H	5	0.15
(1,551)	1:104:A:CYS:HB3	1:104:A:CYS:H	5	0.15
(1,550)	1:104:A:CYS:HB2	1:104:A:CYS:H	5	0.15
(1,550)	1:104:A:CYS:HB3	1:104:A:CYS:H	5	0.15
(1,534)	1:77:A:GLU:HB2	1:77:A:GLU:H	19	0.15
(1,534)	1:77:A:GLU:HB3	1:77:A:GLU:H	19	0.15
(1,510)	1:48:A:GLU:HB2	1:48:A:GLU:H	3	0.15
(1,510)	1:48:A:GLU:HB3	1:48:A:GLU:H	3	0.15
(1,510)	1:48:A:GLU:HB2	1:48:A:GLU:H	10	0.15
(1,510)	1:48:A:GLU:HB3	1:48:A:GLU:H	10	0.15
(1,510)	1:48:A:GLU:HB2	1:48:A:GLU:H	15	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,510)	1:48:A:GLU:HB3	1:48:A:GLU:H	15	0.15
(1,501)	1:34:A:GLU:HB2	1:34:A:GLU:H	17	0.15
(1,501)	1:34:A:GLU:HB3	1:34:A:GLU:H	17	0.15
(1,499)	1:33:A:ASP:HB2	1:33:A:ASP:H	1	0.15
(1,499)	1:33:A:ASP:HB3	1:33:A:ASP:H	1	0.15
(1,482)	1:11:A:ASN:HD21	1:11:A:ASN:H	1	0.15
(1,482)	1:11:A:ASN:HD21	1:11:A:ASN:H	7	0.15
(1,482)	1:11:A:ASN:HD21	1:11:A:ASN:H	17	0.15
(1,477)	1:9:A:VAL:HA	1:9:A:VAL:H	3	0.15
(1,475)	1:75:A:GLU:H	1:76:A:ASP:H	5	0.15
(1,475)	1:75:A:GLU:H	1:76:A:ASP:H	9	0.15
(1,475)	1:75:A:GLU:H	1:76:A:ASP:H	14	0.15
(1,473)	1:85:A:CYS:H	1:86:A:SER:H	7	0.15
(1,473)	1:85:A:CYS:H	1:86:A:SER:H	15	0.15
(1,473)	1:85:A:CYS:H	1:86:A:SER:H	18	0.15
(1,473)	1:85:A:CYS:H	1:86:A:SER:H	19	0.15
(1,469)	1:78:A:GLU:HB2	1:79:A:ASN:H	14	0.15
(1,469)	1:78:A:GLU:HB2	1:79:A:ASN:H	14	0.15
(1,469)	1:78:A:GLU:HB3	1:79:A:ASN:H	14	0.15
(1,469)	1:78:A:GLU:HB3	1:79:A:ASN:H	14	0.15
(1,462)	1:79:A:ASN:H	1:78:A:GLU:H	7	0.15
(1,454)	1:78:A:GLU:HG2	1:76:A:ASP:H	6	0.15
(1,454)	1:78:A:GLU:HG3	1:76:A:ASP:H	6	0.15
(1,454)	1:78:A:GLU:HG2	1:76:A:ASP:H	11	0.15
(1,454)	1:78:A:GLU:HG3	1:76:A:ASP:H	11	0.15
(1,451)	1:75:A:GLU:H	1:76:A:ASP:H	5	0.15
(1,451)	1:75:A:GLU:H	1:76:A:ASP:H	9	0.15
(1,451)	1:75:A:GLU:H	1:76:A:ASP:H	14	0.15
(1,442)	1:73:A:SER:HB2	1:73:A:SER:H	2	0.15
(1,442)	1:73:A:SER:HB3	1:73:A:SER:H	2	0.15
(1,437)	1:72:A:ASP:H	1:71:A:CYS:H	12	0.15
(1,435)	1:72:A:ASP:HA	1:72:A:ASP:H	1	0.15
(1,435)	1:72:A:ASP:HA	1:72:A:ASP:H	11	0.15
(1,435)	1:72:A:ASP:HA	1:72:A:ASP:H	16	0.15
(1,419)	1:65:A:CYS:HB2	1:66:A:ASP:H	18	0.15
(1,419)	1:65:A:CYS:HB3	1:66:A:ASP:H	18	0.15
(1,409)	1:60:A:PRO:HA	1:61:A:VAL:H	2	0.15
(1,409)	1:60:A:PRO:HA	1:61:A:VAL:H	7	0.15
(1,409)	1:60:A:PRO:HA	1:61:A:VAL:H	16	0.15
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB1	5	0.15
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB2	5	0.15
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB3	5	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,390)	1:51:A:CYS:HB2	1:52:A:GLY:H	19	0.15
(1,390)	1:51:A:CYS:HB3	1:52:A:GLY:H	19	0.15
(1,386)	1:51:A:CYS:HB2	1:51:A:CYS:H	4	0.15
(1,386)	1:51:A:CYS:HB3	1:51:A:CYS:H	4	0.15
(1,383)	1:51:A:CYS:H	1:50:A:SER:HA	20	0.15
(1,378)	1:48:A:GLU:HG2	1:49:A:ILE:H	5	0.15
(1,378)	1:48:A:GLU:HG3	1:49:A:ILE:H	5	0.15
(1,369)	1:43:A:THR:HB	1:44:A:CYS:H	6	0.15
(1,369)	1:43:A:THR:HB	1:44:A:CYS:H	11	0.15
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB2	2	0.15
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB3	2	0.15
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB2	3	0.15
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB3	3	0.15
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB2	13	0.15
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB3	13	0.15
(1,357)	1:40:A:HIS:H	1:39:A:CYS:HA	4	0.15
(1,350)	1:31:A:GLY:H	1:32:A:SER:H	7	0.15
(1,346)	1:32:A:SER:H	1:31:A:GLY:H	5	0.15
(1,343)	1:28:A:CYS:HB2	1:28:A:CYS:H	15	0.15
(1,343)	1:28:A:CYS:HB3	1:28:A:CYS:H	15	0.15
(1,329)	1:25:A:ASP:H	1:23:A:ASP:H	7	0.15
(1,320)	1:7:A:ASP:HA	1:18:A:SER:H	18	0.15
(1,313)	1:14:A:GLN:HG2	1:14:A:GLN:H	11	0.15
(1,313)	1:14:A:GLN:HG3	1:14:A:GLN:H	11	0.15
(1,302)	1:14:A:GLN:H	1:12:A:ASN:H	10	0.15
(1,293)	1:8:A:PHE:HB2	1:9:A:VAL:H	7	0.15
(1,293)	1:8:A:PHE:HB3	1:9:A:VAL:H	7	0.15
(1,290)	1:8:A:PHE:HA	1:9:A:VAL:H	2	0.15
(1,279)	1:6:A:SER:HB2	1:6:A:SER:H	6	0.15
(1,279)	1:6:A:SER:HB3	1:6:A:SER:H	6	0.15
(1,277)	1:6:A:SER:HB2	1:6:A:SER:H	6	0.15
(1,277)	1:6:A:SER:HB3	1:6:A:SER:H	6	0.15
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	1	0.15
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	1	0.15
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	1	0.15
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	1	0.15
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	2	0.15
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	2	0.15
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	2	0.15
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	2	0.15
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	3	0.15
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	3	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	3	0.15
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	3	0.15
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	15	0.15
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	15	0.15
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	15	0.15
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	15	0.15
(1,248)	1:83:A:ILE:HB	1:84:A:THR:H	3	0.15
(1,241)	1:86:A:SER:H	1:89:A:GLU:H	8	0.15
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD11	1	0.15
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD12	1	0.15
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD13	1	0.15
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD11	14	0.15
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD12	14	0.15
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD13	14	0.15
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD11	17	0.15
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD12	17	0.15
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD13	17	0.15
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD11	20	0.15
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD12	20	0.15
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD13	20	0.15
(1,228)	1:92:A:CYS:HB2	1:93:A:SER:H	3	0.15
(1,228)	1:92:A:CYS:HB3	1:93:A:SER:H	3	0.15
(1,226)	1:92:A:CYS:HB2	1:94:A:SER:H	11	0.15
(1,226)	1:92:A:CYS:HB3	1:94:A:SER:H	11	0.15
(1,215)	1:96:A:ARG:H	1:92:A:CYS:HB2	17	0.15
(1,215)	1:96:A:ARG:H	1:92:A:CYS:HB3	17	0.15
(1,190)	1:101:A:ASN:HB2	1:101:A:ASN:H	8	0.15
(1,190)	1:101:A:ASN:HB3	1:101:A:ASN:H	8	0.15
(1,190)	1:101:A:ASN:HB2	1:101:A:ASN:H	19	0.15
(1,190)	1:101:A:ASN:HB3	1:101:A:ASN:H	19	0.15
(1,184)	1:103:A:VAL:HB	1:102:A:PHE:H	9	0.15
(1,180)	1:99:A:SER:HB2	1:102:A:PHE:H	19	0.15
(1,180)	1:99:A:SER:HB3	1:102:A:PHE:H	19	0.15
(1,134)	1:110:A:CYS:H	1:109:A:ASP:HB2	6	0.15
(1,134)	1:110:A:CYS:H	1:109:A:ASP:HB2	6	0.15
(1,134)	1:110:A:CYS:H	1:109:A:ASP:HB3	6	0.15
(1,134)	1:110:A:CYS:H	1:109:A:ASP:HB3	6	0.15
(1,128)	1:114:A:SER:HA	1:114:A:SER:H	7	0.15
(1,128)	1:114:A:SER:HA	1:114:A:SER:H	12	0.15
(1,128)	1:114:A:SER:HA	1:114:A:SER:H	18	0.15
(1,127)	1:114:A:SER:H	1:114:A:SER:HB2	7	0.15
(1,127)	1:114:A:SER:H	1:114:A:SER:HB3	7	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,125)	1:114:A:SER:H	1:113:A:GLY:HA2	12	0.15
(1,125)	1:114:A:SER:H	1:113:A:GLY:HA3	12	0.15
(1,125)	1:114:A:SER:H	1:113:A:GLY:HA2	20	0.15
(1,125)	1:114:A:SER:H	1:113:A:GLY:HA3	20	0.15
(1,123)	1:115:A:ASP:HB2	1:115:A:ASP:H	14	0.15
(1,123)	1:115:A:ASP:HB3	1:115:A:ASP:H	14	0.15
(1,109)	1:119:A:CYS:H	1:117:A:LEU:HG	12	0.15
(1,98)	1:98:A:ILE:HG12	1:99:A:SER:H	16	0.15
(1,98)	1:98:A:ILE:HG13	1:99:A:SER:H	16	0.15
(1,94)	1:120:A:ALA:H	1:119:A:CYS:HB2	19	0.15
(1,94)	1:120:A:ALA:H	1:119:A:CYS:HB3	19	0.15
(1,93)	1:8:A:PHE:H	1:7:A:ASP:HA	20	0.15
(1,92)	1:7:A:ASP:HB2	1:8:A:PHE:H	10	0.15
(1,92)	1:7:A:ASP:HB3	1:8:A:PHE:H	10	0.15
(1,92)	1:7:A:ASP:HB2	1:8:A:PHE:H	14	0.15
(1,92)	1:7:A:ASP:HB3	1:8:A:PHE:H	14	0.15
(1,74)	1:65:A:CYS:H	1:65:A:CYS:HB2	8	0.15
(1,74)	1:65:A:CYS:H	1:65:A:CYS:HB3	8	0.15
(1,59)	1:65:A:CYS:H	1:66:A:ASP:H	1	0.15
(1,59)	1:65:A:CYS:H	1:66:A:ASP:H	5	0.15
(1,59)	1:65:A:CYS:H	1:66:A:ASP:H	7	0.15
(1,59)	1:65:A:CYS:H	1:66:A:ASP:H	11	0.15
(1,59)	1:65:A:CYS:H	1:66:A:ASP:H	18	0.15
(1,57)	1:66:A:ASP:H	1:67:A:GLY:H	10	0.15
(1,55)	1:71:A:CYS:H	1:70:A:ASP:H	12	0.15
(1,49)	1:94:A:SER:H	1:93:A:SER:H	14	0.15
(1,42)	1:96:A:ARG:H	1:97:A:CYS:H	9	0.15
(1,42)	1:96:A:ARG:H	1:97:A:CYS:H	16	0.15
(1,41)	1:96:A:ARG:H	1:97:A:CYS:H	9	0.15
(1,41)	1:96:A:ARG:H	1:97:A:CYS:H	16	0.15
(1,33)	1:115:A:ASP:H	1:114:A:SER:H	6	0.15
(1,28)	1:118:A:ASP:H	1:117:A:LEU:H	12	0.15
(1,12)	1:34:A:GLU:H	1:33:A:ASP:H	3	0.15
(1,7)	1:22:A:CYS:H	1:23:A:ASP:H	16	0.15
(1,1)	1:112:A:ASP:H	1:113:A:GLY:H	5	0.15
(4,5)	1:49:A:ILE:O	1:59:A:ILE:H	13	0.14
(4,3)	1:92:A:CYS:H	1:96:A:ARG:O	8	0.14
(3,7)	2:202:A:CA:CA	1:63:A:TRP:O	6	0.14
(3,7)	2:202:A:CA:CA	1:63:A:TRP:O	14	0.14
(3,7)	2:202:A:CA:CA	1:63:A:TRP:O	18	0.14
(2,382)	1:72:A:ASP:HB2	1:73:A:SER:H	8	0.14
(2,382)	1:72:A:ASP:HB3	1:73:A:SER:H	8	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,382)	1:72:A:ASP:HB2	1:73:A:SER:H	16	0.14
(2,382)	1:72:A:ASP:HB3	1:73:A:SER:H	16	0.14
(2,382)	1:72:A:ASP:HB2	1:73:A:SER:H	18	0.14
(2,382)	1:72:A:ASP:HB3	1:73:A:SER:H	18	0.14
(2,382)	1:72:A:ASP:HB2	1:73:A:SER:H	20	0.14
(2,382)	1:72:A:ASP:HB3	1:73:A:SER:H	20	0.14
(2,370)	1:38:A:GLN:HG2	1:38:A:GLN:HE22	9	0.14
(2,370)	1:38:A:GLN:HG2	1:38:A:GLN:HE22	10	0.14
(2,370)	1:38:A:GLN:HG2	1:38:A:GLN:HE22	15	0.14
(2,339)	1:9:A:VAL:HG11	1:13:A:GLY:H	14	0.14
(2,339)	1:9:A:VAL:HG12	1:13:A:GLY:H	14	0.14
(2,339)	1:9:A:VAL:HG13	1:13:A:GLY:H	14	0.14
(2,339)	1:9:A:VAL:HG21	1:13:A:GLY:H	14	0.14
(2,339)	1:9:A:VAL:HG22	1:13:A:GLY:H	14	0.14
(2,339)	1:9:A:VAL:HG23	1:13:A:GLY:H	14	0.14
(2,339)	1:9:A:VAL:HG11	1:13:A:GLY:H	15	0.14
(2,339)	1:9:A:VAL:HG12	1:13:A:GLY:H	15	0.14
(2,339)	1:9:A:VAL:HG13	1:13:A:GLY:H	15	0.14
(2,339)	1:9:A:VAL:HG21	1:13:A:GLY:H	15	0.14
(2,339)	1:9:A:VAL:HG22	1:13:A:GLY:H	15	0.14
(2,339)	1:9:A:VAL:HG23	1:13:A:GLY:H	15	0.14
(2,331)	1:101:A:ASN:H	1:99:A:SER:H	9	0.14
(2,320)	1:59:A:ILE:HA	1:58:A:CYS:H	12	0.14
(2,313)	1:17:A:PRO:HB2	1:20:A:TRP:H	3	0.14
(2,307)	1:59:A:ILE:HD12	1:63:A:TRP:H	9	0.14
(2,295)	1:38:A:GLN:HA	1:38:A:GLN:HE21	4	0.14
(2,285)	1:112:A:ASP:HB2	1:112:A:ASP:H	6	0.14
(2,276)	1:43:A:THR:HA	1:57:A:GLN:H	6	0.14
(2,276)	1:43:A:THR:HA	1:57:A:GLN:H	20	0.14
(2,236)	1:21:A:LYS:HB2	1:21:A:LYS:H	5	0.14
(2,236)	1:21:A:LYS:HB2	1:21:A:LYS:H	8	0.14
(2,236)	1:21:A:LYS:HB2	1:21:A:LYS:H	11	0.14
(2,236)	1:21:A:LYS:HB2	1:21:A:LYS:H	13	0.14
(2,233)	1:14:A:GLN:HB2	1:14:A:GLN:HE22	1	0.14
(2,233)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	1	0.14
(2,233)	1:14:A:GLN:HB2	1:14:A:GLN:HE22	15	0.14
(2,233)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	15	0.14
(2,233)	1:14:A:GLN:HB2	1:14:A:GLN:HE22	19	0.14
(2,233)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	19	0.14
(2,218)	1:36:A:PRO:HD2	1:37:A:GLU:H	2	0.14
(2,218)	1:36:A:PRO:HD2	1:37:A:GLU:H	13	0.14
(2,188)	1:16:A:VAL:HG11	1:19:A:ARG:H	18	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,188)	1:16:A:VAL:HG12	1:19:A:ARG:H	18	0.14
(2,188)	1:16:A:VAL:HG13	1:19:A:ARG:H	18	0.14
(2,188)	1:16:A:VAL:HG21	1:19:A:ARG:H	18	0.14
(2,188)	1:16:A:VAL:HG22	1:19:A:ARG:H	18	0.14
(2,188)	1:16:A:VAL:HG23	1:19:A:ARG:H	18	0.14
(2,181)	1:41:A:MET:HG3	1:41:A:MET:H	7	0.14
(2,181)	1:39:A:CYS:HB3	1:41:A:MET:H	16	0.14
(2,179)	1:9:A:VAL:HG11	1:10:A:CYS:H	18	0.14
(2,179)	1:9:A:VAL:HG12	1:10:A:CYS:H	18	0.14
(2,179)	1:9:A:VAL:HG13	1:10:A:CYS:H	18	0.14
(2,179)	1:9:A:VAL:HG21	1:10:A:CYS:H	18	0.14
(2,179)	1:9:A:VAL:HG22	1:10:A:CYS:H	18	0.14
(2,179)	1:9:A:VAL:HG23	1:10:A:CYS:H	18	0.14
(2,164)	1:14:A:GLN:HB2	1:14:A:GLN:H	11	0.14
(2,164)	1:14:A:GLN:HB3	1:14:A:GLN:H	11	0.14
(2,159)	1:42:A:ARG:HD2	1:43:A:THR:H	17	0.14
(2,150)	1:28:A:CYS:HB3	1:31:A:GLY:H	19	0.14
(2,104)	1:80:A:CYS:HB3	1:80:A:CYS:H	12	0.14
(2,98)	1:32:A:SER:HB3	1:11:A:ASN:H	6	0.14
(2,89)	1:107:A:GLN:HB2	1:108:A:ASP:H	13	0.14
(2,89)	1:107:A:GLN:HB3	1:108:A:ASP:H	13	0.14
(2,89)	1:107:A:GLN:HB2	1:108:A:ASP:H	20	0.14
(2,89)	1:107:A:GLN:HB3	1:108:A:ASP:H	20	0.14
(2,75)	1:108:A:ASP:HA	1:108:A:ASP:H	11	0.14
(2,75)	1:108:A:ASP:HA	1:108:A:ASP:H	15	0.14
(2,75)	1:108:A:ASP:HA	1:108:A:ASP:H	20	0.14
(2,74)	1:46:A:ILE:HB	1:46:A:ILE:H	13	0.14
(2,49)	1:35:A:SER:HB3	1:39:A:CYS:H	5	0.14
(2,22)	1:75:A:GLU:HA	1:78:A:GLU:H	17	0.14
(1,931)	1:99:A:SER:HB2	1:102:A:PHE:HD1	9	0.14
(1,931)	1:99:A:SER:HB2	1:102:A:PHE:HD2	9	0.14
(1,931)	1:99:A:SER:HB3	1:102:A:PHE:HD1	9	0.14
(1,931)	1:99:A:SER:HB3	1:102:A:PHE:HD2	9	0.14
(1,930)	1:102:A:PHE:HE2	1:107:A:GLN:HG2	10	0.14
(1,926)	1:16:A:VAL:HG11	1:20:A:TRP:HZ3	16	0.14
(1,926)	1:16:A:VAL:HG12	1:20:A:TRP:HZ3	16	0.14
(1,926)	1:16:A:VAL:HG13	1:20:A:TRP:HZ3	16	0.14
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG11	19	0.14
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG12	19	0.14
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG13	19	0.14
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG21	19	0.14
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG22	19	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG23	19	0.14
(1,907)	1:39:A:CYS:H	1:41:A:MET:H	10	0.14
(1,902)	1:94:A:SER:HB2	1:82:A:ASN:HD21	19	0.14
(1,902)	1:94:A:SER:HB3	1:82:A:ASN:HD21	19	0.14
(1,897)	1:77:A:GLU:HB2	1:69:A:ASN:HD22	14	0.14
(1,897)	1:77:A:GLU:HB3	1:69:A:ASN:HD22	14	0.14
(1,895)	1:77:A:GLU:HG2	1:66:A:ASP:H	12	0.14
(1,895)	1:77:A:GLU:HG3	1:66:A:ASP:H	12	0.14
(1,894)	1:66:A:ASP:H	1:77:A:GLU:HG2	12	0.14
(1,894)	1:66:A:ASP:H	1:77:A:GLU:HG3	12	0.14
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB2	14	0.14
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB3	14	0.14
(1,886)	1:51:A:CYS:H	1:58:A:CYS:H	3	0.14
(1,884)	1:50:A:SER:H	1:59:A:ILE:H	4	0.14
(1,882)	1:58:A:CYS:HA	1:50:A:SER:H	19	0.14
(1,876)	1:39:A:CYS:HB2	1:43:A:THR:H	19	0.14
(1,876)	1:39:A:CYS:HB3	1:43:A:THR:H	19	0.14
(1,872)	1:32:A:SER:H	1:33:A:ASP:HB2	11	0.14
(1,872)	1:32:A:SER:H	1:33:A:ASP:HB3	11	0.14
(1,869)	1:14:A:GLN:HE22	1:28:A:CYS:H	5	0.14
(1,869)	1:14:A:GLN:HE22	1:28:A:CYS:H	9	0.14
(1,869)	1:14:A:GLN:HE22	1:28:A:CYS:H	15	0.14
(1,863)	1:17:A:PRO:HD2	1:20:A:TRP:HE1	2	0.14
(1,863)	1:17:A:PRO:HD3	1:20:A:TRP:HE1	2	0.14
(1,844)	1:79:A:ASN:HB2	1:92:A:CYS:H	3	0.14
(1,844)	1:79:A:ASN:HB3	1:92:A:CYS:H	3	0.14
(1,842)	1:80:A:CYS:HA	1:84:A:THR:H	7	0.14
(1,842)	1:80:A:CYS:HA	1:84:A:THR:H	12	0.14
(1,838)	1:58:A:CYS:HA	1:52:A:GLY:H	2	0.14
(1,832)	1:35:A:SER:H	1:38:A:GLN:H	8	0.14
(1,832)	1:35:A:SER:H	1:38:A:GLN:H	12	0.14
(1,832)	1:35:A:SER:H	1:38:A:GLN:H	20	0.14
(1,828)	1:85:A:CYS:HA	1:86:A:SER:H	20	0.14
(1,826)	1:114:A:SER:H	1:117:A:LEU:H	5	0.14
(1,810)	1:101:A:ASN:HD21	1:105:A:ASN:HD22	3	0.14
(1,809)	1:106:A:GLY:H	1:104:A:CYS:H	13	0.14
(1,803)	1:101:A:ASN:HD21	1:99:A:SER:H	9	0.14
(1,803)	1:101:A:ASN:HD21	1:99:A:SER:H	18	0.14
(1,800)	1:85:A:CYS:HB2	1:98:A:ILE:H	13	0.14
(1,800)	1:85:A:CYS:HB3	1:98:A:ILE:H	13	0.14
(1,799)	1:85:A:CYS:HA	1:97:A:CYS:H	12	0.14
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG21	8	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG22	8	0.14
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG23	8	0.14
(1,786)	1:71:A:CYS:H	1:76:A:ASP:H	18	0.14
(1,781)	1:73:A:SER:H	1:71:A:CYS:HB2	9	0.14
(1,781)	1:73:A:SER:H	1:71:A:CYS:HB3	9	0.14
(1,781)	1:73:A:SER:H	1:71:A:CYS:HB2	19	0.14
(1,781)	1:73:A:SER:H	1:71:A:CYS:HB3	19	0.14
(1,780)	1:72:A:ASP:H	1:57:A:GLN:HE22	20	0.14
(1,753)	1:51:A:CYS:H	1:57:A:GLN:H	10	0.14
(1,749)	1:51:A:CYS:H	1:57:A:GLN:H	10	0.14
(1,745)	1:48:A:GLU:HB2	1:49:A:ILE:H	18	0.14
(1,745)	1:48:A:GLU:HB3	1:49:A:ILE:H	18	0.14
(1,734)	1:32:A:SER:H	1:11:A:ASN:H	10	0.14
(1,719)	1:19:A:ARG:HH21	1:20:A:TRP:HE1	7	0.14
(1,719)	1:19:A:ARG:HH21	1:20:A:TRP:HE1	16	0.14
(1,712)	1:32:A:SER:H	1:11:A:ASN:H	10	0.14
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG2	6	0.14
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG3	6	0.14
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG2	20	0.14
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG3	20	0.14
(1,682)	1:79:A:ASN:HD22	1:87:A:PRO:HD2	4	0.14
(1,682)	1:79:A:ASN:HD22	1:87:A:PRO:HD3	4	0.14
(1,680)	1:79:A:ASN:HD22	1:79:A:ASN:HB2	12	0.14
(1,680)	1:79:A:ASN:HD22	1:79:A:ASN:HB3	12	0.14
(1,679)	1:78:A:GLU:HG2	1:79:A:ASN:HD22	3	0.14
(1,679)	1:78:A:GLU:HG3	1:79:A:ASN:HD22	3	0.14
(1,679)	1:78:A:GLU:HG2	1:79:A:ASN:HD22	18	0.14
(1,679)	1:78:A:GLU:HG3	1:79:A:ASN:HD22	18	0.14
(1,674)	1:17:A:PRO:HG2	1:20:A:TRP:HE1	12	0.14
(1,674)	1:17:A:PRO:HG3	1:20:A:TRP:HE1	12	0.14
(1,674)	1:17:A:PRO:HG2	1:20:A:TRP:HE1	15	0.14
(1,674)	1:17:A:PRO:HG3	1:20:A:TRP:HE1	15	0.14
(1,674)	1:17:A:PRO:HG2	1:20:A:TRP:HE1	20	0.14
(1,674)	1:17:A:PRO:HG3	1:20:A:TRP:HE1	20	0.14
(1,673)	1:17:A:PRO:HB2	1:20:A:TRP:HE1	15	0.14
(1,673)	1:17:A:PRO:HB3	1:20:A:TRP:HE1	15	0.14
(1,625)	1:72:A:ASP:H	1:57:A:GLN:HE22	20	0.14
(1,623)	1:30:A:ASP:HB2	1:12:A:ASN:HD22	10	0.14
(1,623)	1:30:A:ASP:HB3	1:12:A:ASN:HD22	10	0.14
(1,623)	1:30:A:ASP:HB2	1:12:A:ASN:HD22	14	0.14
(1,623)	1:30:A:ASP:HB3	1:12:A:ASN:HD22	14	0.14
(1,612)	1:15:A:CYS:H	1:14:A:GLN:HE22	4	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,607)	1:11:A:ASN:HB2	1:11:A:ASN:HD21	1	0.14
(1,607)	1:11:A:ASN:HB3	1:11:A:ASN:HD21	1	0.14
(1,607)	1:11:A:ASN:HB2	1:11:A:ASN:HD21	2	0.14
(1,607)	1:11:A:ASN:HB3	1:11:A:ASN:HD21	2	0.14
(1,603)	1:32:A:SER:HB2	1:11:A:ASN:HD22	10	0.14
(1,603)	1:32:A:SER:HB3	1:11:A:ASN:HD22	10	0.14
(1,598)	1:74:A:GLY:HA2	1:69:A:ASN:HD22	12	0.14
(1,598)	1:74:A:GLY:HA3	1:69:A:ASN:HD22	12	0.14
(1,597)	1:74:A:GLY:HA2	1:69:A:ASN:HD22	12	0.14
(1,597)	1:74:A:GLY:HA3	1:69:A:ASN:HD22	12	0.14
(1,596)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	7	0.14
(1,596)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	7	0.14
(1,592)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	3	0.14
(1,592)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	3	0.14
(1,591)	1:69:A:ASN:HB2	1:69:A:ASN:HD21	5	0.14
(1,591)	1:69:A:ASN:HB3	1:69:A:ASN:HD21	5	0.14
(1,591)	1:69:A:ASN:HB2	1:69:A:ASN:HD21	6	0.14
(1,591)	1:69:A:ASN:HB3	1:69:A:ASN:HD21	6	0.14
(1,591)	1:69:A:ASN:HB2	1:69:A:ASN:HD21	20	0.14
(1,591)	1:69:A:ASN:HB3	1:69:A:ASN:HD21	20	0.14
(1,575)	1:57:A:GLN:H	1:56:A:THR:H	10	0.14
(1,574)	1:64:A:ARG:H	1:65:A:CYS:H	5	0.14
(1,565)	1:91:A:THR:HG1	1:91:A:THR:H	3	0.14
(1,562)	1:102:A:PHE:HB2	1:99:A:SER:H	15	0.14
(1,562)	1:102:A:PHE:HB3	1:99:A:SER:H	15	0.14
(1,560)	1:90:A:PHE:H	1:99:A:SER:H	9	0.14
(1,560)	1:90:A:PHE:H	1:99:A:SER:H	18	0.14
(1,549)	1:115:A:ASP:HA	1:104:A:CYS:H	11	0.14
(1,518)	1:49:A:ILE:H	1:61:A:VAL:H	11	0.14
(1,518)	1:49:A:ILE:H	1:61:A:VAL:H	12	0.14
(1,516)	1:49:A:ILE:H	1:59:A:ILE:H	5	0.14
(1,516)	1:49:A:ILE:H	1:59:A:ILE:H	14	0.14
(1,513)	1:61:A:VAL:HA	1:49:A:ILE:H	12	0.14
(1,512)	1:59:A:ILE:H	1:49:A:ILE:H	6	0.14
(1,512)	1:59:A:ILE:H	1:49:A:ILE:H	18	0.14
(1,496)	1:31:A:GLY:HA2	1:31:A:GLY:H	3	0.14
(1,496)	1:31:A:GLY:HA3	1:31:A:GLY:H	3	0.14
(1,496)	1:31:A:GLY:HA2	1:31:A:GLY:H	14	0.14
(1,496)	1:31:A:GLY:HA3	1:31:A:GLY:H	14	0.14
(1,496)	1:31:A:GLY:HA2	1:31:A:GLY:H	18	0.14
(1,496)	1:31:A:GLY:HA3	1:31:A:GLY:H	18	0.14
(1,478)	1:9:A:VAL:HB	1:9:A:VAL:H	3	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,478)	1:9:A:VAL:HB	1:9:A:VAL:H	8	0.14
(1,475)	1:75:A:GLU:H	1:76:A:ASP:H	4	0.14
(1,473)	1:85:A:CYS:H	1:86:A:SER:H	3	0.14
(1,473)	1:85:A:CYS:H	1:86:A:SER:H	5	0.14
(1,473)	1:85:A:CYS:H	1:86:A:SER:H	10	0.14
(1,473)	1:85:A:CYS:H	1:86:A:SER:H	13	0.14
(1,473)	1:85:A:CYS:H	1:86:A:SER:H	14	0.14
(1,473)	1:85:A:CYS:H	1:86:A:SER:H	17	0.14
(1,468)	1:78:A:GLU:HG2	1:79:A:ASN:H	5	0.14
(1,468)	1:78:A:GLU:HG3	1:79:A:ASN:H	5	0.14
(1,462)	1:79:A:ASN:H	1:78:A:GLU:H	1	0.14
(1,462)	1:79:A:ASN:H	1:78:A:GLU:H	9	0.14
(1,462)	1:79:A:ASN:H	1:78:A:GLU:H	11	0.14
(1,462)	1:79:A:ASN:H	1:78:A:GLU:H	17	0.14
(1,454)	1:78:A:GLU:HG2	1:76:A:ASP:H	8	0.14
(1,454)	1:78:A:GLU:HG3	1:76:A:ASP:H	8	0.14
(1,451)	1:75:A:GLU:H	1:76:A:ASP:H	4	0.14
(1,439)	1:75:A:GLU:H	1:73:A:SER:H	12	0.14
(1,439)	1:75:A:GLU:H	1:73:A:SER:H	14	0.14
(1,439)	1:75:A:GLU:H	1:73:A:SER:H	15	0.14
(1,432)	1:70:A:ASP:HB2	1:70:A:ASP:H	11	0.14
(1,432)	1:70:A:ASP:HB3	1:70:A:ASP:H	11	0.14
(1,419)	1:65:A:CYS:HB2	1:66:A:ASP:H	1	0.14
(1,419)	1:65:A:CYS:HB3	1:66:A:ASP:H	1	0.14
(1,419)	1:65:A:CYS:HB2	1:66:A:ASP:H	6	0.14
(1,419)	1:65:A:CYS:HB3	1:66:A:ASP:H	6	0.14
(1,418)	1:64:A:ARG:HA	1:66:A:ASP:H	2	0.14
(1,415)	1:64:A:ARG:HA	1:65:A:CYS:H	19	0.14
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB2	6	0.14
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB3	6	0.14
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB2	18	0.14
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB3	18	0.14
(1,409)	1:60:A:PRO:HA	1:61:A:VAL:H	6	0.14
(1,409)	1:60:A:PRO:HA	1:61:A:VAL:H	14	0.14
(1,409)	1:60:A:PRO:HA	1:61:A:VAL:H	19	0.14
(1,392)	1:52:A:GLY:HA2	1:53:A:ALA:H	13	0.14
(1,392)	1:52:A:GLY:HA3	1:53:A:ALA:H	13	0.14
(1,390)	1:51:A:CYS:HB2	1:52:A:GLY:H	10	0.14
(1,390)	1:51:A:CYS:HB3	1:52:A:GLY:H	10	0.14
(1,386)	1:51:A:CYS:HB2	1:51:A:CYS:H	15	0.14
(1,386)	1:51:A:CYS:HB3	1:51:A:CYS:H	15	0.14
(1,383)	1:51:A:CYS:H	1:50:A:SER:HA	6	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,383)	1:51:A:CYS:H	1:50:A:SER:HA	14	0.14
(1,375)	1:48:A:GLU:HA	1:49:A:ILE:H	19	0.14
(1,374)	1:61:A:VAL:H	1:49:A:ILE:H	20	0.14
(1,369)	1:43:A:THR:HB	1:44:A:CYS:H	13	0.14
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB2	6	0.14
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB3	6	0.14
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB2	7	0.14
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB3	7	0.14
(1,357)	1:40:A:HIS:H	1:39:A:CYS:HA	9	0.14
(1,329)	1:25:A:ASP:H	1:23:A:ASP:H	13	0.14
(1,320)	1:7:A:ASP:HA	1:18:A:SER:H	12	0.14
(1,319)	1:16:A:VAL:H	1:9:A:VAL:HA	6	0.14
(1,313)	1:14:A:GLN:HG2	1:14:A:GLN:H	13	0.14
(1,313)	1:14:A:GLN:HG3	1:14:A:GLN:H	13	0.14
(1,299)	1:11:A:ASN:H	1:12:A:ASN:H	19	0.14
(1,296)	1:10:A:CYS:HB2	1:10:A:CYS:H	4	0.14
(1,296)	1:10:A:CYS:HB3	1:10:A:CYS:H	4	0.14
(1,295)	1:15:A:CYS:HA	1:10:A:CYS:H	14	0.14
(1,295)	1:15:A:CYS:HA	1:10:A:CYS:H	16	0.14
(1,290)	1:8:A:PHE:HA	1:9:A:VAL:H	13	0.14
(1,286)	1:7:A:ASP:HB2	1:7:A:ASP:H	16	0.14
(1,286)	1:7:A:ASP:HB3	1:7:A:ASP:H	16	0.14
(1,279)	1:6:A:SER:HB2	1:6:A:SER:H	11	0.14
(1,279)	1:6:A:SER:HB3	1:6:A:SER:H	11	0.14
(1,277)	1:6:A:SER:HB2	1:6:A:SER:H	11	0.14
(1,277)	1:6:A:SER:HB3	1:6:A:SER:H	11	0.14
(1,273)	1:7:A:ASP:HB2	1:4:A:ALA:H	1	0.14
(1,273)	1:7:A:ASP:HB3	1:4:A:ALA:H	1	0.14
(1,273)	1:7:A:ASP:HB2	1:4:A:ALA:H	5	0.14
(1,273)	1:7:A:ASP:HB3	1:4:A:ALA:H	5	0.14
(1,248)	1:83:A:ILE:HB	1:84:A:THR:H	8	0.14
(1,247)	1:83:A:ILE:HA	1:84:A:THR:H	8	0.14
(1,241)	1:86:A:SER:H	1:89:A:GLU:H	4	0.14
(1,241)	1:86:A:SER:H	1:89:A:GLU:H	11	0.14
(1,215)	1:96:A:ARG:H	1:92:A:CYS:HB2	16	0.14
(1,215)	1:96:A:ARG:H	1:92:A:CYS:HB3	16	0.14
(1,204)	1:98:A:ILE:HG12	1:98:A:ILE:H	5	0.14
(1,204)	1:98:A:ILE:HG13	1:98:A:ILE:H	5	0.14
(1,204)	1:98:A:ILE:HG12	1:98:A:ILE:H	18	0.14
(1,204)	1:98:A:ILE:HG13	1:98:A:ILE:H	18	0.14
(1,196)	1:98:A:ILE:HA	1:99:A:SER:H	7	0.14
(1,190)	1:101:A:ASN:HB2	1:101:A:ASN:H	1	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,190)	1:101:A:ASN:HB3	1:101:A:ASN:H	1	0.14
(1,190)	1:101:A:ASN:HB2	1:101:A:ASN:H	17	0.14
(1,190)	1:101:A:ASN:HB3	1:101:A:ASN:H	17	0.14
(1,187)	1:103:A:VAL:HG11	1:102:A:PHE:H	2	0.14
(1,187)	1:103:A:VAL:HG12	1:102:A:PHE:H	2	0.14
(1,187)	1:103:A:VAL:HG13	1:102:A:PHE:H	2	0.14
(1,187)	1:103:A:VAL:HG21	1:102:A:PHE:H	2	0.14
(1,187)	1:103:A:VAL:HG22	1:102:A:PHE:H	2	0.14
(1,187)	1:103:A:VAL:HG23	1:102:A:PHE:H	2	0.14
(1,184)	1:103:A:VAL:HB	1:102:A:PHE:H	11	0.14
(1,180)	1:99:A:SER:HB2	1:102:A:PHE:H	13	0.14
(1,180)	1:99:A:SER:HB3	1:102:A:PHE:H	13	0.14
(1,143)	1:106:A:GLY:H	1:107:A:GLN:H	1	0.14
(1,139)	1:109:A:ASP:H	1:109:A:ASP:HB2	8	0.14
(1,139)	1:109:A:ASP:H	1:109:A:ASP:HB3	8	0.14
(1,130)	1:115:A:ASP:HB2	1:113:A:GLY:H	15	0.14
(1,130)	1:115:A:ASP:HB3	1:113:A:GLY:H	15	0.14
(1,129)	1:114:A:SER:H	1:114:A:SER:HG	10	0.14
(1,128)	1:114:A:SER:HA	1:114:A:SER:H	15	0.14
(1,127)	1:114:A:SER:H	1:114:A:SER:HB2	15	0.14
(1,127)	1:114:A:SER:H	1:114:A:SER:HB3	15	0.14
(1,126)	1:117:A:LEU:HD11	1:114:A:SER:H	3	0.14
(1,126)	1:117:A:LEU:HD12	1:114:A:SER:H	3	0.14
(1,126)	1:117:A:LEU:HD13	1:114:A:SER:H	3	0.14
(1,126)	1:117:A:LEU:HD21	1:114:A:SER:H	3	0.14
(1,126)	1:117:A:LEU:HD22	1:114:A:SER:H	3	0.14
(1,126)	1:117:A:LEU:HD23	1:114:A:SER:H	3	0.14
(1,126)	1:117:A:LEU:HD11	1:114:A:SER:H	7	0.14
(1,126)	1:117:A:LEU:HD12	1:114:A:SER:H	7	0.14
(1,126)	1:117:A:LEU:HD13	1:114:A:SER:H	7	0.14
(1,126)	1:117:A:LEU:HD21	1:114:A:SER:H	7	0.14
(1,126)	1:117:A:LEU:HD22	1:114:A:SER:H	7	0.14
(1,126)	1:117:A:LEU:HD23	1:114:A:SER:H	7	0.14
(1,125)	1:114:A:SER:H	1:113:A:GLY:HA2	15	0.14
(1,125)	1:114:A:SER:H	1:113:A:GLY:HA3	15	0.14
(1,123)	1:115:A:ASP:HB2	1:115:A:ASP:H	6	0.14
(1,123)	1:115:A:ASP:HB3	1:115:A:ASP:H	6	0.14
(1,122)	1:115:A:ASP:HB2	1:115:A:ASP:H	5	0.14
(1,122)	1:115:A:ASP:HB3	1:115:A:ASP:H	5	0.14
(1,121)	1:114:A:SER:HA	1:115:A:ASP:H	14	0.14
(1,96)	1:100:A:ARG:H	1:89:A:GLU:HA	1	0.14
(1,94)	1:120:A:ALA:H	1:119:A:CYS:HB2	8	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,94)	1:120:A:ALA:H	1:119:A:CYS:HB3	8	0.14
(1,84)	1:14:A:GLN:HG2	1:29:A:GLU:H	13	0.14
(1,84)	1:14:A:GLN:HG3	1:29:A:GLU:H	13	0.14
(1,59)	1:65:A:CYS:H	1:66:A:ASP:H	9	0.14
(1,57)	1:66:A:ASP:H	1:67:A:GLY:H	4	0.14
(1,57)	1:66:A:ASP:H	1:67:A:GLY:H	18	0.14
(1,55)	1:71:A:CYS:H	1:70:A:ASP:H	19	0.14
(1,28)	1:118:A:ASP:H	1:117:A:LEU:H	15	0.14
(1,18)	1:81:A:GLY:H	1:82:A:ASN:H	15	0.14
(1,12)	1:34:A:GLU:H	1:33:A:ASP:H	18	0.14
(1,7)	1:22:A:CYS:H	1:23:A:ASP:H	4	0.14
(1,7)	1:22:A:CYS:H	1:23:A:ASP:H	18	0.14
(1,1)	1:112:A:ASP:H	1:113:A:GLY:H	19	0.14
(4,2)	1:90:A:PHE:O	1:98:A:ILE:H	19	0.13
(3,10)	2:202:A:CA:CA	1:70:A:ASP:OD2	17	0.13
(2,370)	1:38:A:GLN:HG3	1:38:A:GLN:HE22	4	0.13
(2,370)	1:38:A:GLN:HG3	1:38:A:GLN:HE22	5	0.13
(2,370)	1:38:A:GLN:HG3	1:38:A:GLN:HE22	7	0.13
(2,370)	1:38:A:GLN:HG3	1:38:A:GLN:HE22	19	0.13
(2,370)	1:38:A:GLN:HG2	1:38:A:GLN:HE22	20	0.13
(2,362)	1:14:A:GLN:HB2	1:10:A:CYS:H	1	0.13
(2,362)	1:14:A:GLN:HB3	1:10:A:CYS:H	1	0.13
(2,339)	1:9:A:VAL:HG11	1:13:A:GLY:H	4	0.13
(2,339)	1:9:A:VAL:HG12	1:13:A:GLY:H	4	0.13
(2,339)	1:9:A:VAL:HG13	1:13:A:GLY:H	4	0.13
(2,339)	1:9:A:VAL:HG21	1:13:A:GLY:H	4	0.13
(2,339)	1:9:A:VAL:HG22	1:13:A:GLY:H	4	0.13
(2,339)	1:9:A:VAL:HG23	1:13:A:GLY:H	4	0.13
(2,322)	1:69:A:ASN:HB3	1:71:A:CYS:H	4	0.13
(2,320)	1:59:A:ILE:HA	1:58:A:CYS:H	14	0.13
(2,301)	1:11:A:ASN:HD22	1:32:A:SER:H	19	0.13
(2,289)	1:41:A:MET:HB2	1:41:A:MET:H	10	0.13
(2,285)	1:112:A:ASP:HB2	1:112:A:ASP:H	7	0.13
(2,280)	1:92:A:CYS:H	1:91:A:THR:H	1	0.13
(2,276)	1:43:A:THR:HA	1:57:A:GLN:H	19	0.13
(2,270)	1:113:A:GLY:HA2	1:110:A:CYS:H	5	0.13
(2,263)	1:63:A:TRP:HB2	1:63:A:TRP:H	1	0.13
(2,236)	1:21:A:LYS:HB2	1:21:A:LYS:H	2	0.13
(2,233)	1:14:A:GLN:HB2	1:14:A:GLN:HE22	2	0.13
(2,233)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	2	0.13
(2,233)	1:14:A:GLN:HB2	1:14:A:GLN:HE22	4	0.13
(2,233)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	4	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,233)	1:14:A:GLN:HB2	1:14:A:GLN:HE22	5	0.13
(2,233)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	5	0.13
(2,233)	1:14:A:GLN:HB2	1:14:A:GLN:HE22	10	0.13
(2,233)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	10	0.13
(2,233)	1:14:A:GLN:HB2	1:14:A:GLN:HE22	11	0.13
(2,233)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	11	0.13
(2,233)	1:14:A:GLN:HB2	1:14:A:GLN:HE22	14	0.13
(2,233)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	14	0.13
(2,226)	1:98:A:ILE:H	1:97:A:CYS:H	1	0.13
(2,218)	1:36:A:PRO:HD2	1:37:A:GLU:H	8	0.13
(2,188)	1:16:A:VAL:HG11	1:19:A:ARG:H	6	0.13
(2,188)	1:16:A:VAL:HG12	1:19:A:ARG:H	6	0.13
(2,188)	1:16:A:VAL:HG13	1:19:A:ARG:H	6	0.13
(2,188)	1:16:A:VAL:HG21	1:19:A:ARG:H	6	0.13
(2,188)	1:16:A:VAL:HG22	1:19:A:ARG:H	6	0.13
(2,188)	1:16:A:VAL:HG23	1:19:A:ARG:H	6	0.13
(2,181)	1:41:A:MET:HG2	1:41:A:MET:H	3	0.13
(2,179)	1:9:A:VAL:HG11	1:10:A:CYS:H	15	0.13
(2,179)	1:9:A:VAL:HG12	1:10:A:CYS:H	15	0.13
(2,179)	1:9:A:VAL:HG13	1:10:A:CYS:H	15	0.13
(2,179)	1:9:A:VAL:HG21	1:10:A:CYS:H	15	0.13
(2,179)	1:9:A:VAL:HG22	1:10:A:CYS:H	15	0.13
(2,179)	1:9:A:VAL:HG23	1:10:A:CYS:H	15	0.13
(2,174)	1:117:A:LEU:HB2	1:116:A:GLU:H	8	0.13
(2,164)	1:14:A:GLN:HB2	1:14:A:GLN:H	12	0.13
(2,164)	1:14:A:GLN:HB3	1:14:A:GLN:H	12	0.13
(2,123)	1:16:A:VAL:HG11	1:33:A:ASP:H	11	0.13
(2,123)	1:16:A:VAL:HG12	1:33:A:ASP:H	11	0.13
(2,123)	1:16:A:VAL:HG13	1:33:A:ASP:H	11	0.13
(2,123)	1:16:A:VAL:HG21	1:33:A:ASP:H	11	0.13
(2,123)	1:16:A:VAL:HG22	1:33:A:ASP:H	11	0.13
(2,123)	1:16:A:VAL:HG23	1:33:A:ASP:H	11	0.13
(2,117)	1:14:A:GLN:HB2	1:12:A:ASN:HD21	7	0.13
(2,117)	1:14:A:GLN:HB3	1:12:A:ASN:HD21	7	0.13
(2,117)	1:14:A:GLN:HB2	1:12:A:ASN:HD21	17	0.13
(2,117)	1:14:A:GLN:HB3	1:12:A:ASN:HD21	17	0.13
(2,115)	1:80:A:CYS:H	1:81:A:GLY:H	12	0.13
(2,112)	1:84:A:THR:HG1	1:84:A:THR:H	8	0.13
(2,83)	1:35:A:SER:HB2	1:38:A:GLN:H	16	0.13
(2,75)	1:108:A:ASP:HA	1:108:A:ASP:H	12	0.13
(2,75)	1:108:A:ASP:HA	1:108:A:ASP:H	13	0.13
(2,75)	1:108:A:ASP:HA	1:108:A:ASP:H	18	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,74)	1:46:A:ILE:HB	1:46:A:ILE:H	2	0.13
(2,74)	1:46:A:ILE:HB	1:46:A:ILE:H	6	0.13
(2,74)	1:46:A:ILE:HB	1:46:A:ILE:H	8	0.13
(2,61)	1:4:A:ALA:HA	1:5:A:GLU:H	6	0.13
(2,56)	1:114:A:SER:HA	1:117:A:LEU:H	14	0.13
(2,30)	1:9:A:VAL:H	1:10:A:CYS:H	17	0.13
(2,8)	1:45:A:ARG:HA	1:46:A:ILE:H	15	0.13
(1,928)	1:102:A:PHE:HA	1:103:A:VAL:HG11	9	0.13
(1,928)	1:102:A:PHE:HA	1:103:A:VAL:HG12	9	0.13
(1,928)	1:102:A:PHE:HA	1:103:A:VAL:HG13	9	0.13
(1,921)	1:8:A:PHE:HA	1:16:A:VAL:HG21	7	0.13
(1,921)	1:8:A:PHE:HA	1:16:A:VAL:HG22	7	0.13
(1,921)	1:8:A:PHE:HA	1:16:A:VAL:HG23	7	0.13
(1,906)	1:13:A:GLY:HA2	1:12:A:ASN:HD22	6	0.13
(1,906)	1:13:A:GLY:HA3	1:12:A:ASN:HD22	6	0.13
(1,890)	1:81:A:GLY:HA2	1:63:A:TRP:HE1	17	0.13
(1,890)	1:81:A:GLY:HA2	1:63:A:TRP:HE1	17	0.13
(1,890)	1:81:A:GLY:HA3	1:63:A:TRP:HE1	17	0.13
(1,890)	1:81:A:GLY:HA3	1:63:A:TRP:HE1	17	0.13
(1,882)	1:58:A:CYS:HA	1:50:A:SER:H	8	0.13
(1,882)	1:58:A:CYS:HA	1:50:A:SER:H	17	0.13
(1,876)	1:39:A:CYS:HB2	1:43:A:THR:H	14	0.13
(1,876)	1:39:A:CYS:HB3	1:43:A:THR:H	14	0.13
(1,875)	1:38:A:GLN:HE22	1:38:A:GLN:H	8	0.13
(1,869)	1:14:A:GLN:HE22	1:28:A:CYS:H	19	0.13
(1,867)	1:34:A:GLU:HG2	1:24:A:GLY:H	4	0.13
(1,867)	1:34:A:GLU:HG3	1:24:A:GLY:H	4	0.13
(1,867)	1:34:A:GLU:HG2	1:24:A:GLY:H	11	0.13
(1,867)	1:34:A:GLU:HG3	1:24:A:GLY:H	11	0.13
(1,867)	1:34:A:GLU:HG2	1:24:A:GLY:H	16	0.13
(1,867)	1:34:A:GLU:HG3	1:24:A:GLY:H	16	0.13
(1,862)	1:21:A:LYS:HE2	1:19:A:ARG:H	10	0.13
(1,862)	1:21:A:LYS:HE3	1:19:A:ARG:H	10	0.13
(1,861)	1:17:A:PRO:HD2	1:19:A:ARG:H	8	0.13
(1,861)	1:17:A:PRO:HD3	1:19:A:ARG:H	8	0.13
(1,851)	1:32:A:SER:H	1:11:A:ASN:HD22	19	0.13
(1,842)	1:80:A:CYS:HA	1:84:A:THR:H	1	0.13
(1,842)	1:80:A:CYS:HA	1:84:A:THR:H	16	0.13
(1,840)	1:71:A:CYS:HB2	1:77:A:GLU:H	1	0.13
(1,840)	1:71:A:CYS:HB3	1:77:A:GLU:H	1	0.13
(1,840)	1:71:A:CYS:HB2	1:77:A:GLU:H	16	0.13
(1,840)	1:71:A:CYS:HB3	1:77:A:GLU:H	16	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,828)	1:85:A:CYS:HA	1:86:A:SER:H	3	0.13
(1,828)	1:85:A:CYS:HA	1:86:A:SER:H	10	0.13
(1,828)	1:85:A:CYS:HA	1:86:A:SER:H	19	0.13
(1,813)	1:107:A:GLN:HE21	1:108:A:ASP:HA	11	0.13
(1,811)	1:107:A:GLN:H	1:105:A:ASN:HD21	12	0.13
(1,810)	1:101:A:ASN:HD21	1:105:A:ASN:HD22	12	0.13
(1,809)	1:106:A:GLY:H	1:104:A:CYS:H	19	0.13
(1,808)	1:116:A:GLU:HB2	1:104:A:CYS:H	14	0.13
(1,808)	1:116:A:GLU:HB3	1:104:A:CYS:H	14	0.13
(1,806)	1:101:A:ASN:HD21	1:102:A:PHE:H	12	0.13
(1,806)	1:101:A:ASN:HD21	1:102:A:PHE:H	13	0.13
(1,800)	1:85:A:CYS:HB2	1:98:A:ILE:H	8	0.13
(1,800)	1:85:A:CYS:HB3	1:98:A:ILE:H	8	0.13
(1,799)	1:85:A:CYS:HA	1:97:A:CYS:H	11	0.13
(1,798)	1:85:A:CYS:HB2	1:97:A:CYS:H	18	0.13
(1,798)	1:85:A:CYS:HB3	1:97:A:CYS:H	18	0.13
(1,792)	1:97:A:CYS:HB2	1:91:A:THR:H	1	0.13
(1,792)	1:97:A:CYS:HB3	1:91:A:THR:H	1	0.13
(1,788)	1:80:A:CYS:H	1:78:A:GLU:H	9	0.13
(1,788)	1:80:A:CYS:H	1:78:A:GLU:H	11	0.13
(1,784)	1:71:A:CYS:HB2	1:76:A:ASP:H	18	0.13
(1,784)	1:71:A:CYS:HB3	1:76:A:ASP:H	18	0.13
(1,777)	1:77:A:GLU:HB2	1:70:A:ASP:H	11	0.13
(1,777)	1:77:A:GLU:HB3	1:70:A:ASP:H	11	0.13
(1,776)	1:77:A:GLU:HG2	1:70:A:ASP:H	1	0.13
(1,776)	1:77:A:GLU:HG3	1:70:A:ASP:H	1	0.13
(1,761)	1:72:A:ASP:H	1:57:A:GLN:HE21	4	0.13
(1,745)	1:48:A:GLU:HB2	1:49:A:ILE:H	1	0.13
(1,745)	1:48:A:GLU:HB3	1:49:A:ILE:H	1	0.13
(1,745)	1:48:A:GLU:HB2	1:49:A:ILE:H	17	0.13
(1,745)	1:48:A:GLU:HB3	1:49:A:ILE:H	17	0.13
(1,744)	1:48:A:GLU:H	1:47:A:HIS:H	8	0.13
(1,734)	1:32:A:SER:H	1:11:A:ASN:H	4	0.13
(1,726)	1:34:A:GLU:HG2	1:27:A:ASP:H	11	0.13
(1,726)	1:34:A:GLU:HG3	1:27:A:ASP:H	11	0.13
(1,724)	1:34:A:GLU:HB2	1:25:A:ASP:H	5	0.13
(1,724)	1:34:A:GLU:HB3	1:25:A:ASP:H	5	0.13
(1,718)	1:16:A:VAL:HB	1:20:A:TRP:HE1	1	0.13
(1,718)	1:16:A:VAL:HB	1:20:A:TRP:HE1	9	0.13
(1,717)	1:20:A:TRP:HE1	1:20:A:TRP:H	4	0.13
(1,717)	1:20:A:TRP:HE1	1:20:A:TRP:H	14	0.13
(1,717)	1:20:A:TRP:HE1	1:20:A:TRP:H	18	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,716)	1:28:A:CYS:HB2	1:14:A:GLN:HE22	4	0.13
(1,716)	1:28:A:CYS:HB3	1:14:A:GLN:HE22	4	0.13
(1,712)	1:32:A:SER:H	1:11:A:ASN:H	4	0.13
(1,709)	1:45:A:ARG:HD2	1:45:A:ARG:H	16	0.13
(1,709)	1:45:A:ARG:HD3	1:45:A:ARG:H	16	0.13
(1,707)	1:45:A:ARG:HD2	1:45:A:ARG:H	16	0.13
(1,707)	1:45:A:ARG:HD3	1:45:A:ARG:H	16	0.13
(1,705)	1:100:A:ARG:H	1:100:A:ARG:HD2	12	0.13
(1,705)	1:100:A:ARG:H	1:100:A:ARG:HD3	12	0.13
(1,705)	1:100:A:ARG:H	1:100:A:ARG:HD2	18	0.13
(1,705)	1:100:A:ARG:H	1:100:A:ARG:HD3	18	0.13
(1,699)	1:64:A:ARG:HD2	1:64:A:ARG:H	18	0.13
(1,699)	1:64:A:ARG:HD3	1:64:A:ARG:H	18	0.13
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG2	4	0.13
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG3	4	0.13
(1,694)	1:21:A:LYS:HE2	1:21:A:LYS:H	8	0.13
(1,694)	1:21:A:LYS:HE3	1:21:A:LYS:H	8	0.13
(1,679)	1:78:A:GLU:HG2	1:79:A:ASN:HD22	13	0.13
(1,679)	1:78:A:GLU:HG3	1:79:A:ASN:HD22	13	0.13
(1,658)	1:102:A:PHE:HA	1:105:A:ASN:HD22	20	0.13
(1,639)	1:82:A:ASN:H	1:82:A:ASN:HD21	16	0.13
(1,631)	1:79:A:ASN:HD22	1:79:A:ASN:H	20	0.13
(1,627)	1:72:A:ASP:HA	1:57:A:GLN:HE22	18	0.13
(1,612)	1:15:A:CYS:H	1:14:A:GLN:HE22	7	0.13
(1,610)	1:14:A:GLN:HE22	1:29:A:GLU:H	12	0.13
(1,603)	1:32:A:SER:HB2	1:11:A:ASN:HD22	1	0.13
(1,603)	1:32:A:SER:HB3	1:11:A:ASN:HD22	1	0.13
(1,603)	1:32:A:SER:HB2	1:11:A:ASN:HD22	20	0.13
(1,603)	1:32:A:SER:HB3	1:11:A:ASN:HD22	20	0.13
(1,601)	1:11:A:ASN:H	1:11:A:ASN:HD22	1	0.13
(1,596)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	2	0.13
(1,596)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	2	0.13
(1,585)	1:28:A:CYS:H	1:27:A:ASP:H	6	0.13
(1,585)	1:28:A:CYS:H	1:27:A:ASP:H	8	0.13
(1,585)	1:28:A:CYS:H	1:27:A:ASP:H	9	0.13
(1,580)	1:48:A:GLU:HG2	1:49:A:ILE:H	3	0.13
(1,580)	1:48:A:GLU:HG3	1:49:A:ILE:H	3	0.13
(1,580)	1:48:A:GLU:HG2	1:49:A:ILE:H	11	0.13
(1,580)	1:48:A:GLU:HG3	1:49:A:ILE:H	11	0.13
(1,562)	1:102:A:PHE:HB2	1:99:A:SER:H	3	0.13
(1,562)	1:102:A:PHE:HB3	1:99:A:SER:H	3	0.13
(1,560)	1:90:A:PHE:H	1:99:A:SER:H	3	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,560)	1:90:A:PHE:H	1:99:A:SER:H	20	0.13
(1,551)	1:104:A:CYS:HB2	1:104:A:CYS:H	1	0.13
(1,551)	1:104:A:CYS:HB3	1:104:A:CYS:H	1	0.13
(1,551)	1:104:A:CYS:HB2	1:104:A:CYS:H	3	0.13
(1,551)	1:104:A:CYS:HB3	1:104:A:CYS:H	3	0.13
(1,550)	1:104:A:CYS:HB2	1:104:A:CYS:H	1	0.13
(1,550)	1:104:A:CYS:HB3	1:104:A:CYS:H	1	0.13
(1,550)	1:104:A:CYS:HB2	1:104:A:CYS:H	3	0.13
(1,550)	1:104:A:CYS:HB3	1:104:A:CYS:H	3	0.13
(1,547)	1:104:A:CYS:HB2	1:105:A:ASN:H	2	0.13
(1,547)	1:104:A:CYS:HB3	1:105:A:ASN:H	2	0.13
(1,547)	1:104:A:CYS:HB2	1:105:A:ASN:H	9	0.13
(1,547)	1:104:A:CYS:HB3	1:105:A:ASN:H	9	0.13
(1,547)	1:104:A:CYS:HB2	1:105:A:ASN:H	16	0.13
(1,547)	1:104:A:CYS:HB3	1:105:A:ASN:H	16	0.13
(1,541)	1:115:A:ASP:HB2	1:116:A:GLU:H	16	0.13
(1,541)	1:115:A:ASP:HB3	1:116:A:GLU:H	16	0.13
(1,516)	1:49:A:ILE:H	1:59:A:ILE:H	4	0.13
(1,509)	1:46:A:ILE:HA	1:46:A:ILE:H	14	0.13
(1,501)	1:34:A:GLU:HB2	1:34:A:GLU:H	15	0.13
(1,501)	1:34:A:GLU:HB3	1:34:A:GLU:H	15	0.13
(1,496)	1:31:A:GLY:HA2	1:31:A:GLY:H	4	0.13
(1,496)	1:31:A:GLY:HA3	1:31:A:GLY:H	4	0.13
(1,496)	1:31:A:GLY:HA2	1:31:A:GLY:H	10	0.13
(1,496)	1:31:A:GLY:HA3	1:31:A:GLY:H	10	0.13
(1,496)	1:31:A:GLY:HA2	1:31:A:GLY:H	15	0.13
(1,496)	1:31:A:GLY:HA3	1:31:A:GLY:H	15	0.13
(1,496)	1:31:A:GLY:HA2	1:31:A:GLY:H	17	0.13
(1,496)	1:31:A:GLY:HA3	1:31:A:GLY:H	17	0.13
(1,495)	1:31:A:GLY:H	1:29:A:GLU:H	11	0.13
(1,482)	1:11:A:ASN:HD21	1:11:A:ASN:H	12	0.13
(1,479)	1:9:A:VAL:HG11	1:9:A:VAL:H	18	0.13
(1,479)	1:9:A:VAL:HG12	1:9:A:VAL:H	18	0.13
(1,479)	1:9:A:VAL:HG13	1:9:A:VAL:H	18	0.13
(1,479)	1:9:A:VAL:HG21	1:9:A:VAL:H	18	0.13
(1,479)	1:9:A:VAL:HG22	1:9:A:VAL:H	18	0.13
(1,479)	1:9:A:VAL:HG23	1:9:A:VAL:H	18	0.13
(1,478)	1:9:A:VAL:HB	1:9:A:VAL:H	18	0.13
(1,475)	1:75:A:GLU:H	1:76:A:ASP:H	3	0.13
(1,475)	1:75:A:GLU:H	1:76:A:ASP:H	13	0.13
(1,473)	1:85:A:CYS:H	1:86:A:SER:H	8	0.13
(1,473)	1:85:A:CYS:H	1:86:A:SER:H	11	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,473)	1:85:A:CYS:H	1:86:A:SER:H	12	0.13
(1,466)	1:80:A:CYS:HA	1:79:A:ASN:H	11	0.13
(1,462)	1:79:A:ASN:H	1:78:A:GLU:H	2	0.13
(1,462)	1:79:A:ASN:H	1:78:A:GLU:H	3	0.13
(1,462)	1:79:A:ASN:H	1:78:A:GLU:H	6	0.13
(1,462)	1:79:A:ASN:H	1:78:A:GLU:H	10	0.13
(1,462)	1:79:A:ASN:H	1:78:A:GLU:H	16	0.13
(1,462)	1:79:A:ASN:H	1:78:A:GLU:H	20	0.13
(1,451)	1:75:A:GLU:H	1:76:A:ASP:H	3	0.13
(1,451)	1:75:A:GLU:H	1:76:A:ASP:H	13	0.13
(1,444)	1:76:A:ASP:H	1:74:A:GLY:H	4	0.13
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB2	4	0.13
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB3	4	0.13
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB2	7	0.13
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB3	7	0.13
(1,437)	1:72:A:ASP:H	1:71:A:CYS:H	2	0.13
(1,437)	1:72:A:ASP:H	1:71:A:CYS:H	19	0.13
(1,435)	1:72:A:ASP:HA	1:72:A:ASP:H	3	0.13
(1,435)	1:72:A:ASP:HA	1:72:A:ASP:H	13	0.13
(1,435)	1:72:A:ASP:HA	1:72:A:ASP:H	19	0.13
(1,432)	1:70:A:ASP:HB2	1:70:A:ASP:H	20	0.13
(1,432)	1:70:A:ASP:HB3	1:70:A:ASP:H	20	0.13
(1,419)	1:65:A:CYS:HB2	1:66:A:ASP:H	14	0.13
(1,419)	1:65:A:CYS:HB3	1:66:A:ASP:H	14	0.13
(1,418)	1:64:A:ARG:HA	1:66:A:ASP:H	13	0.13
(1,409)	1:60:A:PRO:HA	1:61:A:VAL:H	3	0.13
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB1	13	0.13
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB2	13	0.13
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB3	13	0.13
(1,392)	1:52:A:GLY:HA2	1:53:A:ALA:H	2	0.13
(1,392)	1:52:A:GLY:HA3	1:53:A:ALA:H	2	0.13
(1,392)	1:52:A:GLY:HA2	1:53:A:ALA:H	6	0.13
(1,392)	1:52:A:GLY:HA3	1:53:A:ALA:H	6	0.13
(1,392)	1:52:A:GLY:HA2	1:53:A:ALA:H	7	0.13
(1,392)	1:52:A:GLY:HA3	1:53:A:ALA:H	7	0.13
(1,392)	1:52:A:GLY:HA2	1:53:A:ALA:H	17	0.13
(1,392)	1:52:A:GLY:HA3	1:53:A:ALA:H	17	0.13
(1,390)	1:51:A:CYS:HB2	1:52:A:GLY:H	18	0.13
(1,390)	1:51:A:CYS:HB3	1:52:A:GLY:H	18	0.13
(1,387)	1:51:A:CYS:H	1:51:A:CYS:HB2	8	0.13
(1,387)	1:51:A:CYS:H	1:51:A:CYS:HB3	8	0.13
(1,383)	1:51:A:CYS:H	1:50:A:SER:HA	9	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,383)	1:51:A:CYS:H	1:50:A:SER:HA	19	0.13
(1,378)	1:48:A:GLU:HG2	1:49:A:ILE:H	3	0.13
(1,378)	1:48:A:GLU:HG3	1:49:A:ILE:H	3	0.13
(1,378)	1:48:A:GLU:HG2	1:49:A:ILE:H	11	0.13
(1,378)	1:48:A:GLU:HG3	1:49:A:ILE:H	11	0.13
(1,377)	1:60:A:PRO:HA	1:49:A:ILE:H	6	0.13
(1,372)	1:48:A:GLU:H	1:48:A:GLU:HA	14	0.13
(1,372)	1:48:A:GLU:H	1:48:A:GLU:HA	18	0.13
(1,369)	1:43:A:THR:HB	1:44:A:CYS:H	8	0.13
(1,367)	1:42:A:ARG:HG2	1:43:A:THR:H	19	0.13
(1,367)	1:42:A:ARG:HG2	1:43:A:THR:H	19	0.13
(1,367)	1:42:A:ARG:HG3	1:43:A:THR:H	19	0.13
(1,367)	1:42:A:ARG:HG3	1:43:A:THR:H	19	0.13
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB2	11	0.13
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB3	11	0.13
(1,357)	1:40:A:HIS:H	1:39:A:CYS:HA	12	0.13
(1,357)	1:40:A:HIS:H	1:39:A:CYS:HA	16	0.13
(1,350)	1:31:A:GLY:H	1:32:A:SER:H	11	0.13
(1,335)	1:45:A:ARG:HD2	1:24:A:GLY:H	13	0.13
(1,335)	1:45:A:ARG:HD3	1:24:A:GLY:H	13	0.13
(1,329)	1:25:A:ASP:H	1:23:A:ASP:H	12	0.13
(1,320)	1:7:A:ASP:HA	1:18:A:SER:H	4	0.13
(1,312)	1:14:A:GLN:HG2	1:14:A:GLN:H	2	0.13
(1,312)	1:14:A:GLN:HG3	1:14:A:GLN:H	2	0.13
(1,308)	1:13:A:GLY:H	1:14:A:GLN:H	16	0.13
(1,302)	1:14:A:GLN:H	1:12:A:ASN:H	4	0.13
(1,302)	1:14:A:GLN:H	1:12:A:ASN:H	6	0.13
(1,295)	1:15:A:CYS:HA	1:10:A:CYS:H	2	0.13
(1,295)	1:15:A:CYS:HA	1:10:A:CYS:H	9	0.13
(1,290)	1:8:A:PHE:HA	1:9:A:VAL:H	3	0.13
(1,290)	1:8:A:PHE:HA	1:9:A:VAL:H	18	0.13
(1,290)	1:8:A:PHE:HA	1:9:A:VAL:H	19	0.13
(1,287)	1:7:A:ASP:H	1:4:A:ALA:HB1	17	0.13
(1,287)	1:7:A:ASP:H	1:4:A:ALA:HB2	17	0.13
(1,287)	1:7:A:ASP:H	1:4:A:ALA:HB3	17	0.13
(1,280)	1:5:A:GLU:HG2	1:6:A:SER:H	2	0.13
(1,280)	1:5:A:GLU:HG2	1:6:A:SER:H	2	0.13
(1,280)	1:5:A:GLU:HG3	1:6:A:SER:H	2	0.13
(1,280)	1:5:A:GLU:HG3	1:6:A:SER:H	2	0.13
(1,279)	1:6:A:SER:HB2	1:6:A:SER:H	18	0.13
(1,279)	1:6:A:SER:HB3	1:6:A:SER:H	18	0.13
(1,279)	1:6:A:SER:HB2	1:6:A:SER:H	19	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,279)	1:6:A:SER:HB3	1:6:A:SER:H	19	0.13
(1,277)	1:6:A:SER:HB2	1:6:A:SER:H	18	0.13
(1,277)	1:6:A:SER:HB3	1:6:A:SER:H	18	0.13
(1,277)	1:6:A:SER:HB2	1:6:A:SER:H	19	0.13
(1,277)	1:6:A:SER:HB3	1:6:A:SER:H	19	0.13
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	9	0.13
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	9	0.13
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	9	0.13
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	9	0.13
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	20	0.13
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	20	0.13
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	20	0.13
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	20	0.13
(1,248)	1:83:A:ILE:HB	1:84:A:THR:H	4	0.13
(1,247)	1:83:A:ILE:HA	1:84:A:THR:H	19	0.13
(1,241)	1:86:A:SER:H	1:89:A:GLU:H	12	0.13
(1,241)	1:86:A:SER:H	1:89:A:GLU:H	16	0.13
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD11	6	0.13
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD12	6	0.13
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD13	6	0.13
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD11	15	0.13
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD12	15	0.13
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD13	15	0.13
(1,226)	1:92:A:CYS:HB2	1:94:A:SER:H	3	0.13
(1,226)	1:92:A:CYS:HB3	1:94:A:SER:H	3	0.13
(1,226)	1:92:A:CYS:HB2	1:94:A:SER:H	14	0.13
(1,226)	1:92:A:CYS:HB3	1:94:A:SER:H	14	0.13
(1,222)	1:92:A:CYS:HB2	1:95:A:GLY:H	10	0.13
(1,222)	1:92:A:CYS:HB3	1:95:A:GLY:H	10	0.13
(1,196)	1:98:A:ILE:HA	1:99:A:SER:H	4	0.13
(1,196)	1:98:A:ILE:HA	1:99:A:SER:H	6	0.13
(1,190)	1:101:A:ASN:HB2	1:101:A:ASN:H	4	0.13
(1,190)	1:101:A:ASN:HB3	1:101:A:ASN:H	4	0.13
(1,180)	1:99:A:SER:HB2	1:102:A:PHE:H	18	0.13
(1,180)	1:99:A:SER:HB3	1:102:A:PHE:H	18	0.13
(1,143)	1:106:A:GLY:H	1:107:A:GLN:H	8	0.13
(1,128)	1:114:A:SER:HA	1:114:A:SER:H	13	0.13
(1,128)	1:114:A:SER:HA	1:114:A:SER:H	20	0.13
(1,127)	1:114:A:SER:H	1:114:A:SER:HB2	12	0.13
(1,127)	1:114:A:SER:H	1:114:A:SER:HB3	12	0.13
(1,126)	1:117:A:LEU:HD11	1:114:A:SER:H	4	0.13
(1,126)	1:117:A:LEU:HD12	1:114:A:SER:H	4	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,126)	1:117:A:LEU:HD13	1:114:A:SER:H	4	0.13
(1,126)	1:117:A:LEU:HD21	1:114:A:SER:H	4	0.13
(1,126)	1:117:A:LEU:HD22	1:114:A:SER:H	4	0.13
(1,126)	1:117:A:LEU:HD23	1:114:A:SER:H	4	0.13
(1,116)	1:116:A:GLU:HG2	1:116:A:GLU:H	17	0.13
(1,116)	1:116:A:GLU:HG3	1:116:A:GLU:H	17	0.13
(1,96)	1:100:A:ARG:H	1:89:A:GLU:HA	3	0.13
(1,94)	1:120:A:ALA:H	1:119:A:CYS:HB2	10	0.13
(1,94)	1:120:A:ALA:H	1:119:A:CYS:HB3	10	0.13
(1,94)	1:120:A:ALA:H	1:119:A:CYS:HB2	13	0.13
(1,94)	1:120:A:ALA:H	1:119:A:CYS:HB3	13	0.13
(1,83)	1:28:A:CYS:HB2	1:29:A:GLU:H	9	0.13
(1,83)	1:28:A:CYS:HB3	1:29:A:GLU:H	9	0.13
(1,74)	1:65:A:CYS:H	1:65:A:CYS:HB2	3	0.13
(1,74)	1:65:A:CYS:H	1:65:A:CYS:HB3	3	0.13
(1,69)	1:78:A:GLU:HG2	1:78:A:GLU:H	13	0.13
(1,69)	1:78:A:GLU:HG3	1:78:A:GLU:H	13	0.13
(1,67)	1:19:A:ARG:H	1:18:A:SER:H	19	0.13
(1,63)	1:39:A:CYS:H	1:40:A:HIS:H	10	0.13
(1,63)	1:39:A:CYS:H	1:40:A:HIS:H	14	0.13
(1,59)	1:65:A:CYS:H	1:66:A:ASP:H	10	0.13
(1,59)	1:65:A:CYS:H	1:66:A:ASP:H	14	0.13
(1,57)	1:66:A:ASP:H	1:67:A:GLY:H	14	0.13
(1,56)	1:70:A:ASP:H	1:71:A:CYS:H	9	0.13
(1,49)	1:94:A:SER:H	1:93:A:SER:H	4	0.13
(1,49)	1:94:A:SER:H	1:93:A:SER:H	10	0.13
(1,22)	1:91:A:THR:H	1:92:A:CYS:H	1	0.13
(1,15)	1:109:A:ASP:H	1:110:A:CYS:H	14	0.13
(1,9)	1:12:A:ASN:H	1:11:A:ASN:H	11	0.13
(1,7)	1:22:A:CYS:H	1:23:A:ASP:H	3	0.13
(1,7)	1:22:A:CYS:H	1:23:A:ASP:H	6	0.13
(1,7)	1:22:A:CYS:H	1:23:A:ASP:H	7	0.13
(1,7)	1:22:A:CYS:H	1:23:A:ASP:H	19	0.13
(1,6)	1:23:A:ASP:H	1:24:A:GLY:H	17	0.13
(1,1)	1:112:A:ASP:H	1:113:A:GLY:H	17	0.13
(4,7)	1:8:A:PHE:H	1:16:A:VAL:O	19	0.12
(4,2)	1:90:A:PHE:O	1:98:A:ILE:H	5	0.12
(3,9)	2:202:A:CA:CA	1:68:A:GLU:O	6	0.12
(3,7)	2:202:A:CA:CA	1:63:A:TRP:O	4	0.12
(2,385)	1:66:A:ASP:HA	1:68:A:GLU:H	1	0.12
(2,385)	1:66:A:ASP:HA	1:68:A:GLU:H	9	0.12
(2,382)	1:72:A:ASP:HB2	1:73:A:SER:H	15	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,382)	1:72:A:ASP:HB3	1:73:A:SER:H	15	0.12
(2,370)	1:38:A:GLN:HG3	1:38:A:GLN:HE22	11	0.12
(2,370)	1:38:A:GLN:HG3	1:38:A:GLN:HE22	16	0.12
(2,370)	1:38:A:GLN:HG3	1:38:A:GLN:HE22	17	0.12
(2,366)	1:107:A:GLN:HA	1:106:A:GLY:H	5	0.12
(2,359)	1:98:A:ILE:HD12	1:98:A:ILE:H	11	0.12
(2,331)	1:101:A:ASN:H	1:99:A:SER:H	6	0.12
(2,313)	1:17:A:PRO:HB2	1:20:A:TRP:H	9	0.12
(2,307)	1:59:A:ILE:HD12	1:63:A:TRP:H	1	0.12
(2,307)	1:60:A:PRO:HB2	1:63:A:TRP:H	19	0.12
(2,302)	1:119:A:CYS:HA	1:120:A:ALA:H	15	0.12
(2,277)	1:19:A:ARG:HG2	1:19:A:ARG:H	19	0.12
(2,263)	1:63:A:TRP:HB2	1:63:A:TRP:H	5	0.12
(2,245)	1:36:A:PRO:HA	1:39:A:CYS:H	7	0.12
(2,236)	1:21:A:LYS:HB2	1:21:A:LYS:H	9	0.12
(2,236)	1:21:A:LYS:HB2	1:21:A:LYS:H	10	0.12
(2,233)	1:14:A:GLN:HB2	1:14:A:GLN:HE22	3	0.12
(2,233)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	3	0.12
(2,233)	1:14:A:GLN:HB2	1:14:A:GLN:HE22	6	0.12
(2,233)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	6	0.12
(2,233)	1:14:A:GLN:HB2	1:14:A:GLN:HE22	9	0.12
(2,233)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	9	0.12
(2,233)	1:14:A:GLN:HB2	1:14:A:GLN:HE22	13	0.12
(2,233)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	13	0.12
(2,233)	1:14:A:GLN:HB2	1:14:A:GLN:HE22	18	0.12
(2,233)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	18	0.12
(2,233)	1:14:A:GLN:HB2	1:14:A:GLN:HE22	20	0.12
(2,233)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	20	0.12
(2,218)	1:36:A:PRO:HD2	1:37:A:GLU:H	9	0.12
(2,191)	1:54:A:HIS:H	1:55:A:SER:H	1	0.12
(2,188)	1:16:A:VAL:HG11	1:19:A:ARG:H	8	0.12
(2,188)	1:16:A:VAL:HG12	1:19:A:ARG:H	8	0.12
(2,188)	1:16:A:VAL:HG13	1:19:A:ARG:H	8	0.12
(2,188)	1:16:A:VAL:HG21	1:19:A:ARG:H	8	0.12
(2,188)	1:16:A:VAL:HG22	1:19:A:ARG:H	8	0.12
(2,188)	1:16:A:VAL:HG23	1:19:A:ARG:H	8	0.12
(2,188)	1:16:A:VAL:HG11	1:19:A:ARG:H	15	0.12
(2,188)	1:16:A:VAL:HG12	1:19:A:ARG:H	15	0.12
(2,188)	1:16:A:VAL:HG13	1:19:A:ARG:H	15	0.12
(2,188)	1:16:A:VAL:HG21	1:19:A:ARG:H	15	0.12
(2,188)	1:16:A:VAL:HG22	1:19:A:ARG:H	15	0.12
(2,188)	1:16:A:VAL:HG23	1:19:A:ARG:H	15	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,187)	1:118:A:ASP:HA	1:119:A:CYS:H	13	0.12
(2,181)	1:39:A:CYS:HB3	1:41:A:MET:H	19	0.12
(2,168)	1:38:A:GLN:HG3	1:38:A:GLN:H	12	0.12
(2,122)	1:16:A:VAL:HA	1:16:A:VAL:H	12	0.12
(2,117)	1:14:A:GLN:HB2	1:12:A:ASN:HD21	9	0.12
(2,117)	1:14:A:GLN:HB3	1:12:A:ASN:HD21	9	0.12
(2,115)	1:80:A:CYS:H	1:81:A:GLY:H	7	0.12
(2,111)	1:72:A:ASP:H	1:71:A:CYS:H	18	0.12
(2,83)	1:35:A:SER:HB3	1:38:A:GLN:H	5	0.12
(2,75)	1:108:A:ASP:HA	1:108:A:ASP:H	5	0.12
(2,61)	1:4:A:ALA:HA	1:5:A:GLU:H	20	0.12
(2,22)	1:75:A:GLU:HA	1:78:A:GLU:H	19	0.12
(2,10)	1:14:A:GLN:HB2	1:15:A:CYS:H	1	0.12
(2,10)	1:14:A:GLN:HB3	1:15:A:CYS:H	1	0.12
(1,930)	1:102:A:PHE:HE2	1:107:A:GLN:HG2	8	0.12
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG21	14	0.12
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG22	14	0.12
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG23	14	0.12
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG21	17	0.12
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG22	17	0.12
(1,925)	1:8:A:PHE:HB3	1:16:A:VAL:HG23	17	0.12
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG11	11	0.12
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG12	11	0.12
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG13	11	0.12
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG21	11	0.12
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG22	11	0.12
(1,924)	1:8:A:PHE:HB2	1:16:A:VAL:HG23	11	0.12
(1,920)	1:16:A:VAL:HG11	1:20:A:TRP:HE3	11	0.12
(1,920)	1:16:A:VAL:HG12	1:20:A:TRP:HE3	11	0.12
(1,920)	1:16:A:VAL:HG13	1:20:A:TRP:HE3	11	0.12
(1,920)	1:16:A:VAL:HG21	1:20:A:TRP:HE3	11	0.12
(1,920)	1:16:A:VAL:HG22	1:20:A:TRP:HE3	11	0.12
(1,920)	1:16:A:VAL:HG23	1:20:A:TRP:HE3	11	0.12
(1,917)	1:28:A:CYS:H	1:14:A:GLN:HG2	14	0.12
(1,916)	1:77:A:GLU:HB2	1:77:A:GLU:H	1	0.12
(1,916)	1:77:A:GLU:HB3	1:77:A:GLU:H	1	0.12
(1,906)	1:13:A:GLY:HA2	1:12:A:ASN:HD22	5	0.12
(1,906)	1:13:A:GLY:HA3	1:12:A:ASN:HD22	5	0.12
(1,906)	1:13:A:GLY:HA2	1:12:A:ASN:HD22	11	0.12
(1,906)	1:13:A:GLY:HA3	1:12:A:ASN:HD22	11	0.12
(1,905)	1:101:A:ASN:HD21	1:105:A:ASN:HD21	19	0.12
(1,900)	1:83:A:ILE:HG12	1:82:A:ASN:H	5	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,900)	1:83:A:ILE:HG13	1:82:A:ASN:H	5	0.12
(1,882)	1:58:A:CYS:HA	1:50:A:SER:H	9	0.12
(1,882)	1:58:A:CYS:HA	1:50:A:SER:H	16	0.12
(1,876)	1:39:A:CYS:HB2	1:43:A:THR:H	13	0.12
(1,876)	1:39:A:CYS:HB3	1:43:A:THR:H	13	0.12
(1,875)	1:38:A:GLN:HE22	1:38:A:GLN:H	6	0.12
(1,873)	1:34:A:GLU:HB2	1:33:A:ASP:H	5	0.12
(1,873)	1:34:A:GLU:HB3	1:33:A:ASP:H	5	0.12
(1,872)	1:32:A:SER:H	1:33:A:ASP:HB2	19	0.12
(1,872)	1:32:A:SER:H	1:33:A:ASP:HB3	19	0.12
(1,869)	1:14:A:GLN:HE22	1:28:A:CYS:H	1	0.12
(1,867)	1:34:A:GLU:HG2	1:24:A:GLY:H	6	0.12
(1,867)	1:34:A:GLU:HG3	1:24:A:GLY:H	6	0.12
(1,843)	1:4:A:ALA:H	1:17:A:PRO:HB2	18	0.12
(1,843)	1:4:A:ALA:H	1:17:A:PRO:HB3	18	0.12
(1,838)	1:58:A:CYS:HA	1:52:A:GLY:H	14	0.12
(1,829)	1:85:A:CYS:HB2	1:86:A:SER:H	19	0.12
(1,829)	1:85:A:CYS:HB3	1:86:A:SER:H	19	0.12
(1,828)	1:85:A:CYS:HA	1:86:A:SER:H	5	0.12
(1,828)	1:85:A:CYS:HA	1:86:A:SER:H	13	0.12
(1,820)	1:110:A:CYS:H	1:115:A:ASP:H	4	0.12
(1,820)	1:110:A:CYS:H	1:115:A:ASP:H	7	0.12
(1,813)	1:107:A:GLN:HE21	1:108:A:ASP:HA	12	0.12
(1,813)	1:107:A:GLN:HE21	1:108:A:ASP:HA	18	0.12
(1,811)	1:107:A:GLN:H	1:105:A:ASN:HD21	20	0.12
(1,809)	1:106:A:GLY:H	1:104:A:CYS:H	17	0.12
(1,807)	1:98:A:ILE:HG12	1:103:A:VAL:H	2	0.12
(1,807)	1:98:A:ILE:HG13	1:103:A:VAL:H	2	0.12
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG21	6	0.12
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG22	6	0.12
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG23	6	0.12
(1,794)	1:82:A:ASN:HD22	1:94:A:SER:H	18	0.12
(1,792)	1:97:A:CYS:HB2	1:91:A:THR:H	6	0.12
(1,792)	1:97:A:CYS:HB3	1:91:A:THR:H	6	0.12
(1,792)	1:97:A:CYS:HB2	1:91:A:THR:H	11	0.12
(1,792)	1:97:A:CYS:HB3	1:91:A:THR:H	11	0.12
(1,766)	1:48:A:GLU:HB2	1:58:A:CYS:H	19	0.12
(1,766)	1:48:A:GLU:HB3	1:58:A:CYS:H	19	0.12
(1,759)	1:57:A:GLN:HE21	1:71:A:CYS:HA	5	0.12
(1,751)	1:52:A:GLY:H	1:57:A:GLN:HG2	9	0.12
(1,751)	1:52:A:GLY:H	1:57:A:GLN:HG3	9	0.12
(1,751)	1:52:A:GLY:H	1:57:A:GLN:HG2	20	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,751)	1:52:A:GLY:H	1:57:A:GLN:HG3	20	0.12
(1,745)	1:48:A:GLU:HB2	1:49:A:ILE:H	4	0.12
(1,745)	1:48:A:GLU:HB3	1:49:A:ILE:H	4	0.12
(1,745)	1:48:A:GLU:HB2	1:49:A:ILE:H	12	0.12
(1,745)	1:48:A:GLU:HB3	1:49:A:ILE:H	12	0.12
(1,744)	1:48:A:GLU:H	1:47:A:HIS:H	5	0.12
(1,744)	1:48:A:GLU:H	1:47:A:HIS:H	10	0.12
(1,741)	1:9:A:VAL:HG11	1:38:A:GLN:HE21	20	0.12
(1,741)	1:9:A:VAL:HG12	1:38:A:GLN:HE21	20	0.12
(1,741)	1:9:A:VAL:HG13	1:38:A:GLN:HE21	20	0.12
(1,741)	1:9:A:VAL:HG21	1:38:A:GLN:HE21	20	0.12
(1,741)	1:9:A:VAL:HG22	1:38:A:GLN:HE21	20	0.12
(1,741)	1:9:A:VAL:HG23	1:38:A:GLN:HE21	20	0.12
(1,739)	1:34:A:GLU:HB2	1:35:A:SER:H	6	0.12
(1,739)	1:34:A:GLU:HB3	1:35:A:SER:H	6	0.12
(1,734)	1:32:A:SER:H	1:11:A:ASN:H	8	0.12
(1,718)	1:16:A:VAL:HB	1:20:A:TRP:HE1	5	0.12
(1,712)	1:32:A:SER:H	1:11:A:ASN:H	8	0.12
(1,709)	1:45:A:ARG:HD2	1:45:A:ARG:H	6	0.12
(1,709)	1:45:A:ARG:HD3	1:45:A:ARG:H	6	0.12
(1,707)	1:45:A:ARG:HD2	1:45:A:ARG:H	6	0.12
(1,707)	1:45:A:ARG:HD3	1:45:A:ARG:H	6	0.12
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG2	1	0.12
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG3	1	0.12
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG2	16	0.12
(1,698)	1:64:A:ARG:H	1:64:A:ARG:HG3	16	0.12
(1,680)	1:79:A:ASN:HD22	1:79:A:ASN:HB2	18	0.12
(1,680)	1:79:A:ASN:HD22	1:79:A:ASN:HB3	18	0.12
(1,679)	1:78:A:GLU:HG2	1:79:A:ASN:HD22	11	0.12
(1,679)	1:78:A:GLU:HG3	1:79:A:ASN:HD22	11	0.12
(1,678)	1:63:A:TRP:HE1	1:63:A:TRP:HA	10	0.12
(1,670)	1:107:A:GLN:HB2	1:105:A:ASN:HD22	12	0.12
(1,670)	1:107:A:GLN:HB2	1:105:A:ASN:HD22	12	0.12
(1,670)	1:107:A:GLN:HB3	1:105:A:ASN:HD22	12	0.12
(1,670)	1:107:A:GLN:HB3	1:105:A:ASN:HD22	12	0.12
(1,662)	1:102:A:PHE:HB2	1:105:A:ASN:HD21	11	0.12
(1,662)	1:102:A:PHE:HB3	1:105:A:ASN:HD21	11	0.12
(1,662)	1:102:A:PHE:HB2	1:105:A:ASN:HD21	17	0.12
(1,662)	1:102:A:PHE:HB3	1:105:A:ASN:HD21	17	0.12
(1,658)	1:102:A:PHE:HA	1:105:A:ASN:HD22	10	0.12
(1,645)	1:101:A:ASN:HD22	1:101:A:ASN:H	12	0.12
(1,627)	1:72:A:ASP:HA	1:57:A:GLN:HE22	4	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,627)	1:72:A:ASP:HA	1:57:A:GLN:HE22	10	0.12
(1,613)	1:28:A:CYS:HA	1:14:A:GLN:HE22	1	0.12
(1,607)	1:11:A:ASN:HB2	1:11:A:ASN:HD21	18	0.12
(1,607)	1:11:A:ASN:HB3	1:11:A:ASN:HD21	18	0.12
(1,602)	1:32:A:SER:HB2	1:11:A:ASN:HD21	5	0.12
(1,602)	1:32:A:SER:HB3	1:11:A:ASN:HD21	5	0.12
(1,601)	1:11:A:ASN:H	1:11:A:ASN:HD22	2	0.12
(1,596)	1:74:A:GLY:HA2	1:69:A:ASN:HD21	19	0.12
(1,596)	1:74:A:GLY:HA3	1:69:A:ASN:HD21	19	0.12
(1,591)	1:69:A:ASN:HB2	1:69:A:ASN:HD21	9	0.12
(1,591)	1:69:A:ASN:HB3	1:69:A:ASN:HD21	9	0.12
(1,591)	1:69:A:ASN:HB2	1:69:A:ASN:HD21	13	0.12
(1,591)	1:69:A:ASN:HB3	1:69:A:ASN:HD21	13	0.12
(1,588)	1:12:A:ASN:HA	1:13:A:GLY:H	17	0.12
(1,574)	1:64:A:ARG:H	1:65:A:CYS:H	1	0.12
(1,574)	1:64:A:ARG:H	1:65:A:CYS:H	11	0.12
(1,574)	1:64:A:ARG:H	1:65:A:CYS:H	16	0.12
(1,560)	1:90:A:PHE:H	1:99:A:SER:H	4	0.12
(1,553)	1:115:A:ASP:HB2	1:104:A:CYS:H	19	0.12
(1,553)	1:115:A:ASP:HB3	1:104:A:CYS:H	19	0.12
(1,551)	1:104:A:CYS:HB2	1:104:A:CYS:H	4	0.12
(1,551)	1:104:A:CYS:HB3	1:104:A:CYS:H	4	0.12
(1,551)	1:104:A:CYS:HB2	1:104:A:CYS:H	7	0.12
(1,551)	1:104:A:CYS:HB3	1:104:A:CYS:H	7	0.12
(1,551)	1:104:A:CYS:HB2	1:104:A:CYS:H	8	0.12
(1,551)	1:104:A:CYS:HB3	1:104:A:CYS:H	8	0.12
(1,551)	1:104:A:CYS:HB2	1:104:A:CYS:H	12	0.12
(1,551)	1:104:A:CYS:HB3	1:104:A:CYS:H	12	0.12
(1,551)	1:104:A:CYS:HB2	1:104:A:CYS:H	14	0.12
(1,551)	1:104:A:CYS:HB3	1:104:A:CYS:H	14	0.12
(1,551)	1:104:A:CYS:HB2	1:104:A:CYS:H	16	0.12
(1,551)	1:104:A:CYS:HB3	1:104:A:CYS:H	16	0.12
(1,551)	1:104:A:CYS:HB2	1:104:A:CYS:H	20	0.12
(1,551)	1:104:A:CYS:HB3	1:104:A:CYS:H	20	0.12
(1,550)	1:104:A:CYS:HB2	1:104:A:CYS:H	4	0.12
(1,550)	1:104:A:CYS:HB3	1:104:A:CYS:H	4	0.12
(1,550)	1:104:A:CYS:HB2	1:104:A:CYS:H	7	0.12
(1,550)	1:104:A:CYS:HB3	1:104:A:CYS:H	7	0.12
(1,550)	1:104:A:CYS:HB2	1:104:A:CYS:H	8	0.12
(1,550)	1:104:A:CYS:HB3	1:104:A:CYS:H	8	0.12
(1,550)	1:104:A:CYS:HB2	1:104:A:CYS:H	12	0.12
(1,550)	1:104:A:CYS:HB3	1:104:A:CYS:H	12	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,550)	1:104:A:CYS:HB2	1:104:A:CYS:H	14	0.12
(1,550)	1:104:A:CYS:HB3	1:104:A:CYS:H	14	0.12
(1,550)	1:104:A:CYS:HB2	1:104:A:CYS:H	16	0.12
(1,550)	1:104:A:CYS:HB3	1:104:A:CYS:H	16	0.12
(1,550)	1:104:A:CYS:HB2	1:104:A:CYS:H	20	0.12
(1,550)	1:104:A:CYS:HB3	1:104:A:CYS:H	20	0.12
(1,542)	1:112:A:ASP:H	1:114:A:SER:H	10	0.12
(1,536)	1:89:A:GLU:HB2	1:86:A:SER:H	3	0.12
(1,536)	1:89:A:GLU:HB3	1:86:A:SER:H	3	0.12
(1,536)	1:89:A:GLU:HB2	1:86:A:SER:H	19	0.12
(1,536)	1:89:A:GLU:HB3	1:86:A:SER:H	19	0.12
(1,527)	1:67:A:GLY:HA2	1:67:A:GLY:H	6	0.12
(1,527)	1:67:A:GLY:HA3	1:67:A:GLY:H	6	0.12
(1,518)	1:49:A:ILE:H	1:61:A:VAL:H	18	0.12
(1,510)	1:48:A:GLU:HB2	1:48:A:GLU:H	17	0.12
(1,510)	1:48:A:GLU:HB3	1:48:A:GLU:H	17	0.12
(1,496)	1:31:A:GLY:HA2	1:31:A:GLY:H	1	0.12
(1,496)	1:31:A:GLY:HA3	1:31:A:GLY:H	1	0.12
(1,496)	1:31:A:GLY:HA2	1:31:A:GLY:H	2	0.12
(1,496)	1:31:A:GLY:HA3	1:31:A:GLY:H	2	0.12
(1,496)	1:31:A:GLY:HA2	1:31:A:GLY:H	9	0.12
(1,496)	1:31:A:GLY:HA3	1:31:A:GLY:H	9	0.12
(1,483)	1:10:A:CYS:HB2	1:14:A:GLN:H	12	0.12
(1,483)	1:10:A:CYS:HB3	1:14:A:GLN:H	12	0.12
(1,482)	1:11:A:ASN:HD21	1:11:A:ASN:H	2	0.12
(1,482)	1:11:A:ASN:HD21	1:11:A:ASN:H	4	0.12
(1,477)	1:9:A:VAL:HA	1:9:A:VAL:H	8	0.12
(1,477)	1:9:A:VAL:HA	1:9:A:VAL:H	14	0.12
(1,476)	1:7:A:ASP:H	1:3:A:CYS:HB2	7	0.12
(1,476)	1:7:A:ASP:H	1:3:A:CYS:HB3	7	0.12
(1,475)	1:75:A:GLU:H	1:76:A:ASP:H	17	0.12
(1,473)	1:85:A:CYS:H	1:86:A:SER:H	4	0.12
(1,473)	1:85:A:CYS:H	1:86:A:SER:H	16	0.12
(1,470)	1:79:A:ASN:HB2	1:79:A:ASN:H	14	0.12
(1,470)	1:79:A:ASN:HB3	1:79:A:ASN:H	14	0.12
(1,466)	1:80:A:CYS:HA	1:79:A:ASN:H	20	0.12
(1,463)	1:71:A:CYS:HB2	1:78:A:GLU:H	7	0.12
(1,463)	1:71:A:CYS:HB3	1:78:A:GLU:H	7	0.12
(1,454)	1:78:A:GLU:HG2	1:76:A:ASP:H	18	0.12
(1,454)	1:78:A:GLU:HG3	1:76:A:ASP:H	18	0.12
(1,451)	1:75:A:GLU:H	1:76:A:ASP:H	17	0.12
(1,444)	1:76:A:ASP:H	1:74:A:GLY:H	1	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,444)	1:76:A:ASP:H	1:74:A:GLY:H	9	0.12
(1,444)	1:76:A:ASP:H	1:74:A:GLY:H	14	0.12
(1,444)	1:76:A:ASP:H	1:74:A:GLY:H	18	0.12
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB2	18	0.12
(1,443)	1:73:A:SER:H	1:71:A:CYS:HB3	18	0.12
(1,437)	1:72:A:ASP:H	1:71:A:CYS:H	3	0.12
(1,435)	1:72:A:ASP:HA	1:72:A:ASP:H	2	0.12
(1,433)	1:74:A:GLY:HA2	1:71:A:CYS:H	8	0.12
(1,433)	1:74:A:GLY:HA3	1:71:A:CYS:H	8	0.12
(1,432)	1:70:A:ASP:HB2	1:70:A:ASP:H	3	0.12
(1,432)	1:70:A:ASP:HB3	1:70:A:ASP:H	3	0.12
(1,432)	1:70:A:ASP:HB2	1:70:A:ASP:H	9	0.12
(1,432)	1:70:A:ASP:HB3	1:70:A:ASP:H	9	0.12
(1,431)	1:72:A:ASP:H	1:70:A:ASP:H	7	0.12
(1,424)	1:68:A:GLU:HA	1:67:A:GLY:H	6	0.12
(1,419)	1:65:A:CYS:HB2	1:66:A:ASP:H	12	0.12
(1,419)	1:65:A:CYS:HB3	1:66:A:ASP:H	12	0.12
(1,418)	1:64:A:ARG:HA	1:66:A:ASP:H	18	0.12
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB2	8	0.12
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB3	8	0.12
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB2	17	0.12
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB3	17	0.12
(1,409)	1:60:A:PRO:HA	1:61:A:VAL:H	4	0.12
(1,392)	1:52:A:GLY:HA2	1:53:A:ALA:H	8	0.12
(1,392)	1:52:A:GLY:HA3	1:53:A:ALA:H	8	0.12
(1,387)	1:51:A:CYS:H	1:51:A:CYS:HB2	10	0.12
(1,387)	1:51:A:CYS:H	1:51:A:CYS:HB3	10	0.12
(1,383)	1:51:A:CYS:H	1:50:A:SER:HA	5	0.12
(1,383)	1:51:A:CYS:H	1:50:A:SER:HA	11	0.12
(1,383)	1:51:A:CYS:H	1:50:A:SER:HA	16	0.12
(1,374)	1:61:A:VAL:H	1:49:A:ILE:H	1	0.12
(1,372)	1:48:A:GLU:H	1:48:A:GLU:HA	3	0.12
(1,372)	1:48:A:GLU:H	1:48:A:GLU:HA	16	0.12
(1,369)	1:43:A:THR:HB	1:44:A:CYS:H	4	0.12
(1,369)	1:43:A:THR:HB	1:44:A:CYS:H	12	0.12
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB2	20	0.12
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB3	20	0.12
(1,357)	1:40:A:HIS:H	1:39:A:CYS:HA	1	0.12
(1,357)	1:40:A:HIS:H	1:39:A:CYS:HA	3	0.12
(1,357)	1:40:A:HIS:H	1:39:A:CYS:HA	5	0.12
(1,357)	1:40:A:HIS:H	1:39:A:CYS:HA	17	0.12
(1,357)	1:40:A:HIS:H	1:39:A:CYS:HA	18	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,350)	1:31:A:GLY:H	1:32:A:SER:H	13	0.12
(1,350)	1:31:A:GLY:H	1:32:A:SER:H	16	0.12
(1,350)	1:31:A:GLY:H	1:32:A:SER:H	20	0.12
(1,347)	1:31:A:GLY:H	1:28:A:CYS:H	12	0.12
(1,335)	1:45:A:ARG:HD2	1:24:A:GLY:H	4	0.12
(1,335)	1:45:A:ARG:HD3	1:24:A:GLY:H	4	0.12
(1,315)	1:15:A:CYS:H	1:15:A:CYS:HB2	11	0.12
(1,315)	1:15:A:CYS:H	1:15:A:CYS:HB3	11	0.12
(1,313)	1:14:A:GLN:HG2	1:14:A:GLN:H	9	0.12
(1,313)	1:14:A:GLN:HG3	1:14:A:GLN:H	9	0.12
(1,313)	1:14:A:GLN:HG2	1:14:A:GLN:H	19	0.12
(1,313)	1:14:A:GLN:HG3	1:14:A:GLN:H	19	0.12
(1,312)	1:14:A:GLN:HG2	1:14:A:GLN:H	1	0.12
(1,312)	1:14:A:GLN:HG3	1:14:A:GLN:H	1	0.12
(1,308)	1:13:A:GLY:H	1:14:A:GLN:H	12	0.12
(1,308)	1:13:A:GLY:H	1:14:A:GLN:H	19	0.12
(1,308)	1:13:A:GLY:H	1:14:A:GLN:H	20	0.12
(1,302)	1:14:A:GLN:H	1:12:A:ASN:H	5	0.12
(1,302)	1:14:A:GLN:H	1:12:A:ASN:H	8	0.12
(1,302)	1:14:A:GLN:H	1:12:A:ASN:H	12	0.12
(1,299)	1:11:A:ASN:H	1:12:A:ASN:H	5	0.12
(1,295)	1:15:A:CYS:HA	1:10:A:CYS:H	19	0.12
(1,279)	1:6:A:SER:HB2	1:6:A:SER:H	1	0.12
(1,279)	1:6:A:SER:HB3	1:6:A:SER:H	1	0.12
(1,279)	1:6:A:SER:HB2	1:6:A:SER:H	2	0.12
(1,279)	1:6:A:SER:HB3	1:6:A:SER:H	2	0.12
(1,279)	1:6:A:SER:HB2	1:6:A:SER:H	3	0.12
(1,279)	1:6:A:SER:HB3	1:6:A:SER:H	3	0.12
(1,279)	1:6:A:SER:HB2	1:6:A:SER:H	4	0.12
(1,279)	1:6:A:SER:HB3	1:6:A:SER:H	4	0.12
(1,279)	1:6:A:SER:HB2	1:6:A:SER:H	9	0.12
(1,279)	1:6:A:SER:HB3	1:6:A:SER:H	9	0.12
(1,277)	1:6:A:SER:HB2	1:6:A:SER:H	1	0.12
(1,277)	1:6:A:SER:HB3	1:6:A:SER:H	1	0.12
(1,277)	1:6:A:SER:HB2	1:6:A:SER:H	2	0.12
(1,277)	1:6:A:SER:HB3	1:6:A:SER:H	2	0.12
(1,277)	1:6:A:SER:HB2	1:6:A:SER:H	3	0.12
(1,277)	1:6:A:SER:HB3	1:6:A:SER:H	3	0.12
(1,277)	1:6:A:SER:HB2	1:6:A:SER:H	4	0.12
(1,277)	1:6:A:SER:HB3	1:6:A:SER:H	4	0.12
(1,277)	1:6:A:SER:HB2	1:6:A:SER:H	9	0.12
(1,277)	1:6:A:SER:HB3	1:6:A:SER:H	9	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	13	0.12
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	13	0.12
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	13	0.12
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	13	0.12
(1,248)	1:83:A:ILE:HB	1:84:A:THR:H	19	0.12
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD11	3	0.12
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD12	3	0.12
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD13	3	0.12
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD11	13	0.12
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD12	13	0.12
(1,240)	1:90:A:PHE:H	1:98:A:ILE:HD13	13	0.12
(1,237)	1:89:A:GLU:HB2	1:90:A:PHE:H	5	0.12
(1,237)	1:89:A:GLU:HB3	1:90:A:PHE:H	5	0.12
(1,220)	1:92:A:CYS:HB2	1:95:A:GLY:H	1	0.12
(1,220)	1:92:A:CYS:HB3	1:95:A:GLY:H	1	0.12
(1,220)	1:92:A:CYS:HB2	1:95:A:GLY:H	2	0.12
(1,220)	1:92:A:CYS:HB3	1:95:A:GLY:H	2	0.12
(1,209)	1:97:A:CYS:HB2	1:97:A:CYS:H	1	0.12
(1,209)	1:97:A:CYS:HB3	1:97:A:CYS:H	1	0.12
(1,204)	1:98:A:ILE:HG12	1:98:A:ILE:H	19	0.12
(1,204)	1:98:A:ILE:HG13	1:98:A:ILE:H	19	0.12
(1,203)	1:89:A:GLU:HB2	1:98:A:ILE:H	14	0.12
(1,203)	1:89:A:GLU:HB3	1:98:A:ILE:H	14	0.12
(1,202)	1:97:A:CYS:HB2	1:98:A:ILE:H	15	0.12
(1,202)	1:97:A:CYS:HB3	1:98:A:ILE:H	15	0.12
(1,196)	1:98:A:ILE:HA	1:99:A:SER:H	10	0.12
(1,190)	1:101:A:ASN:HB2	1:101:A:ASN:H	5	0.12
(1,190)	1:101:A:ASN:HB3	1:101:A:ASN:H	5	0.12
(1,187)	1:103:A:VAL:HG11	1:102:A:PHE:H	5	0.12
(1,187)	1:103:A:VAL:HG12	1:102:A:PHE:H	5	0.12
(1,187)	1:103:A:VAL:HG13	1:102:A:PHE:H	5	0.12
(1,187)	1:103:A:VAL:HG21	1:102:A:PHE:H	5	0.12
(1,187)	1:103:A:VAL:HG22	1:102:A:PHE:H	5	0.12
(1,187)	1:103:A:VAL:HG23	1:102:A:PHE:H	5	0.12
(1,184)	1:103:A:VAL:HB	1:102:A:PHE:H	5	0.12
(1,165)	1:104:A:CYS:H	1:116:A:GLU:HA	4	0.12
(1,137)	1:109:A:ASP:H	1:113:A:GLY:HA2	1	0.12
(1,137)	1:109:A:ASP:H	1:113:A:GLY:HA3	1	0.12
(1,125)	1:114:A:SER:H	1:113:A:GLY:HA2	11	0.12
(1,125)	1:114:A:SER:H	1:113:A:GLY:HA3	11	0.12
(1,125)	1:114:A:SER:H	1:113:A:GLY:HA2	13	0.12
(1,125)	1:114:A:SER:H	1:113:A:GLY:HA3	13	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,124)	1:117:A:LEU:HB2	1:115:A:ASP:H	1	0.12
(1,124)	1:117:A:LEU:HB3	1:115:A:ASP:H	1	0.12
(1,121)	1:114:A:SER:HA	1:115:A:ASP:H	13	0.12
(1,121)	1:114:A:SER:HA	1:115:A:ASP:H	15	0.12
(1,121)	1:114:A:SER:HA	1:115:A:ASP:H	20	0.12
(1,116)	1:116:A:GLU:HG2	1:116:A:GLU:H	1	0.12
(1,116)	1:116:A:GLU:HG3	1:116:A:GLU:H	1	0.12
(1,116)	1:116:A:GLU:HG2	1:116:A:GLU:H	3	0.12
(1,116)	1:116:A:GLU:HG3	1:116:A:GLU:H	3	0.12
(1,116)	1:116:A:GLU:HG2	1:116:A:GLU:H	8	0.12
(1,116)	1:116:A:GLU:HG3	1:116:A:GLU:H	8	0.12
(1,96)	1:100:A:ARG:H	1:89:A:GLU:HA	2	0.12
(1,94)	1:120:A:ALA:H	1:119:A:CYS:HB2	1	0.12
(1,94)	1:120:A:ALA:H	1:119:A:CYS:HB3	1	0.12
(1,69)	1:78:A:GLU:HG2	1:78:A:GLU:H	4	0.12
(1,69)	1:78:A:GLU:HG3	1:78:A:GLU:H	4	0.12
(1,69)	1:78:A:GLU:HG2	1:78:A:GLU:H	7	0.12
(1,69)	1:78:A:GLU:HG3	1:78:A:GLU:H	7	0.12
(1,67)	1:19:A:ARG:H	1:18:A:SER:H	12	0.12
(1,42)	1:96:A:ARG:H	1:97:A:CYS:H	11	0.12
(1,41)	1:96:A:ARG:H	1:97:A:CYS:H	11	0.12
(1,9)	1:12:A:ASN:H	1:11:A:ASN:H	16	0.12
(1,9)	1:12:A:ASN:H	1:11:A:ASN:H	20	0.12
(1,7)	1:22:A:CYS:H	1:23:A:ASP:H	8	0.12
(1,7)	1:22:A:CYS:H	1:23:A:ASP:H	11	0.12
(1,7)	1:22:A:CYS:H	1:23:A:ASP:H	12	0.12
(1,7)	1:22:A:CYS:H	1:23:A:ASP:H	13	0.12
(1,1)	1:112:A:ASP:H	1:113:A:GLY:H	14	0.12
(4,6)	1:51:A:CYS:H	1:57:A:GLN:O	4	0.11
(4,5)	1:49:A:ILE:O	1:59:A:ILE:H	20	0.11
(3,11)	2:202:A:CA:CA	1:76:A:ASP:OD2	1	0.11
(2,385)	1:66:A:ASP:HA	1:68:A:GLU:H	5	0.11
(2,382)	1:72:A:ASP:HB2	1:73:A:SER:H	2	0.11
(2,382)	1:72:A:ASP:HB3	1:73:A:SER:H	2	0.11
(2,359)	1:98:A:ILE:HD12	1:98:A:ILE:H	13	0.11
(2,338)	1:97:A:CYS:H	1:98:A:ILE:H	14	0.11
(2,338)	1:99:A:SER:H	1:98:A:ILE:H	18	0.11
(2,338)	1:97:A:CYS:H	1:98:A:ILE:H	20	0.11
(2,288)	1:75:A:GLU:HB2	1:75:A:GLU:H	11	0.11
(2,288)	1:75:A:GLU:HB3	1:75:A:GLU:H	11	0.11
(2,287)	1:5:A:GLU:HB2	1:5:A:GLU:H	3	0.11
(2,287)	1:5:A:GLU:HB3	1:5:A:GLU:H	3	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,287)	1:5:A:GLU:HB2	1:5:A:GLU:H	19	0.11
(2,287)	1:5:A:GLU:HB3	1:5:A:GLU:H	19	0.11
(2,245)	1:36:A:PRO:HA	1:39:A:CYS:H	5	0.11
(2,245)	1:36:A:PRO:HA	1:39:A:CYS:H	13	0.11
(2,236)	1:21:A:LYS:HB2	1:21:A:LYS:H	20	0.11
(2,235)	1:86:A:SER:HA	1:85:A:CYS:H	5	0.11
(2,235)	1:80:A:CYS:HA	1:85:A:CYS:H	20	0.11
(2,233)	1:14:A:GLN:HB2	1:14:A:GLN:HE22	7	0.11
(2,233)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	7	0.11
(2,233)	1:14:A:GLN:HB2	1:14:A:GLN:HE22	8	0.11
(2,233)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	8	0.11
(2,233)	1:14:A:GLN:HB2	1:14:A:GLN:HE22	12	0.11
(2,233)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	12	0.11
(2,233)	1:14:A:GLN:HB2	1:14:A:GLN:HE22	16	0.11
(2,233)	1:14:A:GLN:HB3	1:14:A:GLN:HE22	16	0.11
(2,232)	1:51:A:CYS:H	1:59:A:ILE:H	18	0.11
(2,226)	1:92:A:CYS:H	1:97:A:CYS:H	4	0.11
(2,226)	1:98:A:ILE:H	1:97:A:CYS:H	14	0.11
(2,226)	1:98:A:ILE:H	1:97:A:CYS:H	18	0.11
(2,226)	1:98:A:ILE:H	1:97:A:CYS:H	20	0.11
(2,222)	1:24:A:GLY:HA3	1:45:A:ARG:H	10	0.11
(2,188)	1:16:A:VAL:HG11	1:19:A:ARG:H	12	0.11
(2,188)	1:16:A:VAL:HG12	1:19:A:ARG:H	12	0.11
(2,188)	1:16:A:VAL:HG13	1:19:A:ARG:H	12	0.11
(2,188)	1:16:A:VAL:HG21	1:19:A:ARG:H	12	0.11
(2,188)	1:16:A:VAL:HG22	1:19:A:ARG:H	12	0.11
(2,188)	1:16:A:VAL:HG23	1:19:A:ARG:H	12	0.11
(2,188)	1:16:A:VAL:HG11	1:19:A:ARG:H	14	0.11
(2,188)	1:16:A:VAL:HG12	1:19:A:ARG:H	14	0.11
(2,188)	1:16:A:VAL:HG13	1:19:A:ARG:H	14	0.11
(2,188)	1:16:A:VAL:HG21	1:19:A:ARG:H	14	0.11
(2,188)	1:16:A:VAL:HG22	1:19:A:ARG:H	14	0.11
(2,188)	1:16:A:VAL:HG23	1:19:A:ARG:H	14	0.11
(2,179)	1:9:A:VAL:HG11	1:10:A:CYS:H	1	0.11
(2,179)	1:9:A:VAL:HG12	1:10:A:CYS:H	1	0.11
(2,179)	1:9:A:VAL:HG13	1:10:A:CYS:H	1	0.11
(2,179)	1:9:A:VAL:HG21	1:10:A:CYS:H	1	0.11
(2,179)	1:9:A:VAL:HG22	1:10:A:CYS:H	1	0.11
(2,179)	1:9:A:VAL:HG23	1:10:A:CYS:H	1	0.11
(2,173)	1:69:A:ASN:HD21	1:69:A:ASN:H	15	0.11
(2,171)	1:86:A:SER:HB2	1:86:A:SER:H	16	0.11
(2,168)	1:38:A:GLN:HG3	1:38:A:GLN:H	2	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,164)	1:14:A:GLN:HB2	1:14:A:GLN:H	18	0.11
(2,164)	1:14:A:GLN:HB3	1:14:A:GLN:H	18	0.11
(2,123)	1:16:A:VAL:HG11	1:33:A:ASP:H	17	0.11
(2,123)	1:16:A:VAL:HG12	1:33:A:ASP:H	17	0.11
(2,123)	1:16:A:VAL:HG13	1:33:A:ASP:H	17	0.11
(2,123)	1:16:A:VAL:HG21	1:33:A:ASP:H	17	0.11
(2,123)	1:16:A:VAL:HG22	1:33:A:ASP:H	17	0.11
(2,123)	1:16:A:VAL:HG23	1:33:A:ASP:H	17	0.11
(2,122)	1:16:A:VAL:HA	1:16:A:VAL:H	4	0.11
(2,122)	1:16:A:VAL:HA	1:16:A:VAL:H	20	0.11
(2,117)	1:14:A:GLN:HB2	1:12:A:ASN:HD21	6	0.11
(2,117)	1:14:A:GLN:HB3	1:12:A:ASN:HD21	6	0.11
(2,80)	1:41:A:MET:HA	1:56:A:THR:H	13	0.11
(2,75)	1:108:A:ASP:HA	1:108:A:ASP:H	19	0.11
(2,70)	1:19:A:ARG:HG3	1:18:A:SER:H	20	0.11
(2,61)	1:4:A:ALA:HA	1:5:A:GLU:H	10	0.11
(2,52)	1:60:A:PRO:HD2	1:63:A:TRP:HE1	1	0.11
(2,49)	1:35:A:SER:HB2	1:39:A:CYS:H	1	0.11
(2,49)	1:35:A:SER:HB3	1:39:A:CYS:H	8	0.11
(2,2)	1:32:A:SER:HB2	1:35:A:SER:H	13	0.11
(1,931)	1:99:A:SER:HB2	1:102:A:PHE:HD1	16	0.11
(1,931)	1:99:A:SER:HB2	1:102:A:PHE:HD2	16	0.11
(1,931)	1:99:A:SER:HB3	1:102:A:PHE:HD1	16	0.11
(1,931)	1:99:A:SER:HB3	1:102:A:PHE:HD2	16	0.11
(1,916)	1:77:A:GLU:HB2	1:77:A:GLU:H	5	0.11
(1,916)	1:77:A:GLU:HB3	1:77:A:GLU:H	5	0.11
(1,915)	1:51:A:CYS:HA	1:71:A:CYS:H	5	0.11
(1,911)	1:57:A:GLN:HE21	1:71:A:CYS:H	12	0.11
(1,906)	1:13:A:GLY:HA2	1:12:A:ASN:HD22	8	0.11
(1,906)	1:13:A:GLY:HA3	1:12:A:ASN:HD22	8	0.11
(1,906)	1:13:A:GLY:HA2	1:12:A:ASN:HD22	16	0.11
(1,906)	1:13:A:GLY:HA3	1:12:A:ASN:HD22	16	0.11
(1,905)	1:101:A:ASN:HD21	1:105:A:ASN:HD21	5	0.11
(1,905)	1:101:A:ASN:HD21	1:105:A:ASN:HD21	13	0.11
(1,897)	1:77:A:GLU:HB2	1:69:A:ASN:HD22	10	0.11
(1,897)	1:77:A:GLU:HB3	1:69:A:ASN:HD22	10	0.11
(1,895)	1:77:A:GLU:HG2	1:66:A:ASP:H	6	0.11
(1,895)	1:77:A:GLU:HG3	1:66:A:ASP:H	6	0.11
(1,894)	1:66:A:ASP:H	1:77:A:GLU:HG2	6	0.11
(1,894)	1:66:A:ASP:H	1:77:A:GLU:HG3	6	0.11
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB2	15	0.11
(1,891)	1:64:A:ARG:H	1:80:A:CYS:HB3	15	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,888)	1:49:A:ILE:HA	1:61:A:VAL:H	14	0.11
(1,884)	1:50:A:SER:H	1:59:A:ILE:H	5	0.11
(1,876)	1:39:A:CYS:HB2	1:43:A:THR:H	5	0.11
(1,876)	1:39:A:CYS:HB3	1:43:A:THR:H	5	0.11
(1,876)	1:39:A:CYS:HB2	1:43:A:THR:H	11	0.11
(1,876)	1:39:A:CYS:HB3	1:43:A:THR:H	11	0.11
(1,876)	1:39:A:CYS:HB2	1:43:A:THR:H	12	0.11
(1,876)	1:39:A:CYS:HB3	1:43:A:THR:H	12	0.11
(1,876)	1:39:A:CYS:HB2	1:43:A:THR:H	17	0.11
(1,876)	1:39:A:CYS:HB3	1:43:A:THR:H	17	0.11
(1,872)	1:32:A:SER:H	1:33:A:ASP:HB2	7	0.11
(1,872)	1:32:A:SER:H	1:33:A:ASP:HB3	7	0.11
(1,872)	1:32:A:SER:H	1:33:A:ASP:HB2	20	0.11
(1,872)	1:32:A:SER:H	1:33:A:ASP:HB3	20	0.11
(1,869)	1:14:A:GLN:HE22	1:28:A:CYS:H	2	0.11
(1,867)	1:34:A:GLU:HG2	1:24:A:GLY:H	7	0.11
(1,867)	1:34:A:GLU:HG3	1:24:A:GLY:H	7	0.11
(1,867)	1:34:A:GLU:HG2	1:24:A:GLY:H	13	0.11
(1,867)	1:34:A:GLU:HG3	1:24:A:GLY:H	13	0.11
(1,862)	1:21:A:LYS:HE2	1:19:A:ARG:H	11	0.11
(1,862)	1:21:A:LYS:HE3	1:19:A:ARG:H	11	0.11
(1,852)	1:14:A:GLN:HG2	1:12:A:ASN:H	18	0.11
(1,852)	1:14:A:GLN:HG3	1:12:A:ASN:H	18	0.11
(1,846)	1:38:A:GLN:HE21	1:9:A:VAL:H	4	0.11
(1,838)	1:58:A:CYS:HA	1:52:A:GLY:H	6	0.11
(1,838)	1:58:A:CYS:HA	1:52:A:GLY:H	12	0.11
(1,837)	1:50:A:SER:H	1:45:A:ARG:HD2	3	0.11
(1,837)	1:50:A:SER:H	1:45:A:ARG:HD3	3	0.11
(1,832)	1:35:A:SER:H	1:38:A:GLN:H	16	0.11
(1,832)	1:35:A:SER:H	1:38:A:GLN:H	19	0.11
(1,828)	1:85:A:CYS:HA	1:86:A:SER:H	8	0.11
(1,817)	1:112:A:ASP:HB2	1:114:A:SER:H	9	0.11
(1,817)	1:112:A:ASP:HB3	1:114:A:SER:H	9	0.11
(1,809)	1:106:A:GLY:H	1:104:A:CYS:H	12	0.11
(1,787)	1:73:A:SER:H	1:76:A:ASP:H	8	0.11
(1,787)	1:73:A:SER:H	1:76:A:ASP:H	14	0.11
(1,787)	1:73:A:SER:H	1:76:A:ASP:H	18	0.11
(1,784)	1:71:A:CYS:HB2	1:76:A:ASP:H	13	0.11
(1,784)	1:71:A:CYS:HB3	1:76:A:ASP:H	13	0.11
(1,781)	1:73:A:SER:H	1:71:A:CYS:HB2	3	0.11
(1,781)	1:73:A:SER:H	1:71:A:CYS:HB3	3	0.11
(1,781)	1:73:A:SER:H	1:71:A:CYS:HB2	5	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,781)	1:73:A:SER:H	1:71:A:CYS:HB3	5	0.11
(1,781)	1:73:A:SER:H	1:71:A:CYS:HB2	16	0.11
(1,781)	1:73:A:SER:H	1:71:A:CYS:HB3	16	0.11
(1,750)	1:57:A:GLN:HB2	1:52:A:GLY:H	6	0.11
(1,750)	1:57:A:GLN:HB2	1:52:A:GLY:H	6	0.11
(1,750)	1:57:A:GLN:HB3	1:52:A:GLY:H	6	0.11
(1,750)	1:57:A:GLN:HB3	1:52:A:GLY:H	6	0.11
(1,734)	1:32:A:SER:H	1:11:A:ASN:H	16	0.11
(1,731)	1:28:A:CYS:HB2	1:32:A:SER:H	4	0.11
(1,731)	1:28:A:CYS:HB3	1:32:A:SER:H	4	0.11
(1,726)	1:34:A:GLU:HG2	1:27:A:ASP:H	15	0.11
(1,726)	1:34:A:GLU:HG3	1:27:A:ASP:H	15	0.11
(1,726)	1:34:A:GLU:HG2	1:27:A:ASP:H	20	0.11
(1,726)	1:34:A:GLU:HG3	1:27:A:ASP:H	20	0.11
(1,719)	1:19:A:ARG:HH21	1:20:A:TRP:HE1	13	0.11
(1,717)	1:20:A:TRP:HE1	1:20:A:TRP:H	15	0.11
(1,716)	1:28:A:CYS:HB2	1:14:A:GLN:HE22	3	0.11
(1,716)	1:28:A:CYS:HB3	1:14:A:GLN:HE22	3	0.11
(1,712)	1:32:A:SER:H	1:11:A:ASN:H	16	0.11
(1,709)	1:45:A:ARG:HD2	1:45:A:ARG:H	19	0.11
(1,709)	1:45:A:ARG:HD3	1:45:A:ARG:H	19	0.11
(1,708)	1:44:A:CYS:HB2	1:45:A:ARG:H	20	0.11
(1,708)	1:44:A:CYS:HB3	1:45:A:ARG:H	20	0.11
(1,707)	1:45:A:ARG:HD2	1:45:A:ARG:H	19	0.11
(1,707)	1:45:A:ARG:HD3	1:45:A:ARG:H	19	0.11
(1,696)	1:44:A:CYS:HB2	1:34:A:GLU:H	8	0.11
(1,696)	1:44:A:CYS:HB3	1:34:A:GLU:H	8	0.11
(1,689)	1:69:A:ASN:HD21	1:69:A:ASN:H	15	0.11
(1,682)	1:79:A:ASN:HD22	1:87:A:PRO:HD2	8	0.11
(1,682)	1:79:A:ASN:HD22	1:87:A:PRO:HD3	8	0.11
(1,680)	1:79:A:ASN:HD22	1:79:A:ASN:HB2	13	0.11
(1,680)	1:79:A:ASN:HD22	1:79:A:ASN:HB3	13	0.11
(1,673)	1:17:A:PRO:HB2	1:20:A:TRP:HE1	11	0.11
(1,673)	1:17:A:PRO:HB3	1:20:A:TRP:HE1	11	0.11
(1,662)	1:102:A:PHE:HB2	1:105:A:ASN:HD21	3	0.11
(1,662)	1:102:A:PHE:HB3	1:105:A:ASN:HD21	3	0.11
(1,662)	1:102:A:PHE:HB2	1:105:A:ASN:HD21	4	0.11
(1,662)	1:102:A:PHE:HB3	1:105:A:ASN:HD21	4	0.11
(1,658)	1:102:A:PHE:HA	1:105:A:ASN:HD22	13	0.11
(1,652)	1:101:A:ASN:HD21	1:101:A:ASN:HB2	6	0.11
(1,652)	1:101:A:ASN:HD21	1:101:A:ASN:HB3	6	0.11
(1,652)	1:101:A:ASN:HD21	1:101:A:ASN:HB2	17	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,652)	1:101:A:ASN:HD21	1:101:A:ASN:HB3	17	0.11
(1,645)	1:101:A:ASN:HD22	1:101:A:ASN:H	15	0.11
(1,631)	1:79:A:ASN:HD22	1:79:A:ASN:H	16	0.11
(1,631)	1:79:A:ASN:HD22	1:79:A:ASN:H	19	0.11
(1,627)	1:72:A:ASP:HA	1:57:A:GLN:HE22	3	0.11
(1,627)	1:72:A:ASP:HA	1:57:A:GLN:HE22	6	0.11
(1,626)	1:71:A:CYS:HA	1:57:A:GLN:HE22	10	0.11
(1,623)	1:30:A:ASP:HB2	1:12:A:ASN:HD22	18	0.11
(1,623)	1:30:A:ASP:HB3	1:12:A:ASN:HD22	18	0.11
(1,607)	1:11:A:ASN:HB2	1:11:A:ASN:HD21	3	0.11
(1,607)	1:11:A:ASN:HB3	1:11:A:ASN:HD21	3	0.11
(1,600)	1:11:A:ASN:H	1:11:A:ASN:HD21	8	0.11
(1,600)	1:11:A:ASN:H	1:11:A:ASN:HD21	20	0.11
(1,598)	1:74:A:GLY:HA2	1:69:A:ASN:HD22	15	0.11
(1,598)	1:74:A:GLY:HA3	1:69:A:ASN:HD22	15	0.11
(1,597)	1:74:A:GLY:HA2	1:69:A:ASN:HD22	15	0.11
(1,597)	1:74:A:GLY:HA3	1:69:A:ASN:HD22	15	0.11
(1,588)	1:12:A:ASN:HA	1:13:A:GLY:H	12	0.11
(1,580)	1:48:A:GLU:HG2	1:49:A:ILE:H	18	0.11
(1,580)	1:48:A:GLU:HG3	1:49:A:ILE:H	18	0.11
(1,571)	1:85:A:CYS:HB2	1:85:A:CYS:H	16	0.11
(1,571)	1:85:A:CYS:HB3	1:85:A:CYS:H	16	0.11
(1,551)	1:104:A:CYS:HB2	1:104:A:CYS:H	10	0.11
(1,551)	1:104:A:CYS:HB3	1:104:A:CYS:H	10	0.11
(1,550)	1:104:A:CYS:HB2	1:104:A:CYS:H	10	0.11
(1,550)	1:104:A:CYS:HB3	1:104:A:CYS:H	10	0.11
(1,541)	1:115:A:ASP:HB2	1:116:A:GLU:H	19	0.11
(1,541)	1:115:A:ASP:HB3	1:116:A:GLU:H	19	0.11
(1,534)	1:77:A:GLU:HB2	1:77:A:GLU:H	7	0.11
(1,534)	1:77:A:GLU:HB3	1:77:A:GLU:H	7	0.11
(1,527)	1:67:A:GLY:HA2	1:67:A:GLY:H	2	0.11
(1,527)	1:67:A:GLY:HA3	1:67:A:GLY:H	2	0.11
(1,527)	1:67:A:GLY:HA2	1:67:A:GLY:H	3	0.11
(1,527)	1:67:A:GLY:HA3	1:67:A:GLY:H	3	0.11
(1,527)	1:67:A:GLY:HA2	1:67:A:GLY:H	13	0.11
(1,527)	1:67:A:GLY:HA3	1:67:A:GLY:H	13	0.11
(1,527)	1:67:A:GLY:HA2	1:67:A:GLY:H	20	0.11
(1,527)	1:67:A:GLY:HA3	1:67:A:GLY:H	20	0.11
(1,512)	1:59:A:ILE:H	1:49:A:ILE:H	1	0.11
(1,501)	1:34:A:GLU:HB2	1:34:A:GLU:H	12	0.11
(1,501)	1:34:A:GLU:HB3	1:34:A:GLU:H	12	0.11
(1,496)	1:31:A:GLY:HA2	1:31:A:GLY:H	6	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,496)	1:31:A:GLY:HA3	1:31:A:GLY:H	6	0.11
(1,495)	1:31:A:GLY:H	1:29:A:GLU:H	20	0.11
(1,479)	1:9:A:VAL:HG11	1:9:A:VAL:H	3	0.11
(1,479)	1:9:A:VAL:HG12	1:9:A:VAL:H	3	0.11
(1,479)	1:9:A:VAL:HG13	1:9:A:VAL:H	3	0.11
(1,479)	1:9:A:VAL:HG21	1:9:A:VAL:H	3	0.11
(1,479)	1:9:A:VAL:HG22	1:9:A:VAL:H	3	0.11
(1,479)	1:9:A:VAL:HG23	1:9:A:VAL:H	3	0.11
(1,478)	1:9:A:VAL:HB	1:9:A:VAL:H	15	0.11
(1,477)	1:9:A:VAL:HA	1:9:A:VAL:H	15	0.11
(1,475)	1:75:A:GLU:H	1:76:A:ASP:H	11	0.11
(1,462)	1:79:A:ASN:H	1:78:A:GLU:H	13	0.11
(1,461)	1:76:A:ASP:H	1:78:A:GLU:H	8	0.11
(1,451)	1:75:A:GLU:H	1:76:A:ASP:H	11	0.11
(1,446)	1:73:A:SER:H	1:74:A:GLY:H	18	0.11
(1,437)	1:72:A:ASP:H	1:71:A:CYS:H	1	0.11
(1,437)	1:72:A:ASP:H	1:71:A:CYS:H	5	0.11
(1,435)	1:72:A:ASP:HA	1:72:A:ASP:H	10	0.11
(1,435)	1:72:A:ASP:HA	1:72:A:ASP:H	14	0.11
(1,435)	1:72:A:ASP:HA	1:72:A:ASP:H	18	0.11
(1,431)	1:72:A:ASP:H	1:70:A:ASP:H	20	0.11
(1,418)	1:64:A:ARG:HA	1:66:A:ASP:H	4	0.11
(1,418)	1:64:A:ARG:HA	1:66:A:ASP:H	6	0.11
(1,415)	1:64:A:ARG:HA	1:65:A:CYS:H	12	0.11
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB2	2	0.11
(1,414)	1:63:A:TRP:H	1:63:A:TRP:HB3	2	0.11
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB1	6	0.11
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB2	6	0.11
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB3	6	0.11
(1,392)	1:52:A:GLY:HA2	1:53:A:ALA:H	5	0.11
(1,392)	1:52:A:GLY:HA3	1:53:A:ALA:H	5	0.11
(1,392)	1:52:A:GLY:HA2	1:53:A:ALA:H	10	0.11
(1,392)	1:52:A:GLY:HA3	1:53:A:ALA:H	10	0.11
(1,392)	1:52:A:GLY:HA2	1:53:A:ALA:H	19	0.11
(1,392)	1:52:A:GLY:HA3	1:53:A:ALA:H	19	0.11
(1,392)	1:52:A:GLY:HA2	1:53:A:ALA:H	20	0.11
(1,392)	1:52:A:GLY:HA3	1:53:A:ALA:H	20	0.11
(1,390)	1:51:A:CYS:HB2	1:52:A:GLY:H	14	0.11
(1,390)	1:51:A:CYS:HB3	1:52:A:GLY:H	14	0.11
(1,387)	1:51:A:CYS:H	1:51:A:CYS:HB2	20	0.11
(1,387)	1:51:A:CYS:H	1:51:A:CYS:HB3	20	0.11
(1,383)	1:51:A:CYS:H	1:50:A:SER:HA	1	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,383)	1:51:A:CYS:H	1:50:A:SER:HA	2	0.11
(1,383)	1:51:A:CYS:H	1:50:A:SER:HA	3	0.11
(1,383)	1:51:A:CYS:H	1:50:A:SER:HA	7	0.11
(1,383)	1:51:A:CYS:H	1:50:A:SER:HA	13	0.11
(1,383)	1:51:A:CYS:H	1:50:A:SER:HA	17	0.11
(1,382)	1:51:A:CYS:H	1:59:A:ILE:H	18	0.11
(1,379)	1:50:A:SER:H	1:50:A:SER:HA	10	0.11
(1,378)	1:48:A:GLU:HG2	1:49:A:ILE:H	18	0.11
(1,378)	1:48:A:GLU:HG3	1:49:A:ILE:H	18	0.11
(1,377)	1:60:A:PRO:HA	1:49:A:ILE:H	8	0.11
(1,374)	1:61:A:VAL:H	1:49:A:ILE:H	17	0.11
(1,372)	1:48:A:GLU:H	1:48:A:GLU:HA	10	0.11
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB2	15	0.11
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB3	15	0.11
(1,357)	1:40:A:HIS:H	1:39:A:CYS:HA	7	0.11
(1,357)	1:40:A:HIS:H	1:39:A:CYS:HA	11	0.11
(1,357)	1:40:A:HIS:H	1:39:A:CYS:HA	13	0.11
(1,357)	1:40:A:HIS:H	1:39:A:CYS:HA	15	0.11
(1,352)	1:34:A:GLU:H	1:35:A:SER:HB2	9	0.11
(1,352)	1:34:A:GLU:H	1:35:A:SER:HB3	9	0.11
(1,351)	1:32:A:SER:H	1:33:A:ASP:H	8	0.11
(1,351)	1:32:A:SER:H	1:33:A:ASP:H	19	0.11
(1,349)	1:32:A:SER:H	1:33:A:ASP:H	8	0.11
(1,349)	1:32:A:SER:H	1:33:A:ASP:H	19	0.11
(1,345)	1:29:A:GLU:HB2	1:29:A:GLU:H	2	0.11
(1,345)	1:29:A:GLU:HB3	1:29:A:GLU:H	2	0.11
(1,343)	1:28:A:CYS:HB2	1:28:A:CYS:H	14	0.11
(1,343)	1:28:A:CYS:HB3	1:28:A:CYS:H	14	0.11
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB2	8	0.11
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB3	8	0.11
(1,317)	1:8:A:PHE:H	1:16:A:VAL:H	13	0.11
(1,315)	1:15:A:CYS:H	1:15:A:CYS:HB2	20	0.11
(1,315)	1:15:A:CYS:H	1:15:A:CYS:HB3	20	0.11
(1,313)	1:14:A:GLN:HG2	1:14:A:GLN:H	6	0.11
(1,313)	1:14:A:GLN:HG3	1:14:A:GLN:H	6	0.11
(1,313)	1:14:A:GLN:HG2	1:14:A:GLN:H	12	0.11
(1,313)	1:14:A:GLN:HG3	1:14:A:GLN:H	12	0.11
(1,308)	1:13:A:GLY:H	1:14:A:GLN:H	9	0.11
(1,308)	1:13:A:GLY:H	1:14:A:GLN:H	11	0.11
(1,295)	1:15:A:CYS:HA	1:10:A:CYS:H	18	0.11
(1,286)	1:7:A:ASP:HB2	1:7:A:ASP:H	8	0.11
(1,286)	1:7:A:ASP:HB3	1:7:A:ASP:H	8	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,286)	1:7:A:ASP:HB2	1:7:A:ASP:H	9	0.11
(1,286)	1:7:A:ASP:HB3	1:7:A:ASP:H	9	0.11
(1,286)	1:7:A:ASP:HB2	1:7:A:ASP:H	10	0.11
(1,286)	1:7:A:ASP:HB3	1:7:A:ASP:H	10	0.11
(1,286)	1:7:A:ASP:HB2	1:7:A:ASP:H	14	0.11
(1,286)	1:7:A:ASP:HB3	1:7:A:ASP:H	14	0.11
(1,279)	1:6:A:SER:HB2	1:6:A:SER:H	5	0.11
(1,279)	1:6:A:SER:HB3	1:6:A:SER:H	5	0.11
(1,277)	1:6:A:SER:HB2	1:6:A:SER:H	5	0.11
(1,277)	1:6:A:SER:HB3	1:6:A:SER:H	5	0.11
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	7	0.11
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	7	0.11
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	7	0.11
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	7	0.11
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	14	0.11
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	14	0.11
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	14	0.11
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	14	0.11
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	19	0.11
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	19	0.11
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	19	0.11
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	19	0.11
(1,248)	1:83:A:ILE:HB	1:84:A:THR:H	6	0.11
(1,247)	1:83:A:ILE:HA	1:84:A:THR:H	15	0.11
(1,228)	1:92:A:CYS:HB2	1:93:A:SER:H	18	0.11
(1,228)	1:92:A:CYS:HB3	1:93:A:SER:H	18	0.11
(1,225)	1:92:A:CYS:HB2	1:94:A:SER:H	10	0.11
(1,225)	1:92:A:CYS:HB3	1:94:A:SER:H	10	0.11
(1,220)	1:92:A:CYS:HB2	1:95:A:GLY:H	8	0.11
(1,220)	1:92:A:CYS:HB3	1:95:A:GLY:H	8	0.11
(1,215)	1:96:A:ARG:H	1:92:A:CYS:HB2	9	0.11
(1,215)	1:96:A:ARG:H	1:92:A:CYS:HB3	9	0.11
(1,204)	1:98:A:ILE:HG12	1:98:A:ILE:H	1	0.11
(1,204)	1:98:A:ILE:HG13	1:98:A:ILE:H	1	0.11
(1,204)	1:98:A:ILE:HG12	1:98:A:ILE:H	17	0.11
(1,204)	1:98:A:ILE:HG13	1:98:A:ILE:H	17	0.11
(1,187)	1:103:A:VAL:HG11	1:102:A:PHE:H	17	0.11
(1,187)	1:103:A:VAL:HG12	1:102:A:PHE:H	17	0.11
(1,187)	1:103:A:VAL:HG13	1:102:A:PHE:H	17	0.11
(1,187)	1:103:A:VAL:HG21	1:102:A:PHE:H	17	0.11
(1,187)	1:103:A:VAL:HG22	1:102:A:PHE:H	17	0.11
(1,187)	1:103:A:VAL:HG23	1:102:A:PHE:H	17	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,129)	1:114:A:SER:H	1:114:A:SER:HG	1	0.11
(1,128)	1:114:A:SER:HA	1:114:A:SER:H	14	0.11
(1,122)	1:115:A:ASP:HB2	1:115:A:ASP:H	4	0.11
(1,122)	1:115:A:ASP:HB3	1:115:A:ASP:H	4	0.11
(1,122)	1:115:A:ASP:HB2	1:115:A:ASP:H	7	0.11
(1,122)	1:115:A:ASP:HB3	1:115:A:ASP:H	7	0.11
(1,121)	1:114:A:SER:HA	1:115:A:ASP:H	12	0.11
(1,117)	1:116:A:GLU:HG2	1:116:A:GLU:H	5	0.11
(1,117)	1:116:A:GLU:HG3	1:116:A:GLU:H	5	0.11
(1,99)	1:98:A:ILE:HG12	1:99:A:SER:H	19	0.11
(1,99)	1:98:A:ILE:HG13	1:99:A:SER:H	19	0.11
(1,91)	1:14:A:GLN:HG2	1:15:A:CYS:H	2	0.11
(1,91)	1:14:A:GLN:HG3	1:15:A:CYS:H	2	0.11
(1,79)	1:61:A:VAL:HB	1:61:A:VAL:H	17	0.11
(1,74)	1:65:A:CYS:H	1:65:A:CYS:HB2	19	0.11
(1,74)	1:65:A:CYS:H	1:65:A:CYS:HB3	19	0.11
(1,67)	1:19:A:ARG:H	1:18:A:SER:H	4	0.11
(1,59)	1:65:A:CYS:H	1:66:A:ASP:H	8	0.11
(1,56)	1:70:A:ASP:H	1:71:A:CYS:H	11	0.11
(1,56)	1:70:A:ASP:H	1:71:A:CYS:H	13	0.11
(1,53)	1:77:A:GLU:H	1:76:A:ASP:H	8	0.11
(1,52)	1:76:A:ASP:H	1:77:A:GLU:H	8	0.11
(1,42)	1:96:A:ARG:H	1:97:A:CYS:H	13	0.11
(1,41)	1:96:A:ARG:H	1:97:A:CYS:H	13	0.11
(1,33)	1:115:A:ASP:H	1:114:A:SER:H	1	0.11
(1,33)	1:115:A:ASP:H	1:114:A:SER:H	10	0.11
(1,33)	1:115:A:ASP:H	1:114:A:SER:H	14	0.11
(1,15)	1:109:A:ASP:H	1:110:A:CYS:H	9	0.11
(1,9)	1:12:A:ASN:H	1:11:A:ASN:H	7	0.11
(1,7)	1:22:A:CYS:H	1:23:A:ASP:H	17	0.11
(3,11)	2:202:A:CA:CA	1:76:A:ASP:OD2	9	0.1
(3,10)	2:202:A:CA:CA	1:70:A:ASP:OD2	15	0.1
(3,7)	2:202:A:CA:CA	1:63:A:TRP:O	12	0.1
(2,362)	1:14:A:GLN:HB2	1:10:A:CYS:H	2	0.1
(2,362)	1:14:A:GLN:HB3	1:10:A:CYS:H	2	0.1
(2,313)	1:17:A:PRO:HB2	1:20:A:TRP:H	18	0.1
(2,288)	1:75:A:GLU:HB2	1:75:A:GLU:H	14	0.1
(2,288)	1:75:A:GLU:HB3	1:75:A:GLU:H	14	0.1
(2,280)	1:92:A:CYS:H	1:91:A:THR:H	16	0.1
(2,236)	1:21:A:LYS:HB2	1:21:A:LYS:H	3	0.1
(2,236)	1:21:A:LYS:HB2	1:21:A:LYS:H	7	0.1
(2,236)	1:21:A:LYS:HB2	1:21:A:LYS:H	17	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,236)	1:21:A:LYS:HB2	1:21:A:LYS:H	18	0.1
(2,236)	1:21:A:LYS:HB2	1:21:A:LYS:H	19	0.1
(2,191)	1:54:A:HIS:H	1:55:A:SER:H	18	0.1
(2,187)	1:118:A:ASP:HA	1:119:A:CYS:H	4	0.1
(2,123)	1:16:A:VAL:HG11	1:33:A:ASP:H	18	0.1
(2,123)	1:16:A:VAL:HG12	1:33:A:ASP:H	18	0.1
(2,123)	1:16:A:VAL:HG13	1:33:A:ASP:H	18	0.1
(2,123)	1:16:A:VAL:HG21	1:33:A:ASP:H	18	0.1
(2,123)	1:16:A:VAL:HG22	1:33:A:ASP:H	18	0.1
(2,123)	1:16:A:VAL:HG23	1:33:A:ASP:H	18	0.1
(2,122)	1:16:A:VAL:HA	1:16:A:VAL:H	9	0.1
(2,122)	1:16:A:VAL:HA	1:16:A:VAL:H	14	0.1
(2,117)	1:14:A:GLN:HB2	1:12:A:ASN:HD21	10	0.1
(2,117)	1:14:A:GLN:HB3	1:12:A:ASN:HD21	10	0.1
(2,115)	1:80:A:CYS:H	1:81:A:GLY:H	3	0.1
(2,112)	1:84:A:THR:HG1	1:84:A:THR:H	11	0.1
(2,111)	1:72:A:ASP:H	1:71:A:CYS:H	14	0.1
(2,61)	1:4:A:ALA:HA	1:5:A:GLU:H	16	0.1
(2,56)	1:114:A:SER:HA	1:117:A:LEU:H	12	0.1
(2,44)	1:83:A:ILE:HG22	1:97:A:CYS:H	18	0.1
(2,36)	1:83:A:ILE:H	1:82:A:ASN:H	8	0.1
(2,11)	1:109:A:ASP:HA	1:113:A:GLY:H	20	0.1
(2,8)	1:45:A:ARG:HA	1:46:A:ILE:H	12	0.1
(1,926)	1:16:A:VAL:HG11	1:20:A:TRP:HZ3	2	0.1
(1,926)	1:16:A:VAL:HG12	1:20:A:TRP:HZ3	2	0.1
(1,926)	1:16:A:VAL:HG13	1:20:A:TRP:HZ3	2	0.1
(1,906)	1:13:A:GLY:HA2	1:12:A:ASN:HD22	3	0.1
(1,906)	1:13:A:GLY:HA3	1:12:A:ASN:HD22	3	0.1
(1,906)	1:13:A:GLY:HA2	1:12:A:ASN:HD22	4	0.1
(1,906)	1:13:A:GLY:HA3	1:12:A:ASN:HD22	4	0.1
(1,906)	1:13:A:GLY:HA2	1:12:A:ASN:HD22	10	0.1
(1,906)	1:13:A:GLY:HA3	1:12:A:ASN:HD22	10	0.1
(1,906)	1:13:A:GLY:HA2	1:12:A:ASN:HD22	13	0.1
(1,906)	1:13:A:GLY:HA3	1:12:A:ASN:HD22	13	0.1
(1,897)	1:77:A:GLU:HB2	1:69:A:ASN:HD22	6	0.1
(1,897)	1:77:A:GLU:HB3	1:69:A:ASN:HD22	6	0.1
(1,895)	1:77:A:GLU:HG2	1:66:A:ASP:H	18	0.1
(1,895)	1:77:A:GLU:HG3	1:66:A:ASP:H	18	0.1
(1,894)	1:66:A:ASP:H	1:77:A:GLU:HG2	18	0.1
(1,894)	1:66:A:ASP:H	1:77:A:GLU:HG3	18	0.1
(1,878)	1:48:A:GLU:HB2	1:45:A:ARG:H	15	0.1
(1,878)	1:48:A:GLU:HB3	1:45:A:ARG:H	15	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,874)	1:35:A:SER:H	1:37:A:GLU:H	15	0.1
(1,872)	1:32:A:SER:H	1:33:A:ASP:HB2	4	0.1
(1,872)	1:32:A:SER:H	1:33:A:ASP:HB3	4	0.1
(1,869)	1:14:A:GLN:HE22	1:28:A:CYS:H	10	0.1
(1,864)	1:20:A:TRP:HA	1:20:A:TRP:HE1	17	0.1
(1,861)	1:17:A:PRO:HD2	1:19:A:ARG:H	16	0.1
(1,861)	1:17:A:PRO:HD3	1:19:A:ARG:H	16	0.1
(1,847)	1:13:A:GLY:H	1:10:A:CYS:H	16	0.1
(1,828)	1:85:A:CYS:HA	1:86:A:SER:H	11	0.1
(1,811)	1:107:A:GLN:H	1:105:A:ASN:HD21	5	0.1
(1,809)	1:106:A:GLY:H	1:104:A:CYS:H	16	0.1
(1,806)	1:101:A:ASN:HD21	1:102:A:PHE:H	15	0.1
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG21	2	0.1
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG22	2	0.1
(1,796)	1:96:A:ARG:H	1:83:A:ILE:HG23	2	0.1
(1,787)	1:73:A:SER:H	1:76:A:ASP:H	2	0.1
(1,751)	1:52:A:GLY:H	1:57:A:GLN:HG2	1	0.1
(1,751)	1:52:A:GLY:H	1:57:A:GLN:HG3	1	0.1
(1,734)	1:32:A:SER:H	1:11:A:ASN:H	14	0.1
(1,726)	1:34:A:GLU:HG2	1:27:A:ASP:H	4	0.1
(1,726)	1:34:A:GLU:HG3	1:27:A:ASP:H	4	0.1
(1,724)	1:34:A:GLU:HB2	1:25:A:ASP:H	16	0.1
(1,724)	1:34:A:GLU:HB3	1:25:A:ASP:H	16	0.1
(1,712)	1:32:A:SER:H	1:11:A:ASN:H	14	0.1
(1,684)	1:79:A:ASN:HD21	1:79:A:ASN:HB2	16	0.1
(1,684)	1:79:A:ASN:HD21	1:79:A:ASN:HB3	16	0.1
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD2	19	0.1
(1,681)	1:79:A:ASN:HD21	1:87:A:PRO:HD3	19	0.1
(1,680)	1:79:A:ASN:HD22	1:79:A:ASN:HB2	2	0.1
(1,680)	1:79:A:ASN:HD22	1:79:A:ASN:HB3	2	0.1
(1,662)	1:102:A:PHE:HB2	1:105:A:ASN:HD21	13	0.1
(1,662)	1:102:A:PHE:HB3	1:105:A:ASN:HD21	13	0.1
(1,658)	1:102:A:PHE:HA	1:105:A:ASN:HD22	11	0.1
(1,645)	1:101:A:ASN:HD22	1:101:A:ASN:H	16	0.1
(1,623)	1:30:A:ASP:HB2	1:12:A:ASN:HD22	5	0.1
(1,623)	1:30:A:ASP:HB3	1:12:A:ASN:HD22	5	0.1
(1,603)	1:32:A:SER:HB2	1:11:A:ASN:HD22	6	0.1
(1,603)	1:32:A:SER:HB3	1:11:A:ASN:HD22	6	0.1
(1,602)	1:32:A:SER:HB2	1:11:A:ASN:HD21	12	0.1
(1,602)	1:32:A:SER:HB3	1:11:A:ASN:HD21	12	0.1
(1,588)	1:12:A:ASN:HA	1:13:A:GLY:H	15	0.1
(1,586)	1:69:A:ASN:HA	1:64:A:ARG:H	1	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,586)	1:69:A:ASN:HA	1:64:A:ARG:H	9	0.1
(1,580)	1:48:A:GLU:HG2	1:49:A:ILE:H	9	0.1
(1,580)	1:48:A:GLU:HG3	1:49:A:ILE:H	9	0.1
(1,560)	1:90:A:PHE:H	1:99:A:SER:H	7	0.1
(1,547)	1:104:A:CYS:HB2	1:105:A:ASN:H	5	0.1
(1,547)	1:104:A:CYS:HB3	1:105:A:ASN:H	5	0.1
(1,541)	1:115:A:ASP:HB2	1:116:A:GLU:H	11	0.1
(1,541)	1:115:A:ASP:HB3	1:116:A:GLU:H	11	0.1
(1,527)	1:67:A:GLY:HA2	1:67:A:GLY:H	10	0.1
(1,527)	1:67:A:GLY:HA3	1:67:A:GLY:H	10	0.1
(1,527)	1:67:A:GLY:HA2	1:67:A:GLY:H	17	0.1
(1,527)	1:67:A:GLY:HA3	1:67:A:GLY:H	17	0.1
(1,524)	1:64:A:ARG:HB2	1:64:A:ARG:H	18	0.1
(1,524)	1:64:A:ARG:HB3	1:64:A:ARG:H	18	0.1
(1,519)	1:62:A:SER:H	1:61:A:VAL:H	4	0.1
(1,512)	1:59:A:ILE:H	1:49:A:ILE:H	17	0.1
(1,501)	1:34:A:GLU:HB2	1:34:A:GLU:H	1	0.1
(1,501)	1:34:A:GLU:HB3	1:34:A:GLU:H	1	0.1
(1,496)	1:31:A:GLY:HA2	1:31:A:GLY:H	5	0.1
(1,496)	1:31:A:GLY:HA3	1:31:A:GLY:H	5	0.1
(1,496)	1:31:A:GLY:HA2	1:31:A:GLY:H	8	0.1
(1,496)	1:31:A:GLY:HA3	1:31:A:GLY:H	8	0.1
(1,488)	1:20:A:TRP:HB2	1:20:A:TRP:H	16	0.1
(1,488)	1:20:A:TRP:HB3	1:20:A:TRP:H	16	0.1
(1,482)	1:11:A:ASN:HD21	1:11:A:ASN:H	19	0.1
(1,470)	1:79:A:ASN:HB2	1:79:A:ASN:H	4	0.1
(1,470)	1:79:A:ASN:HB3	1:79:A:ASN:H	4	0.1
(1,444)	1:76:A:ASP:H	1:74:A:GLY:H	2	0.1
(1,444)	1:76:A:ASP:H	1:74:A:GLY:H	10	0.1
(1,442)	1:73:A:SER:HB2	1:73:A:SER:H	19	0.1
(1,442)	1:73:A:SER:HB3	1:73:A:SER:H	19	0.1
(1,409)	1:60:A:PRO:HA	1:61:A:VAL:H	12	0.1
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB1	7	0.1
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB2	7	0.1
(1,399)	1:54:A:HIS:H	1:53:A:ALA:HB3	7	0.1
(1,390)	1:51:A:CYS:HB2	1:52:A:GLY:H	20	0.1
(1,390)	1:51:A:CYS:HB3	1:52:A:GLY:H	20	0.1
(1,387)	1:51:A:CYS:H	1:51:A:CYS:HB2	13	0.1
(1,387)	1:51:A:CYS:H	1:51:A:CYS:HB3	13	0.1
(1,378)	1:48:A:GLU:HG2	1:49:A:ILE:H	9	0.1
(1,378)	1:48:A:GLU:HG3	1:49:A:ILE:H	9	0.1
(1,374)	1:61:A:VAL:H	1:49:A:ILE:H	16	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,367)	1:42:A:ARG:HG2	1:43:A:THR:H	16	0.1
(1,367)	1:42:A:ARG:HG2	1:43:A:THR:H	16	0.1
(1,367)	1:42:A:ARG:HG3	1:43:A:THR:H	16	0.1
(1,367)	1:42:A:ARG:HG3	1:43:A:THR:H	16	0.1
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB2	18	0.1
(1,359)	1:40:A:HIS:H	1:40:A:HIS:HB3	18	0.1
(1,357)	1:40:A:HIS:H	1:39:A:CYS:HA	10	0.1
(1,329)	1:25:A:ASP:H	1:23:A:ASP:H	6	0.1
(1,329)	1:25:A:ASP:H	1:23:A:ASP:H	16	0.1
(1,328)	1:22:A:CYS:HB2	1:22:A:CYS:H	14	0.1
(1,328)	1:22:A:CYS:HB3	1:22:A:CYS:H	14	0.1
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB2	10	0.1
(1,323)	1:64:A:ARG:H	1:80:A:CYS:HB3	10	0.1
(1,315)	1:15:A:CYS:H	1:15:A:CYS:HB2	1	0.1
(1,315)	1:15:A:CYS:H	1:15:A:CYS:HB3	1	0.1
(1,315)	1:15:A:CYS:H	1:15:A:CYS:HB2	16	0.1
(1,315)	1:15:A:CYS:H	1:15:A:CYS:HB3	16	0.1
(1,302)	1:14:A:GLN:H	1:12:A:ASN:H	3	0.1
(1,302)	1:14:A:GLN:H	1:12:A:ASN:H	18	0.1
(1,299)	1:11:A:ASN:H	1:12:A:ASN:H	10	0.1
(1,299)	1:11:A:ASN:H	1:12:A:ASN:H	14	0.1
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	17	0.1
(1,257)	1:82:A:ASN:HB2	1:82:A:ASN:H	17	0.1
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	17	0.1
(1,257)	1:82:A:ASN:HB3	1:82:A:ASN:H	17	0.1
(1,247)	1:83:A:ILE:HA	1:84:A:THR:H	4	0.1
(1,234)	1:100:A:ARG:H	1:90:A:PHE:H	16	0.1
(1,194)	1:90:A:PHE:H	1:100:A:ARG:H	16	0.1
(1,190)	1:101:A:ASN:HB2	1:101:A:ASN:H	9	0.1
(1,190)	1:101:A:ASN:HB3	1:101:A:ASN:H	9	0.1
(1,180)	1:99:A:SER:HB2	1:102:A:PHE:H	20	0.1
(1,180)	1:99:A:SER:HB3	1:102:A:PHE:H	20	0.1
(1,165)	1:104:A:CYS:H	1:116:A:GLU:HA	8	0.1
(1,137)	1:109:A:ASP:H	1:113:A:GLY:HA2	10	0.1
(1,137)	1:109:A:ASP:H	1:113:A:GLY:HA3	10	0.1
(1,129)	1:114:A:SER:H	1:114:A:SER:HG	13	0.1
(1,125)	1:114:A:SER:H	1:113:A:GLY:HA2	14	0.1
(1,125)	1:114:A:SER:H	1:113:A:GLY:HA3	14	0.1
(1,116)	1:116:A:GLU:HG2	1:116:A:GLU:H	10	0.1
(1,116)	1:116:A:GLU:HG3	1:116:A:GLU:H	10	0.1
(1,108)	1:119:A:CYS:H	1:119:A:CYS:HB2	12	0.1
(1,108)	1:119:A:CYS:H	1:119:A:CYS:HB3	12	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,108)	1:119:A:CYS:H	1:119:A:CYS:HB2	15	0.1
(1,108)	1:119:A:CYS:H	1:119:A:CYS:HB3	15	0.1
(1,96)	1:100:A:ARG:H	1:89:A:GLU:HA	6	0.1
(1,84)	1:14:A:GLN:HG2	1:29:A:GLU:H	7	0.1
(1,84)	1:14:A:GLN:HG3	1:29:A:GLU:H	7	0.1
(1,80)	1:44:A:CYS:HB2	1:45:A:ARG:H	10	0.1
(1,80)	1:44:A:CYS:HB3	1:45:A:ARG:H	10	0.1
(1,74)	1:65:A:CYS:H	1:65:A:CYS:HB2	12	0.1
(1,74)	1:65:A:CYS:H	1:65:A:CYS:HB3	12	0.1
(1,74)	1:65:A:CYS:H	1:65:A:CYS:HB2	14	0.1
(1,74)	1:65:A:CYS:H	1:65:A:CYS:HB3	14	0.1
(1,74)	1:65:A:CYS:H	1:65:A:CYS:HB2	18	0.1
(1,74)	1:65:A:CYS:H	1:65:A:CYS:HB3	18	0.1
(1,59)	1:65:A:CYS:H	1:66:A:ASP:H	15	0.1
(1,56)	1:70:A:ASP:H	1:71:A:CYS:H	16	0.1
(1,22)	1:91:A:THR:H	1:92:A:CYS:H	16	0.1
(1,7)	1:22:A:CYS:H	1:23:A:ASP:H	2	0.1
(1,7)	1:22:A:CYS:H	1:23:A:ASP:H	9	0.1
(1,7)	1:22:A:CYS:H	1:23:A:ASP:H	15	0.1
(1,7)	1:22:A:CYS:H	1:23:A:ASP:H	20	0.1

10 Dihedral-angle violation analysis [i](#)

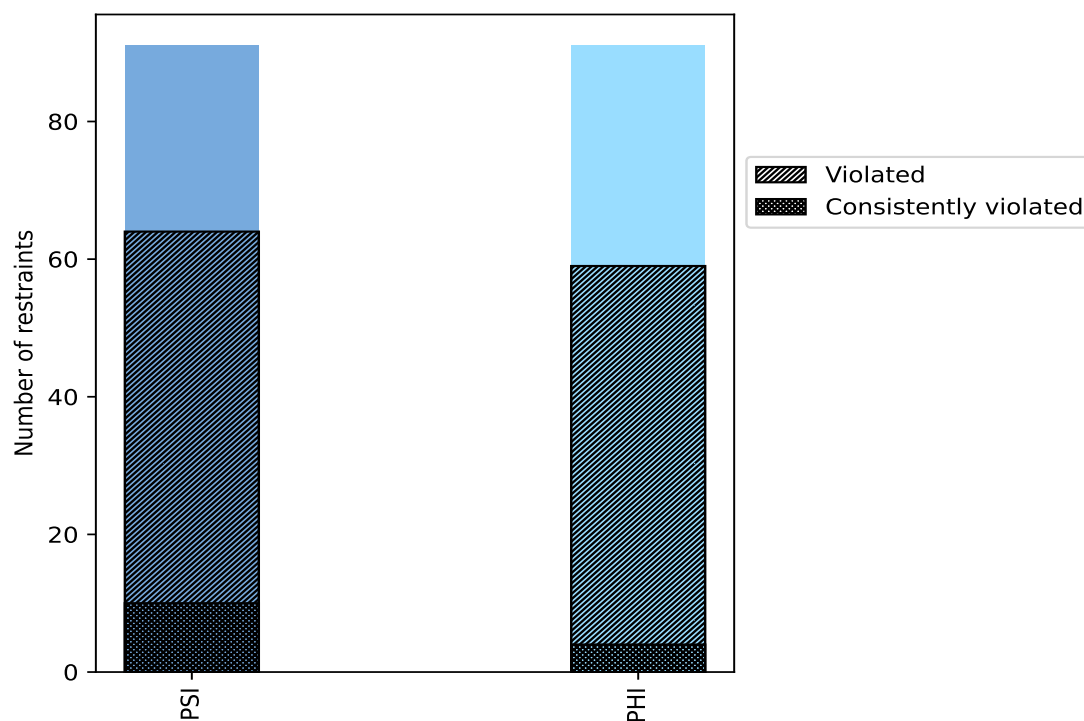
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	91	50.0	64	70.3	35.2	10	11.0	5.5
PHI	91	50.0	59	64.8	32.4	4	4.4	2.2
Total	182	100.0	123	67.6	67.6	14	7.7	7.7

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

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



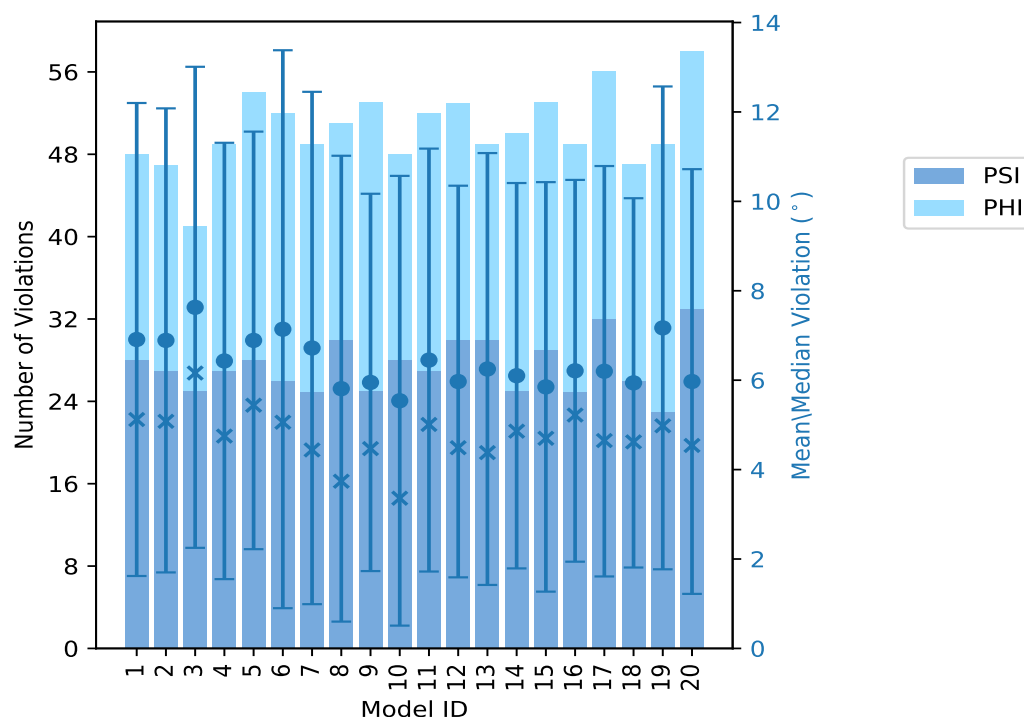
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	28	20	48	6.91	19.31	5.29	5.12
2	27	20	47	6.89	16.65	5.19	5.08
3	25	16	41	7.63	25.7	5.38	6.16
4	27	22	49	6.43	25.38	4.88	4.75
5	28	26	54	6.89	18.29	4.67	5.44
6	26	26	52	7.14	29.08	6.24	5.06
7	25	24	49	6.72	25.24	5.73	4.44
8	30	21	51	5.81	18.76	5.21	3.74
9	25	28	53	5.95	18.92	4.22	4.47
10	28	20	48	5.54	17.84	5.03	3.36
11	27	25	52	6.45	18.74	4.73	5.01
12	30	23	53	5.97	19.89	4.38	4.49
13	30	19	49	6.25	19.89	4.83	4.38
14	25	25	50	6.1	17.99	4.31	4.86
15	29	24	53	5.85	17.09	4.58	4.7
16	25	24	49	6.21	19.02	4.27	5.22
17	32	24	56	6.2	18.21	4.59	4.65
18	26	21	47	5.94	16.63	4.13	4.62
19	23	26	49	7.17	22.63	5.4	4.98
20	33	25	58	5.97	21.26	4.75	4.54

10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



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

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

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
9	10	19	1	5.0
3	10	13	2	10.0
9	7	16	3	15.0
5	3	8	4	20.0
4	1	5	5	25.0
3	1	4	6	30.0
3	1	4	7	35.0
0	0	0	8	40.0
3	4	7	9	45.0
1	2	3	10	50.0
4	2	6	11	55.0

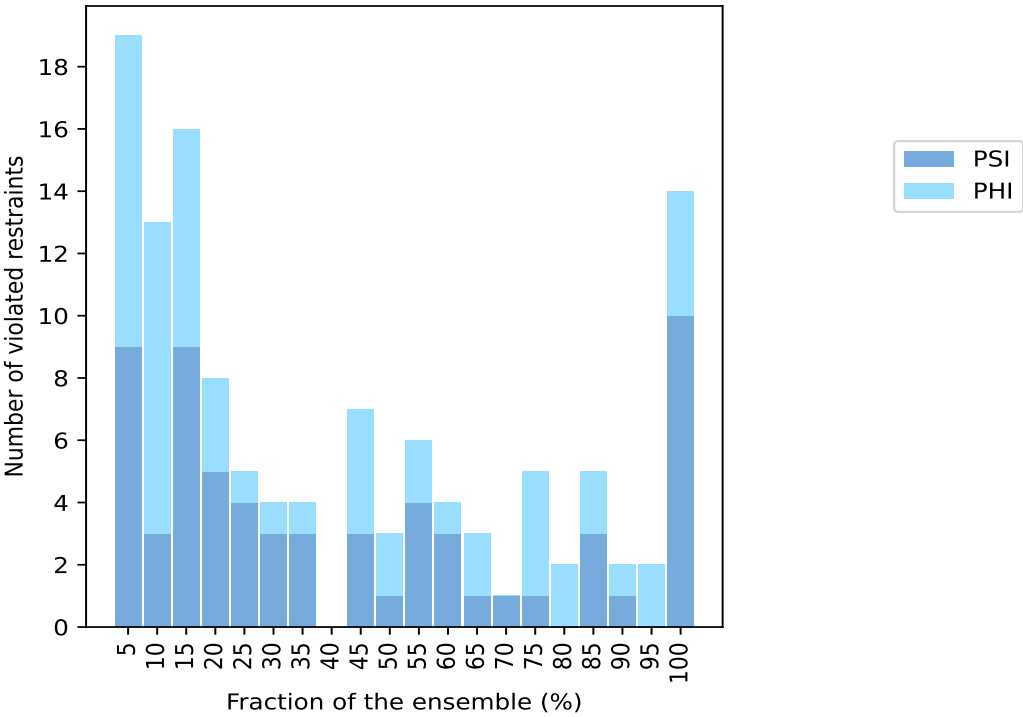
Continued on next page...

Continued from previous page...

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
3	1	4	12	60.0
1	2	3	13	65.0
1	0	1	14	70.0
1	4	5	15	75.0
0	2	2	16	80.0
3	2	5	17	85.0
1	1	2	18	90.0
0	2	2	19	95.0
10	4	14	20	100.0

¹ Number of models with violations

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

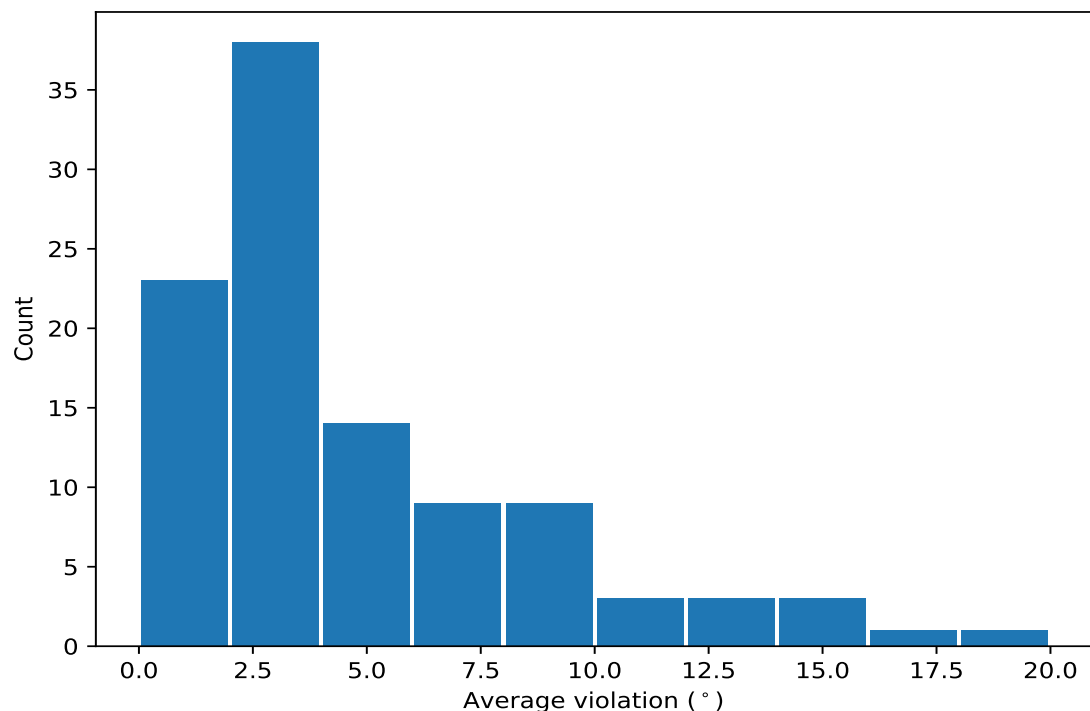


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,40)	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	1:27:A:ASP:N	20	18.3	2.14	17.94
(1,34)	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1:22:A:CYS:N	20	14.39	2.3	15.06
(1,86)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:CYS:N	20	12.85	1.76	13.06
(1,180)	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	1:105:A:ASN:N	20	12.58	1.47	12.44
(1,36)	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	1:23:A:ASP:N	20	12.31	1.25	12.26
(1,162)	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	1:118:A:ASP:N	20	11.76	2.79	11.64
(1,41)	1:26:A:PRO:C	1:27:A:ASP:N	1:27:A:ASP:CA	1:27:A:ASP:C	20	11.63	1.93	11.16
(1,73)	1:56:A:THR:C	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	20	9.66	3.25	10.19
(1,72)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:THR:N	20	8.26	2.17	8.52
(1,93)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	20	7.74	1.77	7.8
(1,58)	1:39:A:CYS:N	1:39:A:CYS:CA	1:39:A:CYS:C	1:40:A:HIS:N	20	7.14	1.89	7.58
(1,33)	1:20:A:TRP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	20	7.07	1.18	7.08
(1,74)	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	1:58:A:CYS:N	20	6.44	2.6	6.3
(1,56)	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	1:39:A:CYS:N	20	4.81	1.06	4.94
(1,95)	1:68:A:GLU:C	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	19	9.47	3.76	11.21
(1,159)	1:115:A:ASP:C	1:116:A:GLU:N	1:116:A:GLU:CA	1:116:A:GLU:C	19	4.37	1.55	4.12
(1,100)	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	1:73:A:SER:N	18	6.24	5.65	5.11
(1,109)	1:82:A:ASN:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	18	4.04	1.63	4.04
(1,153)	1:110:A:CYS:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	17	9.35	6.15	10.04
(1,114)	1:85:A:CYS:N	1:85:A:CYS:CA	1:85:A:CYS:C	1:86:A:SER:N	17	3.37	1.47	3.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,50)	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	1:36:A:PRO:N	17	2.89	1.3	2.69
(1,23)	1:14:A:GLN:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	17	2.51	1.13	2.35
(1,30)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:ARG:N	17	2.5	1.18	2.04
(1,63)	1:48:A:GLU:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	16	14.27	3.48	14.97
(1,143)	1:102:A:PHE:C	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	16	7.21	4.14	4.47
(1,98)	1:71:A:CYS:N	1:71:A:CYS:CA	1:71:A:CYS:C	1:72:A:ASP:N	15	5.75	2.56	6.16
(1,101)	1:74:A:GLY:C	1:75:A:GLU:N	1:75:A:GLU:CA	1:75:A:GLU:C	15	4.39	1.53	4.54
(1,107)	1:77:A:GLU:C	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	15	3.75	1.63	3.4
(1,99)	1:71:A:CYS:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	15	3.43	1.56	3.14
(1,5)	1:4:A:ALA:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	15	2.56	1.43	2.02
(1,108)	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	1:79:A:ASN:N	14	7.72	2.91	7.59
(1,179)	1:103:A:VAL:C	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	13	14.38	3.41	15.6
(1,32)	1:19:A:ARG:N	1:19:A:ARG:CA	1:19:A:ARG:C	1:20:A:TRP:N	13	2.86	2.23	1.76
(1,49)	1:34:A:GLU:C	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	13	2.08	0.75	1.89
(1,154)	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	1:112:A:ASP:N	12	9.68	4.99	11.19
(1,182)	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	1:113:A:GLY:N	12	5.06	2.77	4.5
(1,149)	1:107:A:GLN:C	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	12	3.55	1.41	3.96
(1,138)	1:100:A:ARG:N	1:100:A:ARG:CA	1:100:A:ARG:C	1:101:A:ASN:N	12	2.16	0.54	2.07
(1,152)	1:110:A:CYS:N	1:110:A:CYS:CA	1:110:A:CYS:C	1:111:A:SER:N	11	17.97	6.4	17.49
(1,181)	1:111:A:SER:C	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	11	9.2	4.34	9.23
(1,150)	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	1:109:A:ASP:N	11	5.75	2.75	6.72
(1,64)	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	1:50:A:SER:N	11	3.41	1.72	3.46
(1,80)	1:60:A:PRO:N	1:60:A:PRO:CA	1:60:A:PRO:C	1:61:A:VAL:N	11	2.84	1.36	2.6
(1,35)	1:21:A:LYS:C	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	11	2.41	0.81	2.54
(1,105)	1:76:A:ASP:C	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	10	7.56	2.11	7.56
(1,26)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:PRO:N	10	3.49	2.32	2.88
(1,55)	1:37:A:GLU:C	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	10	1.72	0.58	1.62
(1,156)	1:114:A:SER:N	1:114:A:SER:CA	1:114:A:SER:C	1:115:A:ASP:N	9	11.83	0.54	11.63
(1,104)	1:76:A:ASP:N	1:76:A:ASP:CA	1:76:A:ASP:C	1:77:A:GLU:N	9	5.69	2.6	5.66
(1,144)	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	1:104:A:CYS:N	9	4.49	2.26	3.85
(1,9)	1:7:A:ASP:C	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:C	9	4.34	1.78	3.66
(1,125)	1:93:A:SER:C	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	9	4.27	2.02	5.36
(1,161)	1:116:A:GLU:C	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	9	3.65	2.47	2.07
(1,31)	1:18:A:SER:C	1:19:A:ARG:N	1:19:A:ARG:CA	1:19:A:ARG:C	9	2.61	1.26	2.07
(1,158)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:GLU:N	7	8.57	2.11	8.44
(1,134)	1:98:A:ILE:N	1:98:A:ILE:CA	1:98:A:ILE:C	1:99:A:SER:N	7	3.96	1.13	4.24
(1,103)	1:75:A:GLU:C	1:76:A:ASP:N	1:76:A:ASP:CA	1:76:A:ASP:C	7	3.29	2.22	2.35
(1,122)	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	1:91:A:THR:N	7	2.5	0.93	2.73
(1,127)	1:94:A:SER:C	1:95:A:GLY:N	1:95:A:GLY:CA	1:95:A:GLY:C	6	3.41	2.02	2.89
(1,128)	1:95:A:GLY:N	1:95:A:GLY:CA	1:95:A:GLY:C	1:96:A:ARG:N	6	2.34	1.09	1.8
(1,54)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:GLN:N	6	1.52	0.26	1.62
(1,2)	1:2:A:THR:N	1:2:A:THR:CA	1:2:A:THR:C	1:3:A:CYS:N	6	1.24	0.31	1.14
(1,106)	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	1:78:A:GLU:N	5	4.14	2.91	3.62
(1,42)	1:27:A:ASP:N	1:27:A:ASP:CA	1:27:A:ASP:C	1:28:A:CYS:N	5	2.54	1.24	2.28
(1,44)	1:29:A:GLU:N	1:29:A:GLU:CA	1:29:A:GLU:C	1:30:A:ASP:N	5	2.51	0.75	2.27
(1,120)	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	1:90:A:PHE:N	5	2.18	1.16	1.48
(1,7)	1:5:A:GLU:C	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	5	1.62	0.43	1.56
(1,65)	1:49:A:ILE:C	1:50:A:SER:N	1:50:A:SER:CA	1:50:A:SER:C	4	8.33	2.93	9.3
(1,124)	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	1:94:A:SER:N	4	3.65	1.51	3.12
(1,136)	1:99:A:SER:N	1:99:A:SER:CA	1:99:A:SER:C	1:100:A:ARG:N	4	2.34	0.89	2.0
(1,130)	1:96:A:ARG:N	1:96:A:ARG:CA	1:96:A:ARG:C	1:97:A:CYS:N	4	2.17	0.71	1.98

Continued on next page...

Continued from previous page...

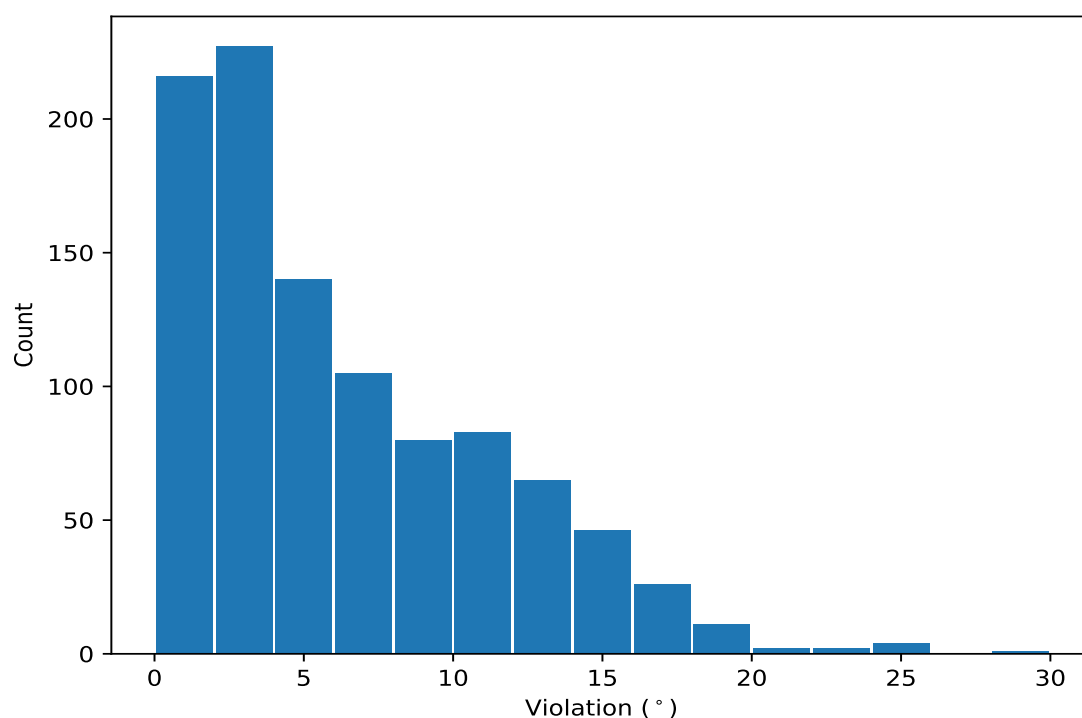
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,13)	1:9:A:VAL:C	1:10:A:CYS:N	1:10:A:CYS:CA	1:10:A:CYS:C	4	1.9	0.21	1.86
(1,4)	1:3:A:CYS:N	1:3:A:CYS:CA	1:3:A:CYS:C	1:4:A:ALA:N	4	1.84	0.7	1.77
(1,70)	1:54:A:HIS:N	1:54:A:HIS:CA	1:54:A:HIS:C	1:55:A:SER:N	4	1.74	0.66	1.58
(1,113)	1:84:A:THR:C	1:85:A:CYS:N	1:85:A:CYS:CA	1:85:A:CYS:C	4	1.5	0.44	1.3
(1,96)	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	1:70:A:ASP:N	3	7.33	0.8	7.56
(1,126)	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	1:95:A:GLY:N	3	4.91	2.62	6.46
(1,97)	1:70:A:ASP:C	1:71:A:CYS:N	1:71:A:CYS:CA	1:71:A:CYS:C	3	4.63	4.23	1.78
(1,121)	1:89:A:GLU:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	3	3.87	1.91	4.87
(1,8)	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	1:7:A:ASP:N	3	3.13	1.32	3.91
(1,147)	1:106:A:GLY:C	1:107:A:GLN:N	1:107:A:GLN:CA	1:107:A:GLN:C	3	3.08	0.17	3.12
(1,68)	1:53:A:ALA:N	1:53:A:ALA:CA	1:53:A:ALA:C	1:54:A:HIS:N	3	2.91	1.65	2.56
(1,90)	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	1:67:A:GLY:N	3	2.9	1.35	2.53
(1,10)	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:C	1:9:A:VAL:N	3	2.78	0.62	2.6
(1,81)	1:60:A:PRO:C	1:61:A:VAL:N	1:61:A:VAL:CA	1:61:A:VAL:C	3	2.38	0.51	2.18
(1,88)	1:65:A:CYS:N	1:65:A:CYS:CA	1:65:A:CYS:C	1:66:A:ASP:N	3	2.37	0.92	2.2
(1,160)	1:116:A:GLU:N	1:116:A:GLU:CA	1:116:A:GLU:C	1:117:A:LEU:N	3	1.78	0.37	1.96
(1,79)	1:59:A:ILE:C	1:60:A:PRO:N	1:60:A:PRO:CA	1:60:A:PRO:C	3	1.77	1.07	1.02
(1,3)	1:2:A:THR:C	1:3:A:CYS:N	1:3:A:CYS:CA	1:3:A:CYS:C	3	1.56	0.39	1.71
(1,131)	1:96:A:ARG:C	1:97:A:CYS:N	1:97:A:CYS:CA	1:97:A:CYS:C	3	1.51	0.36	1.27
(1,132)	1:97:A:CYS:N	1:97:A:CYS:CA	1:97:A:CYS:C	1:98:A:ILE:N	3	1.4	0.11	1.46
(1,102)	1:75:A:GLU:N	1:75:A:GLU:CA	1:75:A:GLU:C	1:76:A:ASP:N	2	9.22	5.6	9.22
(1,123)	1:92:A:CYS:C	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	2	3.2	2.13	3.2
(1,151)	1:109:A:ASP:C	1:110:A:CYS:N	1:110:A:CYS:CA	1:110:A:CYS:C	2	2.02	0.21	2.02
(1,16)	1:11:A:ASN:N	1:11:A:ASN:CA	1:11:A:ASN:C	1:12:A:ASN:N	2	1.92	0.68	1.92
(1,157)	1:114:A:SER:C	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	2	1.78	0.16	1.78
(1,145)	1:105:A:ASN:C	1:106:A:GLY:N	1:106:A:GLY:CA	1:106:A:GLY:C	2	1.76	0.08	1.76
(1,177)	1:91:A:THR:C	1:92:A:CYS:N	1:92:A:CYS:CA	1:92:A:CYS:C	2	1.7	0.32	1.7
(1,19)	1:12:A:ASN:C	1:13:A:GLY:N	1:13:A:GLY:CA	1:13:A:GLY:C	2	1.46	0.1	1.46
(1,133)	1:97:A:CYS:C	1:98:A:ILE:N	1:98:A:ILE:CA	1:98:A:ILE:C	2	1.36	0.26	1.36
(1,21)	1:13:A:GLY:C	1:14:A:GLN:N	1:14:A:GLN:CA	1:14:A:GLN:C	2	1.3	0.02	1.3
(1,27)	1:16:A:VAL:C	1:17:A:PRO:N	1:17:A:PRO:CA	1:17:A:PRO:C	2	1.28	0.04	1.28
(1,61)	1:47:A:HIS:C	1:48:A:GLU:N	1:48:A:GLU:CA	1:48:A:GLU:C	2	1.2	0.09	1.2
(1,116)	1:87:A:PRO:N	1:87:A:PRO:CA	1:87:A:PRO:C	1:88:A:ASP:N	2	1.16	0.06	1.16

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

10.5 All violated dihedral-angle restraints ⓘ

10.5.1 Histogram : Distribution of violations ⓘ

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



10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,100)	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	1:73:A:SER:N	6	29.08
(1,152)	1:110:A:CYS:N	1:110:A:CYS:CA	1:110:A:CYS:C	1:111:A:SER:N	3	25.7
(1,152)	1:110:A:CYS:N	1:110:A:CYS:CA	1:110:A:CYS:C	1:111:A:SER:N	4	25.38
(1,152)	1:110:A:CYS:N	1:110:A:CYS:CA	1:110:A:CYS:C	1:111:A:SER:N	7	25.24
(1,152)	1:110:A:CYS:N	1:110:A:CYS:CA	1:110:A:CYS:C	1:111:A:SER:N	6	24.55
(1,40)	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	1:27:A:ASP:N	7	22.78
(1,40)	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	1:27:A:ASP:N	19	22.63
(1,40)	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	1:27:A:ASP:N	20	21.26
(1,179)	1:103:A:VAL:C	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	6	20.25
(1,40)	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	1:27:A:ASP:N	12	19.89
(1,40)	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	1:27:A:ASP:N	13	19.89
(1,152)	1:110:A:CYS:N	1:110:A:CYS:CA	1:110:A:CYS:C	1:111:A:SER:N	1	19.31
(1,40)	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	1:27:A:ASP:N	16	19.02
(1,40)	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	1:27:A:ASP:N	9	18.92
(1,34)	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1:22:A:CYS:N	8	18.76
(1,40)	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	1:27:A:ASP:N	11	18.74
(1,153)	1:110:A:CYS:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	1	18.7
(1,40)	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	1:27:A:ASP:N	5	18.29
(1,179)	1:103:A:VAL:C	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	17	18.21
(1,153)	1:110:A:CYS:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	8	18.18
(1,40)	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	1:27:A:ASP:N	14	17.99

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,40)	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	1:27:A:ASP:N	6	17.89
(1,179)	1:103:A:VAL:C	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	4	17.86
(1,153)	1:110:A:CYS:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	10	17.84
(1,40)	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	1:27:A:ASP:N	4	17.81
(1,40)	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	1:27:A:ASP:N	10	17.71
(1,152)	1:110:A:CYS:N	1:110:A:CYS:CA	1:110:A:CYS:C	1:111:A:SER:N	8	17.49
(1,34)	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1:22:A:CYS:N	11	17.25
(1,40)	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	1:27:A:ASP:N	15	17.09
(1,63)	1:48:A:GLU:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	20	16.78
(1,63)	1:48:A:GLU:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	13	16.77
(1,40)	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	1:27:A:ASP:N	8	16.77
(1,179)	1:103:A:VAL:C	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	7	16.7
(1,162)	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	1:118:A:ASP:N	15	16.7
(1,40)	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	1:27:A:ASP:N	2	16.65
(1,152)	1:110:A:CYS:N	1:110:A:CYS:CA	1:110:A:CYS:C	1:111:A:SER:N	10	16.64
(1,40)	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	1:27:A:ASP:N	18	16.63
(1,40)	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	1:27:A:ASP:N	3	16.45
(1,63)	1:48:A:GLU:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	5	16.36
(1,179)	1:103:A:VAL:C	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	3	16.29
(1,63)	1:48:A:GLU:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	11	16.26
(1,63)	1:48:A:GLU:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	19	16.23
(1,162)	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	1:118:A:ASP:N	12	16.1
(1,63)	1:48:A:GLU:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	8	16.04
(1,34)	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1:22:A:CYS:N	18	16.03
(1,34)	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1:22:A:CYS:N	1	16.02
(1,180)	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	1:105:A:ASN:N	11	15.88
(1,95)	1:68:A:GLU:C	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	19	15.88
(1,34)	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1:22:A:CYS:N	3	15.81
(1,154)	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	1:112:A:ASP:N	10	15.8
(1,179)	1:103:A:VAL:C	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	2	15.75
(1,181)	1:111:A:SER:C	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	2	15.67
(1,34)	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1:22:A:CYS:N	2	15.65
(1,86)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:CYS:N	15	15.63
(1,179)	1:103:A:VAL:C	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	19	15.6
(1,154)	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	1:112:A:ASP:N	2	15.52
(1,86)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:CYS:N	17	15.5
(1,40)	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	1:27:A:ASP:N	1	15.4
(1,41)	1:26:A:PRO:C	1:27:A:ASP:N	1:27:A:ASP:CA	1:27:A:ASP:C	7	15.35
(1,34)	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1:22:A:CYS:N	13	15.3
(1,162)	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	1:118:A:ASP:N	11	15.29
(1,63)	1:48:A:GLU:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	3	15.27
(1,34)	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1:22:A:CYS:N	20	15.27
(1,34)	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1:22:A:CYS:N	14	15.14
(1,153)	1:110:A:CYS:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	19	15.09
(1,34)	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1:22:A:CYS:N	5	15.09
(1,34)	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1:22:A:CYS:N	10	15.02
(1,152)	1:110:A:CYS:N	1:110:A:CYS:CA	1:110:A:CYS:C	1:111:A:SER:N	19	15.01
(1,63)	1:48:A:GLU:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	6	14.98
(1,63)	1:48:A:GLU:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	2	14.96
(1,154)	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	1:112:A:ASP:N	1	14.91
(1,36)	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	1:23:A:ASP:N	5	14.91

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,86)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:CYS:N	12	14.87
(1,102)	1:75:A:GLU:N	1:75:A:GLU:CA	1:75:A:GLU:C	1:76:A:ASP:N	6	14.82
(1,34)	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1:22:A:CYS:N	15	14.74
(1,162)	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	1:118:A:ASP:N	20	14.7
(1,108)	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	1:79:A:ASN:N	19	14.7
(1,95)	1:68:A:GLU:C	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	7	14.7
(1,41)	1:26:A:PRO:C	1:27:A:ASP:N	1:27:A:ASP:CA	1:27:A:ASP:C	20	14.68
(1,63)	1:48:A:GLU:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	7	14.65
(1,86)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:CYS:N	19	14.57
(1,73)	1:56:A:THR:C	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	1	14.56
(1,63)	1:48:A:GLU:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	9	14.53
(1,180)	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	1:105:A:ASN:N	13	14.41
(1,180)	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	1:105:A:ASN:N	15	14.4
(1,34)	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1:22:A:CYS:N	19	14.38
(1,34)	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1:22:A:CYS:N	17	14.33
(1,73)	1:56:A:THR:C	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	17	14.29
(1,40)	1:26:A:PRO:N	1:26:A:PRO:CA	1:26:A:PRO:C	1:27:A:ASP:N	17	14.29
(1,180)	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	1:105:A:ASN:N	18	14.23
(1,63)	1:48:A:GLU:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	14	14.13
(1,181)	1:111:A:SER:C	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	19	14.1
(1,86)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:CYS:N	2	13.95
(1,180)	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	1:105:A:ASN:N	14	13.93
(1,86)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:CYS:N	1	13.91
(1,162)	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	1:118:A:ASP:N	18	13.86
(1,41)	1:26:A:PRO:C	1:27:A:ASP:N	1:27:A:ASP:CA	1:27:A:ASP:C	13	13.86
(1,181)	1:111:A:SER:C	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	5	13.79
(1,180)	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	1:105:A:ASN:N	12	13.79
(1,162)	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	1:118:A:ASP:N	14	13.79
(1,179)	1:103:A:VAL:C	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	5	13.76
(1,86)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:CYS:N	20	13.75
(1,36)	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	1:23:A:ASP:N	1	13.75
(1,73)	1:56:A:THR:C	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	2	13.72
(1,41)	1:26:A:PRO:C	1:27:A:ASP:N	1:27:A:ASP:CA	1:27:A:ASP:C	11	13.7
(1,154)	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	1:112:A:ASP:N	8	13.69
(1,153)	1:110:A:CYS:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	5	13.63
(1,36)	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	1:23:A:ASP:N	20	13.63
(1,41)	1:26:A:PRO:C	1:27:A:ASP:N	1:27:A:ASP:CA	1:27:A:ASP:C	12	13.49
(1,154)	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	1:112:A:ASP:N	5	13.47
(1,63)	1:48:A:GLU:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	17	13.42
(1,63)	1:48:A:GLU:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	16	13.41
(1,86)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:CYS:N	5	13.4
(1,36)	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	1:23:A:ASP:N	9	13.36
(1,36)	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	1:23:A:ASP:N	17	13.33
(1,180)	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	1:105:A:ASN:N	20	13.29
(1,156)	1:114:A:SER:N	1:114:A:SER:CA	1:114:A:SER:C	1:115:A:ASP:N	14	13.15
(1,86)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:CYS:N	13	13.15
(1,86)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:CYS:N	3	13.1
(1,41)	1:26:A:PRO:C	1:27:A:ASP:N	1:27:A:ASP:CA	1:27:A:ASP:C	16	13.06
(1,36)	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	1:23:A:ASP:N	3	13.04
(1,86)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:CYS:N	10	13.02
(1,73)	1:56:A:THR:C	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	6	13.0

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,36)	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	1:23:A:ASP:N	2	12.98
(1,41)	1:26:A:PRO:C	1:27:A:ASP:N	1:27:A:ASP:CA	1:27:A:ASP:C	5	12.94
(1,180)	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	1:105:A:ASN:N	8	12.92
(1,34)	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1:22:A:CYS:N	9	12.91
(1,86)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:CYS:N	6	12.87
(1,63)	1:48:A:GLU:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	1	12.84
(1,143)	1:102:A:PHE:C	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	15	12.81
(1,162)	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	1:118:A:ASP:N	5	12.8
(1,180)	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	1:105:A:ASN:N	1	12.78
(1,143)	1:102:A:PHE:C	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	13	12.76
(1,34)	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1:22:A:CYS:N	7	12.71
(1,180)	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	1:105:A:ASN:N	10	12.67
(1,73)	1:56:A:THR:C	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	7	12.67
(1,95)	1:68:A:GLU:C	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	3	12.66
(1,36)	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	1:23:A:ASP:N	19	12.6
(1,36)	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	1:23:A:ASP:N	14	12.57
(1,86)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:CYS:N	7	12.55
(1,36)	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	1:23:A:ASP:N	8	12.46
(1,143)	1:102:A:PHE:C	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	14	12.44
(1,154)	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	1:112:A:ASP:N	19	12.43
(1,153)	1:110:A:CYS:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	2	12.43
(1,86)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:CYS:N	11	12.42
(1,74)	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	1:58:A:CYS:N	15	12.4
(1,34)	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1:22:A:CYS:N	16	12.33
(1,41)	1:26:A:PRO:C	1:27:A:ASP:N	1:27:A:ASP:CA	1:27:A:ASP:C	9	12.31
(1,180)	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	1:105:A:ASN:N	4	12.21
(1,86)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:CYS:N	16	12.2
(1,156)	1:114:A:SER:N	1:114:A:SER:CA	1:114:A:SER:C	1:115:A:ASP:N	12	12.19
(1,143)	1:102:A:PHE:C	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	20	12.15
(1,86)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:CYS:N	8	12.11
(1,162)	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	1:118:A:ASP:N	6	12.09
(1,36)	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	1:23:A:ASP:N	13	12.07
(1,36)	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	1:23:A:ASP:N	15	12.07
(1,73)	1:56:A:THR:C	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	13	12.0
(1,156)	1:114:A:SER:N	1:114:A:SER:CA	1:114:A:SER:C	1:115:A:ASP:N	18	11.99
(1,36)	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	1:23:A:ASP:N	6	11.97
(1,162)	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	1:118:A:ASP:N	7	11.96
(1,95)	1:68:A:GLU:C	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	5	11.92
(1,36)	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	1:23:A:ASP:N	7	11.91
(1,34)	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1:22:A:CYS:N	4	11.89
(1,105)	1:76:A:ASP:C	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	3	11.86
(1,162)	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	1:118:A:ASP:N	4	11.84
(1,36)	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	1:23:A:ASP:N	11	11.84
(1,156)	1:114:A:SER:N	1:114:A:SER:CA	1:114:A:SER:C	1:115:A:ASP:N	13	11.82
(1,180)	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	1:105:A:ASN:N	7	11.79
(1,95)	1:68:A:GLU:C	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	1	11.73
(1,158)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:GLU:N	18	11.71
(1,180)	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	1:105:A:ASN:N	6	11.69
(1,95)	1:68:A:GLU:C	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	20	11.66
(1,41)	1:26:A:PRO:C	1:27:A:ASP:N	1:27:A:ASP:CA	1:27:A:ASP:C	1	11.64
(1,156)	1:114:A:SER:N	1:114:A:SER:CA	1:114:A:SER:C	1:115:A:ASP:N	16	11.63

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,95)	1:68:A:GLU:C	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	9	11.61
(1,74)	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	1:58:A:CYS:N	4	11.6
(1,156)	1:114:A:SER:N	1:114:A:SER:CA	1:114:A:SER:C	1:115:A:ASP:N	15	11.54
(1,36)	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	1:23:A:ASP:N	16	11.5
(1,73)	1:56:A:THR:C	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	5	11.49
(1,95)	1:68:A:GLU:C	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	16	11.47
(1,179)	1:103:A:VAL:C	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	8	11.44
(1,180)	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	1:105:A:ASN:N	3	11.43
(1,162)	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	1:118:A:ASP:N	3	11.43
(1,73)	1:56:A:THR:C	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	9	11.43
(1,156)	1:114:A:SER:N	1:114:A:SER:CA	1:114:A:SER:C	1:115:A:ASP:N	9	11.41
(1,180)	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	1:105:A:ASN:N	9	11.39
(1,156)	1:114:A:SER:N	1:114:A:SER:CA	1:114:A:SER:C	1:115:A:ASP:N	20	11.39
(1,152)	1:110:A:CYS:N	1:110:A:CYS:CA	1:110:A:CYS:C	1:111:A:SER:N	2	11.39
(1,73)	1:56:A:THR:C	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	16	11.39
(1,156)	1:114:A:SER:N	1:114:A:SER:CA	1:114:A:SER:C	1:115:A:ASP:N	11	11.38
(1,36)	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	1:23:A:ASP:N	18	11.38
(1,86)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:CYS:N	9	11.37
(1,180)	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	1:105:A:ASN:N	19	11.35
(1,180)	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	1:105:A:ASN:N	16	11.33
(1,95)	1:68:A:GLU:C	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	2	11.27
(1,95)	1:68:A:GLU:C	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	11	11.21
(1,162)	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	1:118:A:ASP:N	13	11.18
(1,41)	1:26:A:PRO:C	1:27:A:ASP:N	1:27:A:ASP:CA	1:27:A:ASP:C	8	11.17
(1,143)	1:102:A:PHE:C	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	11	11.16
(1,65)	1:49:A:ILE:C	1:50:A:SER:N	1:50:A:SER:CA	1:50:A:SER:C	15	11.15
(1,41)	1:26:A:PRO:C	1:27:A:ASP:N	1:27:A:ASP:CA	1:27:A:ASP:C	6	11.15
(1,162)	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	1:118:A:ASP:N	10	11.13
(1,180)	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	1:105:A:ASN:N	17	11.12
(1,73)	1:56:A:THR:C	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	11	11.1
(1,153)	1:110:A:CYS:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	17	11.08
(1,36)	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	1:23:A:ASP:N	12	11.07
(1,181)	1:111:A:SER:C	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	17	11.05
(1,179)	1:103:A:VAL:C	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	10	11.02
(1,41)	1:26:A:PRO:C	1:27:A:ASP:N	1:27:A:ASP:CA	1:27:A:ASP:C	4	10.96
(1,34)	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1:22:A:CYS:N	12	10.91
(1,182)	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	1:113:A:GLY:N	2	10.86
(1,180)	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	1:105:A:ASN:N	5	10.86
(1,153)	1:110:A:CYS:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	3	10.85
(1,143)	1:102:A:PHE:C	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	12	10.84
(1,36)	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	1:23:A:ASP:N	4	10.79
(1,162)	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	1:118:A:ASP:N	8	10.73
(1,72)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:THR:N	5	10.68
(1,162)	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	1:118:A:ASP:N	2	10.64
(1,97)	1:70:A:ASP:C	1:71:A:CYS:N	1:71:A:CYS:CA	1:71:A:CYS:C	6	10.61
(1,41)	1:26:A:PRO:C	1:27:A:ASP:N	1:27:A:ASP:CA	1:27:A:ASP:C	19	10.58
(1,72)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:THR:N	1	10.51
(1,72)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:THR:N	17	10.48
(1,41)	1:26:A:PRO:C	1:27:A:ASP:N	1:27:A:ASP:CA	1:27:A:ASP:C	14	10.47
(1,108)	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	1:79:A:ASN:N	13	10.45
(1,72)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:THR:N	2	10.43

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,86)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:CYS:N	18	10.42
(1,41)	1:26:A:PRO:C	1:27:A:ASP:N	1:27:A:ASP:CA	1:27:A:ASP:C	10	10.4
(1,179)	1:103:A:VAL:C	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	1	10.36
(1,95)	1:68:A:GLU:C	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	17	10.34
(1,65)	1:49:A:ILE:C	1:50:A:SER:N	1:50:A:SER:CA	1:50:A:SER:C	12	10.32
(1,143)	1:102:A:PHE:C	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	18	10.27
(1,41)	1:26:A:PRO:C	1:27:A:ASP:N	1:27:A:ASP:CA	1:27:A:ASP:C	15	10.18
(1,93)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	5	10.16
(1,72)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:THR:N	20	10.14
(1,98)	1:71:A:CYS:N	1:71:A:CYS:CA	1:71:A:CYS:C	1:72:A:ASP:N	4	10.11
(1,41)	1:26:A:PRO:C	1:27:A:ASP:N	1:27:A:ASP:CA	1:27:A:ASP:C	17	10.11
(1,180)	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	1:105:A:ASN:N	2	10.07
(1,153)	1:110:A:CYS:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	6	10.04
(1,105)	1:76:A:ASP:C	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	11	10.04
(1,179)	1:103:A:VAL:C	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	9	10.01
(1,158)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:GLU:N	12	9.98
(1,158)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:GLU:N	14	9.95
(1,154)	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	1:112:A:ASP:N	17	9.95
(1,108)	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	1:79:A:ASN:N	17	9.95
(1,162)	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	1:118:A:ASP:N	1	9.94
(1,58)	1:39:A:CYS:N	1:39:A:CYS:CA	1:39:A:CYS:C	1:40:A:HIS:N	9	9.94
(1,108)	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	1:79:A:ASN:N	6	9.93
(1,41)	1:26:A:PRO:C	1:27:A:ASP:N	1:27:A:ASP:CA	1:27:A:ASP:C	2	9.86
(1,26)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:PRO:N	15	9.84
(1,93)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	16	9.83
(1,153)	1:110:A:CYS:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	7	9.82
(1,153)	1:110:A:CYS:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	4	9.81
(1,152)	1:110:A:CYS:N	1:110:A:CYS:CA	1:110:A:CYS:C	1:111:A:SER:N	17	9.78
(1,93)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	7	9.76
(1,33)	1:20:A:TRP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	6	9.73
(1,93)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	2	9.69
(1,179)	1:103:A:VAL:C	1:104:A:CYS:N	1:104:A:CYS:CA	1:104:A:CYS:C	16	9.65
(1,93)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	11	9.64
(1,93)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	1	9.54
(1,72)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:THR:N	9	9.53
(1,104)	1:76:A:ASP:N	1:76:A:ASP:CA	1:76:A:ASP:C	1:77:A:GLU:N	3	9.51
(1,106)	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	1:78:A:GLU:N	6	9.47
(1,181)	1:111:A:SER:C	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	10	9.41
(1,58)	1:39:A:CYS:N	1:39:A:CYS:CA	1:39:A:CYS:C	1:40:A:HIS:N	4	9.38
(1,150)	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	1:109:A:ASP:N	17	9.35
(1,73)	1:56:A:THR:C	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	3	9.28
(1,104)	1:76:A:ASP:N	1:76:A:ASP:CA	1:76:A:ASP:C	1:77:A:GLU:N	16	9.25
(1,181)	1:111:A:SER:C	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	1	9.23
(1,86)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:CYS:N	4	9.18
(1,93)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	9	9.17
(1,95)	1:68:A:GLU:C	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	13	9.16
(1,86)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:CYS:N	14	9.11
(1,72)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:THR:N	16	9.1
(1,98)	1:71:A:CYS:N	1:71:A:CYS:CA	1:71:A:CYS:C	1:72:A:ASP:N	18	9.09
(1,93)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	17	9.05
(1,162)	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	1:118:A:ASP:N	17	9.01

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,74)	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	1:58:A:CYS:N	12	9.01
(1,162)	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	1:118:A:ASP:N	9	8.99
(1,58)	1:39:A:CYS:N	1:39:A:CYS:CA	1:39:A:CYS:C	1:40:A:HIS:N	12	8.95
(1,58)	1:39:A:CYS:N	1:39:A:CYS:CA	1:39:A:CYS:C	1:40:A:HIS:N	16	8.95
(1,108)	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	1:79:A:ASN:N	3	8.94
(1,36)	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	1:23:A:ASP:N	10	8.94
(1,58)	1:39:A:CYS:N	1:39:A:CYS:CA	1:39:A:CYS:C	1:40:A:HIS:N	3	8.93
(1,181)	1:111:A:SER:C	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	16	8.85
(1,72)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:THR:N	6	8.85
(1,150)	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	1:109:A:ASP:N	19	8.84
(1,182)	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	1:113:A:GLY:N	19	8.78
(1,72)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:THR:N	15	8.7
(1,72)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:THR:N	19	8.66
(1,98)	1:71:A:CYS:N	1:71:A:CYS:CA	1:71:A:CYS:C	1:72:A:ASP:N	20	8.63
(1,41)	1:26:A:PRO:C	1:27:A:ASP:N	1:27:A:ASP:CA	1:27:A:ASP:C	3	8.61
(1,93)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	19	8.58
(1,73)	1:56:A:THR:C	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	14	8.56
(1,33)	1:20:A:TRP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	12	8.51
(1,33)	1:20:A:TRP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	16	8.46
(1,33)	1:20:A:TRP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	4	8.45
(1,158)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:GLU:N	15	8.44
(1,74)	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	1:58:A:CYS:N	2	8.44
(1,109)	1:82:A:ASN:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	1	8.43
(1,103)	1:75:A:GLU:C	1:76:A:ASP:N	1:76:A:ASP:CA	1:76:A:ASP:C	6	8.4
(1,72)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:THR:N	13	8.37
(1,72)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:THR:N	7	8.35
(1,72)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:THR:N	3	8.34
(1,105)	1:76:A:ASP:C	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	16	8.33
(1,58)	1:39:A:CYS:N	1:39:A:CYS:CA	1:39:A:CYS:C	1:40:A:HIS:N	15	8.33
(1,58)	1:39:A:CYS:N	1:39:A:CYS:CA	1:39:A:CYS:C	1:40:A:HIS:N	17	8.29
(1,181)	1:111:A:SER:C	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	9	8.27
(1,93)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	13	8.27
(1,65)	1:49:A:ILE:C	1:50:A:SER:N	1:50:A:SER:CA	1:50:A:SER:C	4	8.27
(1,161)	1:116:A:GLU:C	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	17	8.25
(1,33)	1:20:A:TRP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	7	8.19
(1,34)	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1:22:A:CYS:N	6	8.18
(1,150)	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	1:109:A:ASP:N	5	8.17
(1,96)	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	1:70:A:ASP:N	14	8.17
(1,159)	1:115:A:ASP:C	1:116:A:GLU:N	1:116:A:GLU:CA	1:116:A:GLU:C	14	8.16
(1,144)	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	1:104:A:CYS:N	18	8.15
(1,158)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:GLU:N	20	8.09
(1,41)	1:26:A:PRO:C	1:27:A:ASP:N	1:27:A:ASP:CA	1:27:A:ASP:C	18	8.09
(1,74)	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	1:58:A:CYS:N	6	8.07
(1,58)	1:39:A:CYS:N	1:39:A:CYS:CA	1:39:A:CYS:C	1:40:A:HIS:N	1	8.02
(1,150)	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	1:109:A:ASP:N	8	7.99
(1,105)	1:76:A:ASP:C	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	5	7.98
(1,95)	1:68:A:GLU:C	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	12	7.98
(1,72)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:THR:N	18	7.97
(1,162)	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	1:118:A:ASP:N	19	7.95
(1,58)	1:39:A:CYS:N	1:39:A:CYS:CA	1:39:A:CYS:C	1:40:A:HIS:N	13	7.94
(1,98)	1:71:A:CYS:N	1:71:A:CYS:CA	1:71:A:CYS:C	1:72:A:ASP:N	14	7.93

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,72)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:THR:N	12	7.91
(1,33)	1:20:A:TRP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	9	7.91
(1,74)	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	1:58:A:CYS:N	18	7.87
(1,108)	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	1:79:A:ASN:N	11	7.84
(1,9)	1:7:A:ASP:C	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:C	14	7.78
(1,58)	1:39:A:CYS:N	1:39:A:CYS:CA	1:39:A:CYS:C	1:40:A:HIS:N	7	7.76
(1,74)	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	1:58:A:CYS:N	20	7.73
(1,108)	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	1:79:A:ASN:N	2	7.69
(1,73)	1:56:A:THR:C	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	19	7.67
(1,105)	1:76:A:ASP:C	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	9	7.62
(1,73)	1:56:A:THR:C	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	10	7.62
(1,72)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:THR:N	11	7.61
(1,107)	1:77:A:GLU:C	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	12	7.56
(1,96)	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	1:70:A:ASP:N	18	7.56
(1,105)	1:76:A:ASP:C	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	20	7.51
(1,33)	1:20:A:TRP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	14	7.51
(1,108)	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	1:79:A:ASN:N	1	7.49
(1,104)	1:76:A:ASP:N	1:76:A:ASP:CA	1:76:A:ASP:C	1:77:A:GLU:N	11	7.49
(1,181)	1:111:A:SER:C	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	8	7.42
(1,33)	1:20:A:TRP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	19	7.42
(1,58)	1:39:A:CYS:N	1:39:A:CYS:CA	1:39:A:CYS:C	1:40:A:HIS:N	5	7.4
(1,99)	1:71:A:CYS:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	20	7.33
(1,33)	1:20:A:TRP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	20	7.33
(1,93)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	6	7.32
(1,93)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	3	7.31
(1,73)	1:56:A:THR:C	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	8	7.26
(1,95)	1:68:A:GLU:C	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	6	7.23
(1,33)	1:20:A:TRP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	15	7.23
(1,98)	1:71:A:CYS:N	1:71:A:CYS:CA	1:71:A:CYS:C	1:72:A:ASP:N	7	7.21
(1,58)	1:39:A:CYS:N	1:39:A:CYS:CA	1:39:A:CYS:C	1:40:A:HIS:N	11	7.21
(1,152)	1:110:A:CYS:N	1:110:A:CYS:CA	1:110:A:CYS:C	1:111:A:SER:N	5	7.19
(1,98)	1:71:A:CYS:N	1:71:A:CYS:CA	1:71:A:CYS:C	1:72:A:ASP:N	12	7.19
(1,158)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:GLU:N	13	7.08
(1,32)	1:19:A:ARG:N	1:19:A:ARG:CA	1:19:A:ARG:C	1:20:A:TRP:N	4	7.08
(1,32)	1:19:A:ARG:N	1:19:A:ARG:CA	1:19:A:ARG:C	1:20:A:TRP:N	12	7.08
(1,150)	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	1:109:A:ASP:N	2	7.06
(1,72)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:THR:N	4	7.05
(1,126)	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	1:95:A:GLY:N	16	7.04
(1,98)	1:71:A:CYS:N	1:71:A:CYS:CA	1:71:A:CYS:C	1:72:A:ASP:N	17	7.02
(1,74)	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	1:58:A:CYS:N	10	6.99
(1,73)	1:56:A:THR:C	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	18	6.99
(1,9)	1:7:A:ASP:C	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:C	4	6.98
(1,33)	1:20:A:TRP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	3	6.92
(1,93)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	10	6.87
(1,182)	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	1:113:A:GLY:N	11	6.86
(1,58)	1:39:A:CYS:N	1:39:A:CYS:CA	1:39:A:CYS:C	1:40:A:HIS:N	18	6.83
(1,64)	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	1:50:A:SER:N	14	6.8
(1,58)	1:39:A:CYS:N	1:39:A:CYS:CA	1:39:A:CYS:C	1:40:A:HIS:N	19	6.75
(1,150)	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	1:109:A:ASP:N	1	6.72
(1,161)	1:116:A:GLU:C	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	5	6.71
(1,182)	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	1:113:A:GLY:N	5	6.69

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,50)	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	1:36:A:PRO:N	10	6.69
(1,56)	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	1:39:A:CYS:N	19	6.67
(1,108)	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	1:79:A:ASN:N	20	6.66
(1,144)	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	1:104:A:CYS:N	11	6.65
(1,105)	1:76:A:ASP:C	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	6	6.63
(1,33)	1:20:A:TRP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	18	6.6
(1,72)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:THR:N	14	6.57
(1,127)	1:94:A:SER:C	1:95:A:GLY:N	1:95:A:GLY:CA	1:95:A:GLY:C	16	6.55
(1,74)	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	1:58:A:CYS:N	7	6.52
(1,101)	1:74:A:GLY:C	1:75:A:GLU:N	1:75:A:GLU:CA	1:75:A:GLU:C	4	6.51
(1,100)	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	1:73:A:SER:N	2	6.51
(1,56)	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	1:39:A:CYS:N	20	6.51
(1,73)	1:56:A:THR:C	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	12	6.5
(1,33)	1:20:A:TRP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	10	6.47
(1,126)	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	1:95:A:GLY:N	9	6.46
(1,144)	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	1:104:A:CYS:N	12	6.41
(1,101)	1:74:A:GLY:C	1:75:A:GLU:N	1:75:A:GLU:CA	1:75:A:GLU:C	18	6.41
(1,109)	1:82:A:ASN:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	9	6.39
(1,159)	1:115:A:ASP:C	1:116:A:GLU:N	1:116:A:GLU:CA	1:116:A:GLU:C	18	6.37
(1,74)	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	1:58:A:CYS:N	14	6.36
(1,93)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	4	6.33
(1,5)	1:4:A:ALA:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	15	6.32
(1,108)	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	1:79:A:ASN:N	16	6.3
(1,96)	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	1:70:A:ASP:N	4	6.25
(1,74)	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	1:58:A:CYS:N	17	6.25
(1,80)	1:60:A:PRO:N	1:60:A:PRO:CA	1:60:A:PRO:C	1:61:A:VAL:N	13	6.23
(1,182)	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	1:113:A:GLY:N	18	6.22
(1,125)	1:93:A:SER:C	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	13	6.22
(1,104)	1:76:A:ASP:N	1:76:A:ASP:CA	1:76:A:ASP:C	1:77:A:GLU:N	9	6.22
(1,101)	1:74:A:GLY:C	1:75:A:GLU:N	1:75:A:GLU:CA	1:75:A:GLU:C	20	6.21
(1,100)	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	1:73:A:SER:N	7	6.21
(1,108)	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	1:79:A:ASN:N	7	6.2
(1,95)	1:68:A:GLU:C	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	8	6.2
(1,33)	1:20:A:TRP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	17	6.2
(1,124)	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	1:94:A:SER:N	20	6.17
(1,98)	1:71:A:CYS:N	1:71:A:CYS:CA	1:71:A:CYS:C	1:72:A:ASP:N	15	6.16
(1,56)	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	1:39:A:CYS:N	3	6.16
(1,33)	1:20:A:TRP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	13	6.15
(1,33)	1:20:A:TRP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	5	6.12
(1,93)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	8	6.09
(1,33)	1:20:A:TRP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	2	6.07
(1,58)	1:39:A:CYS:N	1:39:A:CYS:CA	1:39:A:CYS:C	1:40:A:HIS:N	20	6.06
(1,56)	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	1:39:A:CYS:N	17	6.06
(1,154)	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	1:112:A:ASP:N	15	6.05
(1,114)	1:85:A:CYS:N	1:85:A:CYS:CA	1:85:A:CYS:C	1:86:A:SER:N	16	6.05
(1,64)	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	1:50:A:SER:N	3	6.04
(1,144)	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	1:104:A:CYS:N	14	6.0
(1,100)	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	1:73:A:SER:N	15	5.99
(1,161)	1:116:A:GLU:C	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	16	5.98
(1,125)	1:93:A:SER:C	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	15	5.98
(1,159)	1:115:A:ASP:C	1:116:A:GLU:N	1:116:A:GLU:CA	1:116:A:GLU:C	5	5.96

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,100)	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	1:73:A:SER:N	11	5.96
(1,101)	1:74:A:GLY:C	1:75:A:GLU:N	1:75:A:GLU:CA	1:75:A:GLU:C	14	5.95
(1,149)	1:107:A:GLN:C	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	5	5.91
(1,159)	1:115:A:ASP:C	1:116:A:GLU:N	1:116:A:GLU:CA	1:116:A:GLU:C	6	5.89
(1,56)	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	1:39:A:CYS:N	13	5.89
(1,23)	1:14:A:GLN:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	11	5.86
(1,95)	1:68:A:GLU:C	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	15	5.84
(1,100)	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	1:73:A:SER:N	3	5.82
(1,58)	1:39:A:CYS:N	1:39:A:CYS:CA	1:39:A:CYS:C	1:40:A:HIS:N	6	5.77
(1,105)	1:76:A:ASP:C	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	1	5.76
(1,93)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	12	5.75
(1,93)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	14	5.73
(1,100)	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	1:73:A:SER:N	13	5.71
(1,109)	1:82:A:ASN:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	7	5.7
(1,100)	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	1:73:A:SER:N	9	5.7
(1,105)	1:76:A:ASP:C	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	19	5.68
(1,107)	1:77:A:GLU:C	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	4	5.67
(1,104)	1:76:A:ASP:N	1:76:A:ASP:CA	1:76:A:ASP:C	1:77:A:GLU:N	5	5.66
(1,33)	1:20:A:TRP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	11	5.66
(1,150)	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	1:109:A:ASP:N	10	5.62
(1,125)	1:93:A:SER:C	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	20	5.61
(1,93)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	15	5.59
(1,134)	1:98:A:ILE:N	1:98:A:ILE:CA	1:98:A:ILE:C	1:99:A:SER:N	8	5.55
(1,107)	1:77:A:GLU:C	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	11	5.55
(1,125)	1:93:A:SER:C	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	18	5.54
(1,121)	1:89:A:GLU:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	5	5.54
(1,127)	1:94:A:SER:C	1:95:A:GLY:N	1:95:A:GLY:CA	1:95:A:GLY:C	9	5.5
(1,74)	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	1:58:A:CYS:N	1	5.47
(1,114)	1:85:A:CYS:N	1:85:A:CYS:CA	1:85:A:CYS:C	1:86:A:SER:N	4	5.46
(1,101)	1:74:A:GLY:C	1:75:A:GLU:N	1:75:A:GLU:CA	1:75:A:GLU:C	12	5.42
(1,56)	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	1:39:A:CYS:N	16	5.42
(1,125)	1:93:A:SER:C	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	11	5.36
(1,123)	1:92:A:CYS:C	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	20	5.33
(1,109)	1:82:A:ASN:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	5	5.33
(1,125)	1:93:A:SER:C	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	12	5.32
(1,33)	1:20:A:TRP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	8	5.3
(1,74)	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	1:58:A:CYS:N	5	5.27
(1,159)	1:115:A:ASP:C	1:116:A:GLU:N	1:116:A:GLU:CA	1:116:A:GLU:C	15	5.26
(1,33)	1:20:A:TRP:C	1:21:A:LYS:N	1:21:A:LYS:CA	1:21:A:LYS:C	1	5.26
(1,30)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:ARG:N	14	5.24
(1,56)	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	1:39:A:CYS:N	7	5.23
(1,101)	1:74:A:GLY:C	1:75:A:GLU:N	1:75:A:GLU:CA	1:75:A:GLU:C	16	5.22
(1,56)	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	1:39:A:CYS:N	8	5.2
(1,100)	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	1:73:A:SER:N	5	5.14
(1,73)	1:56:A:THR:C	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	20	5.14
(1,159)	1:115:A:ASP:C	1:116:A:GLU:N	1:116:A:GLU:CA	1:116:A:GLU:C	3	5.13
(1,114)	1:85:A:CYS:N	1:85:A:CYS:CA	1:85:A:CYS:C	1:86:A:SER:N	13	5.13
(1,99)	1:71:A:CYS:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	17	5.11
(1,93)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	18	5.1
(1,100)	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	1:73:A:SER:N	16	5.08
(1,68)	1:53:A:ALA:N	1:53:A:ALA:CA	1:53:A:ALA:C	1:54:A:HIS:N	2	5.08

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,32)	1:19:A:ARG:N	1:19:A:ARG:CA	1:19:A:ARG:C	1:20:A:TRP:N	15	5.06
(1,159)	1:115:A:ASP:C	1:116:A:GLU:N	1:116:A:GLU:CA	1:116:A:GLU:C	17	5.02
(1,56)	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	1:39:A:CYS:N	11	5.02
(1,162)	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	1:118:A:ASP:N	16	5.01
(1,93)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	20	5.01
(1,74)	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	1:58:A:CYS:N	13	5.01
(1,32)	1:19:A:ARG:N	1:19:A:ARG:CA	1:19:A:ARG:C	1:20:A:TRP:N	14	5.01
(1,9)	1:7:A:ASP:C	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:C	11	5.0
(1,98)	1:71:A:CYS:N	1:71:A:CYS:CA	1:71:A:CYS:C	1:72:A:ASP:N	5	4.99
(1,159)	1:115:A:ASP:C	1:116:A:GLU:N	1:116:A:GLU:CA	1:116:A:GLU:C	19	4.98
(1,56)	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	1:39:A:CYS:N	1	4.98
(1,108)	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	1:79:A:ASN:N	9	4.96
(1,56)	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	1:39:A:CYS:N	4	4.89
(1,74)	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	1:58:A:CYS:N	8	4.88
(1,121)	1:89:A:GLU:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	9	4.87
(1,107)	1:77:A:GLU:C	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	9	4.83
(1,101)	1:74:A:GLY:C	1:75:A:GLU:N	1:75:A:GLU:CA	1:75:A:GLU:C	5	4.8
(1,100)	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	1:73:A:SER:N	20	4.8
(1,109)	1:82:A:ASN:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	17	4.79
(1,58)	1:39:A:CYS:N	1:39:A:CYS:CA	1:39:A:CYS:C	1:40:A:HIS:N	10	4.79
(1,73)	1:56:A:THR:C	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	4	4.75
(1,107)	1:77:A:GLU:C	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	7	4.74
(1,149)	1:107:A:GLN:C	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	19	4.73
(1,158)	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	1:116:A:GLU:N	11	4.71
(1,149)	1:107:A:GLN:C	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	14	4.71
(1,90)	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	1:67:A:GLY:N	15	4.7
(1,58)	1:39:A:CYS:N	1:39:A:CYS:CA	1:39:A:CYS:C	1:40:A:HIS:N	8	4.7
(1,56)	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	1:39:A:CYS:N	15	4.7
(1,42)	1:27:A:ASP:N	1:27:A:ASP:CA	1:27:A:ASP:C	1:28:A:CYS:N	8	4.7
(1,149)	1:107:A:GLN:C	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	20	4.66
(1,100)	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	1:73:A:SER:N	19	4.66
(1,128)	1:95:A:GLY:N	1:95:A:GLY:CA	1:95:A:GLY:C	1:96:A:ARG:N	18	4.62
(1,100)	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	1:73:A:SER:N	12	4.62
(1,108)	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	1:79:A:ASN:N	5	4.61
(1,72)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:THR:N	8	4.61
(1,100)	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	1:73:A:SER:N	1	4.58
(1,31)	1:18:A:SER:C	1:19:A:ARG:N	1:19:A:ARG:CA	1:19:A:ARG:C	19	4.58
(1,134)	1:98:A:ILE:N	1:98:A:ILE:CA	1:98:A:ILE:C	1:99:A:SER:N	3	4.54
(1,101)	1:74:A:GLY:C	1:75:A:GLU:N	1:75:A:GLU:CA	1:75:A:GLU:C	11	4.54
(1,99)	1:71:A:CYS:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	18	4.53
(1,30)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:ARG:N	4	4.53
(1,182)	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	1:113:A:GLY:N	17	4.52
(1,95)	1:68:A:GLU:C	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	14	4.52
(1,74)	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	1:58:A:CYS:N	19	4.52
(1,5)	1:4:A:ALA:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	12	4.5
(1,182)	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	1:113:A:GLY:N	12	4.49
(1,143)	1:102:A:PHE:C	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	9	4.47
(1,143)	1:102:A:PHE:C	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	17	4.47
(1,149)	1:107:A:GLN:C	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	11	4.46
(1,104)	1:76:A:ASP:N	1:76:A:ASP:CA	1:76:A:ASP:C	1:77:A:GLU:N	7	4.44
(1,114)	1:85:A:CYS:N	1:85:A:CYS:CA	1:85:A:CYS:C	1:86:A:SER:N	20	4.42

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,114)	1:85:A:CYS:N	1:85:A:CYS:CA	1:85:A:CYS:C	1:86:A:SER:N	11	4.41
(1,26)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:PRO:N	12	4.4
(1,159)	1:115:A:ASP:C	1:116:A:GLU:N	1:116:A:GLU:CA	1:116:A:GLU:C	13	4.38
(1,106)	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	1:78:A:GLU:N	13	4.38
(1,23)	1:14:A:GLN:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	19	4.36
(1,143)	1:102:A:PHE:C	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	6	4.35
(1,31)	1:18:A:SER:C	1:19:A:ARG:N	1:19:A:ARG:CA	1:19:A:ARG:C	16	4.34
(1,109)	1:82:A:ASN:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	18	4.31
(1,134)	1:98:A:ILE:N	1:98:A:ILE:CA	1:98:A:ILE:C	1:99:A:SER:N	4	4.28
(1,114)	1:85:A:CYS:N	1:85:A:CYS:CA	1:85:A:CYS:C	1:86:A:SER:N	8	4.27
(1,56)	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	1:39:A:CYS:N	5	4.27
(1,134)	1:98:A:ILE:N	1:98:A:ILE:CA	1:98:A:ILE:C	1:99:A:SER:N	6	4.24
(1,143)	1:102:A:PHE:C	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	2	4.23
(1,99)	1:71:A:CYS:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	5	4.23
(1,99)	1:71:A:CYS:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	4	4.22
(1,99)	1:71:A:CYS:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	14	4.22
(1,50)	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	1:36:A:PRO:N	5	4.22
(1,8)	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	1:7:A:ASP:N	12	4.21
(1,103)	1:75:A:GLU:C	1:76:A:ASP:N	1:76:A:ASP:CA	1:76:A:ASP:C	4	4.19
(1,101)	1:74:A:GLY:C	1:75:A:GLU:N	1:75:A:GLU:CA	1:75:A:GLU:C	3	4.18
(1,109)	1:82:A:ASN:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	11	4.17
(1,105)	1:76:A:ASP:C	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	7	4.16
(1,143)	1:102:A:PHE:C	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	7	4.14
(1,104)	1:76:A:ASP:N	1:76:A:ASP:CA	1:76:A:ASP:C	1:77:A:GLU:N	20	4.13
(1,159)	1:115:A:ASP:C	1:116:A:GLU:N	1:116:A:GLU:CA	1:116:A:GLU:C	1	4.12
(1,149)	1:107:A:GLN:C	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	15	4.11
(1,120)	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	1:90:A:PHE:N	9	4.11
(1,114)	1:85:A:CYS:N	1:85:A:CYS:CA	1:85:A:CYS:C	1:86:A:SER:N	10	4.09
(1,109)	1:82:A:ASN:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	4	4.09
(1,159)	1:115:A:ASP:C	1:116:A:GLU:N	1:116:A:GLU:CA	1:116:A:GLU:C	12	4.07
(1,114)	1:85:A:CYS:N	1:85:A:CYS:CA	1:85:A:CYS:C	1:86:A:SER:N	3	4.07
(1,109)	1:82:A:ASN:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	3	4.05
(1,109)	1:82:A:ASN:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	19	4.04
(1,31)	1:18:A:SER:C	1:19:A:ARG:N	1:19:A:ARG:CA	1:19:A:ARG:C	5	4.04
(1,159)	1:115:A:ASP:C	1:116:A:GLU:N	1:116:A:GLU:CA	1:116:A:GLU:C	4	3.99
(1,159)	1:115:A:ASP:C	1:116:A:GLU:N	1:116:A:GLU:CA	1:116:A:GLU:C	7	3.99
(1,64)	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	1:50:A:SER:N	17	3.96
(1,64)	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	1:50:A:SER:N	16	3.95
(1,56)	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	1:39:A:CYS:N	6	3.94
(1,154)	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	1:112:A:ASP:N	20	3.93
(1,107)	1:77:A:GLU:C	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	1	3.93
(1,8)	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	1:7:A:ASP:N	4	3.91
(1,134)	1:98:A:ILE:N	1:98:A:ILE:CA	1:98:A:ILE:C	1:99:A:SER:N	1	3.9
(1,56)	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	1:39:A:CYS:N	10	3.89
(1,5)	1:4:A:ALA:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	14	3.89
(1,100)	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	1:73:A:SER:N	14	3.88
(1,153)	1:110:A:CYS:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	18	3.87
(1,9)	1:7:A:ASP:C	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:C	16	3.87
(1,80)	1:60:A:PRO:N	1:60:A:PRO:CA	1:60:A:PRO:C	1:61:A:VAL:N	5	3.86
(1,50)	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	1:36:A:PRO:N	17	3.86
(1,144)	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	1:104:A:CYS:N	13	3.85

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,98)	1:71:A:CYS:N	1:71:A:CYS:CA	1:71:A:CYS:C	1:72:A:ASP:N	11	3.85
(1,56)	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	1:39:A:CYS:N	12	3.85
(1,74)	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	1:58:A:CYS:N	11	3.84
(1,58)	1:39:A:CYS:N	1:39:A:CYS:CA	1:39:A:CYS:C	1:40:A:HIS:N	14	3.84
(1,136)	1:99:A:SER:N	1:99:A:SER:CA	1:99:A:SER:C	1:100:A:ARG:N	20	3.83
(1,35)	1:21:A:LYS:C	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	19	3.82
(1,149)	1:107:A:GLN:C	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	4	3.81
(1,49)	1:34:A:GLU:C	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	3	3.81
(1,30)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:ARG:N	15	3.81
(1,143)	1:102:A:PHE:C	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	4	3.8
(1,107)	1:77:A:GLU:C	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	5	3.79
(1,143)	1:102:A:PHE:C	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	16	3.78
(1,26)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:PRO:N	20	3.78
(1,73)	1:56:A:THR:C	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	15	3.77
(1,64)	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	1:50:A:SER:N	6	3.75
(1,122)	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	1:91:A:THR:N	8	3.74
(1,92)	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	1:68:A:GLU:N	15	3.7
(1,44)	1:29:A:GLU:N	1:29:A:GLU:CA	1:29:A:GLU:C	1:30:A:ASP:N	12	3.69
(1,26)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:PRO:N	18	3.69
(1,99)	1:71:A:CYS:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	9	3.68
(1,50)	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	1:36:A:PRO:N	6	3.68
(1,9)	1:7:A:ASP:C	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:C	6	3.66
(1,80)	1:60:A:PRO:N	1:60:A:PRO:CA	1:60:A:PRO:C	1:61:A:VAL:N	9	3.64
(1,144)	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	1:104:A:CYS:N	15	3.63
(1,134)	1:98:A:ILE:N	1:98:A:ILE:CA	1:98:A:ILE:C	1:99:A:SER:N	7	3.63
(1,30)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:ARG:N	5	3.63
(1,106)	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	1:78:A:GLU:N	2	3.62
(1,102)	1:75:A:GLU:N	1:75:A:GLU:CA	1:75:A:GLU:C	1:76:A:ASP:N	10	3.62
(1,10)	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:C	1:9:A:VAL:N	4	3.62
(1,98)	1:71:A:CYS:N	1:71:A:CYS:CA	1:71:A:CYS:C	1:72:A:ASP:N	3	3.6
(1,65)	1:49:A:ILE:C	1:50:A:SER:N	1:50:A:SER:CA	1:50:A:SER:C	18	3.59
(1,88)	1:65:A:CYS:N	1:65:A:CYS:CA	1:65:A:CYS:C	1:66:A:ASP:N	8	3.58
(1,56)	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	1:39:A:CYS:N	9	3.58
(1,50)	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	1:36:A:PRO:N	13	3.58
(1,109)	1:82:A:ASN:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	15	3.57
(1,154)	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	1:112:A:ASP:N	13	3.55
(1,127)	1:94:A:SER:C	1:95:A:GLY:N	1:95:A:GLY:CA	1:95:A:GLY:C	14	3.53
(1,35)	1:21:A:LYS:C	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	2	3.52
(1,56)	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	1:39:A:CYS:N	2	3.49
(1,64)	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	1:50:A:SER:N	9	3.46
(1,154)	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	1:112:A:ASP:N	11	3.44
(1,154)	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	1:112:A:ASP:N	12	3.44
(1,50)	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	1:36:A:PRO:N	20	3.44
(1,122)	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	1:91:A:THR:N	10	3.43
(1,5)	1:4:A:ALA:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	9	3.43
(1,56)	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	1:39:A:CYS:N	18	3.42
(1,98)	1:71:A:CYS:N	1:71:A:CYS:CA	1:71:A:CYS:C	1:72:A:ASP:N	9	3.41
(1,107)	1:77:A:GLU:C	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	3	3.4
(1,182)	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	1:113:A:GLY:N	20	3.39
(1,77)	1:58:A:CYS:C	1:59:A:ILE:N	1:59:A:ILE:CA	1:59:A:ILE:C	10	3.37
(1,101)	1:74:A:GLY:C	1:75:A:GLU:N	1:75:A:GLU:CA	1:75:A:GLU:C	10	3.36

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,9)	1:7:A:ASP:C	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:C	10	3.36
(1,104)	1:76:A:ASP:N	1:76:A:ASP:CA	1:76:A:ASP:C	1:77:A:GLU:N	19	3.34
(1,130)	1:96:A:ARG:N	1:96:A:ARG:CA	1:96:A:ARG:C	1:97:A:CYS:N	10	3.33
(1,114)	1:85:A:CYS:N	1:85:A:CYS:CA	1:85:A:CYS:C	1:86:A:SER:N	14	3.33
(1,109)	1:82:A:ASN:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	13	3.33
(1,161)	1:116:A:GLU:C	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	6	3.32
(1,101)	1:74:A:GLY:C	1:75:A:GLU:N	1:75:A:GLU:CA	1:75:A:GLU:C	19	3.32
(1,79)	1:59:A:ILE:C	1:60:A:PRO:N	1:60:A:PRO:CA	1:60:A:PRO:C	8	3.29
(1,147)	1:106:A:GLY:C	1:107:A:GLN:N	1:107:A:GLN:CA	1:107:A:GLN:C	9	3.26
(1,50)	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	1:36:A:PRO:N	16	3.26
(1,80)	1:60:A:PRO:N	1:60:A:PRO:CA	1:60:A:PRO:C	1:61:A:VAL:N	17	3.25
(1,159)	1:115:A:ASP:C	1:116:A:GLU:N	1:116:A:GLU:CA	1:116:A:GLU:C	20	3.23
(1,138)	1:100:A:ARG:N	1:100:A:ARG:CA	1:100:A:ARG:C	1:101:A:ASN:N	17	3.2
(1,23)	1:14:A:GLN:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	2	3.18
(1,107)	1:77:A:GLU:C	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	19	3.17
(1,26)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:PRO:N	3	3.17
(1,5)	1:4:A:ALA:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	11	3.17
(1,124)	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	1:94:A:SER:N	18	3.16
(1,159)	1:115:A:ASP:C	1:116:A:GLU:N	1:116:A:GLU:CA	1:116:A:GLU:C	11	3.15
(1,138)	1:100:A:ARG:N	1:100:A:ARG:CA	1:100:A:ARG:C	1:101:A:ASN:N	5	3.14
(1,99)	1:71:A:CYS:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	1	3.14
(1,50)	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	1:36:A:PRO:N	1	3.14
(1,150)	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	1:109:A:ASP:N	12	3.12
(1,149)	1:107:A:GLN:C	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	13	3.12
(1,147)	1:106:A:GLY:C	1:107:A:GLN:N	1:107:A:GLN:CA	1:107:A:GLN:C	4	3.12
(1,74)	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	1:58:A:CYS:N	16	3.12
(1,122)	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	1:91:A:THR:N	7	3.11
(1,109)	1:82:A:ASN:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	12	3.11
(1,56)	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	1:39:A:CYS:N	14	3.11
(1,100)	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	1:73:A:SER:N	4	3.1
(1,9)	1:7:A:ASP:C	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:C	12	3.1
(1,124)	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	1:94:A:SER:N	13	3.09
(1,182)	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	1:113:A:GLY:N	13	3.08
(1,81)	1:60:A:PRO:C	1:61:A:VAL:N	1:61:A:VAL:CA	1:61:A:VAL:C	17	3.08
(1,99)	1:71:A:CYS:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	16	3.05
(1,30)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:ARG:N	1	3.05
(1,44)	1:29:A:GLU:N	1:29:A:GLU:CA	1:29:A:GLU:C	1:30:A:ASP:N	13	3.03
(1,23)	1:14:A:GLN:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	7	3.03
(1,80)	1:60:A:PRO:N	1:60:A:PRO:CA	1:60:A:PRO:C	1:61:A:VAL:N	2	3.0
(1,9)	1:7:A:ASP:C	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:C	7	3.0
(1,107)	1:77:A:GLU:C	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	18	2.98
(1,42)	1:27:A:ASP:N	1:27:A:ASP:CA	1:27:A:ASP:C	1:28:A:CYS:N	6	2.98
(1,101)	1:74:A:GLY:C	1:75:A:GLU:N	1:75:A:GLU:CA	1:75:A:GLU:C	7	2.97
(1,101)	1:74:A:GLY:C	1:75:A:GLU:N	1:75:A:GLU:CA	1:75:A:GLU:C	15	2.96
(1,150)	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	1:109:A:ASP:N	18	2.95
(1,120)	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	1:90:A:PHE:N	5	2.94
(1,30)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:ARG:N	12	2.94
(1,55)	1:37:A:GLU:C	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	19	2.93
(1,49)	1:34:A:GLU:C	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	13	2.89
(1,58)	1:39:A:CYS:N	1:39:A:CYS:CA	1:39:A:CYS:C	1:40:A:HIS:N	2	2.87
(1,147)	1:106:A:GLY:C	1:107:A:GLN:N	1:107:A:GLN:CA	1:107:A:GLN:C	7	2.86

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,74)	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	1:58:A:CYS:N	9	2.86
(1,35)	1:21:A:LYS:C	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	11	2.83
(1,107)	1:77:A:GLU:C	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	14	2.82
(1,35)	1:21:A:LYS:C	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	1	2.82
(1,95)	1:68:A:GLU:C	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	18	2.81
(1,23)	1:14:A:GLN:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	16	2.81
(1,98)	1:71:A:CYS:N	1:71:A:CYS:CA	1:71:A:CYS:C	1:72:A:ASP:N	16	2.8
(1,70)	1:54:A:HIS:N	1:54:A:HIS:CA	1:54:A:HIS:C	1:55:A:SER:N	2	2.78
(1,49)	1:34:A:GLU:C	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	9	2.78
(1,100)	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	1:73:A:SER:N	18	2.77
(1,23)	1:14:A:GLN:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	12	2.77
(1,107)	1:77:A:GLU:C	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	15	2.76
(1,64)	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	1:50:A:SER:N	1	2.76
(1,5)	1:4:A:ALA:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	6	2.74
(1,122)	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	1:91:A:THR:N	5	2.73
(1,109)	1:82:A:ASN:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	14	2.73
(1,101)	1:74:A:GLY:C	1:75:A:GLU:N	1:75:A:GLU:CA	1:75:A:GLU:C	17	2.73
(1,35)	1:21:A:LYS:C	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	17	2.72
(1,30)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:ARG:N	8	2.71
(1,4)	1:3:A:CYS:N	1:3:A:CYS:CA	1:3:A:CYS:C	1:4:A:ALA:N	20	2.71
(1,128)	1:95:A:GLY:N	1:95:A:GLY:CA	1:95:A:GLY:C	1:96:A:ARG:N	14	2.7
(1,114)	1:85:A:CYS:N	1:85:A:CYS:CA	1:85:A:CYS:C	1:86:A:SER:N	5	2.7
(1,50)	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	1:36:A:PRO:N	9	2.69
(1,99)	1:71:A:CYS:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	7	2.68
(1,100)	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	1:73:A:SER:N	17	2.67
(1,99)	1:71:A:CYS:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	3	2.67
(1,74)	1:57:A:GLN:N	1:57:A:GLN:CA	1:57:A:GLN:C	1:58:A:CYS:N	3	2.63
(1,91)	1:66:A:ASP:C	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	18	2.6
(1,80)	1:60:A:PRO:N	1:60:A:PRO:CA	1:60:A:PRO:C	1:61:A:VAL:N	11	2.6
(1,26)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:PRO:N	17	2.6
(1,10)	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:C	1:9:A:VAL:N	12	2.6
(1,16)	1:11:A:ASN:N	1:11:A:ASN:CA	1:11:A:ASN:C	1:12:A:ASN:N	5	2.59
(1,109)	1:82:A:ASN:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	2	2.57
(1,68)	1:53:A:ALA:N	1:53:A:ALA:CA	1:53:A:ALA:C	1:54:A:HIS:N	17	2.56
(1,114)	1:85:A:CYS:N	1:85:A:CYS:CA	1:85:A:CYS:C	1:86:A:SER:N	12	2.55
(1,99)	1:71:A:CYS:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	11	2.55
(1,35)	1:21:A:LYS:C	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	16	2.54
(1,90)	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	1:67:A:GLY:N	12	2.53
(1,23)	1:14:A:GLN:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	15	2.52
(1,49)	1:34:A:GLU:C	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	7	2.51
(1,144)	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	1:104:A:CYS:N	9	2.5
(1,49)	1:34:A:GLU:C	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	2	2.5
(1,23)	1:14:A:GLN:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	20	2.5
(1,138)	1:100:A:ARG:N	1:100:A:ARG:CA	1:100:A:ARG:C	1:101:A:ASN:N	12	2.49
(1,159)	1:115:A:ASP:C	1:116:A:GLU:N	1:116:A:GLU:CA	1:116:A:GLU:C	2	2.46
(1,31)	1:18:A:SER:C	1:19:A:ARG:N	1:19:A:ARG:CA	1:19:A:ARG:C	7	2.46
(1,114)	1:85:A:CYS:N	1:85:A:CYS:CA	1:85:A:CYS:C	1:86:A:SER:N	17	2.45
(1,55)	1:37:A:GLU:C	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	6	2.45
(1,109)	1:82:A:ASN:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	6	2.44
(1,26)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:PRO:N	14	2.43
(1,159)	1:115:A:ASP:C	1:116:A:GLU:N	1:116:A:GLU:CA	1:116:A:GLU:C	8	2.41

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,182)	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	1:113:A:GLY:N	14	2.4
(1,108)	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	1:79:A:ASN:N	10	2.38
(1,114)	1:85:A:CYS:N	1:85:A:CYS:CA	1:85:A:CYS:C	1:86:A:SER:N	19	2.37
(1,103)	1:75:A:GLU:C	1:76:A:ASP:N	1:76:A:ASP:CA	1:76:A:ASP:C	2	2.36
(1,103)	1:75:A:GLU:C	1:76:A:ASP:N	1:76:A:ASP:CA	1:76:A:ASP:C	14	2.35
(1,23)	1:14:A:GLN:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	4	2.35
(1,4)	1:3:A:CYS:N	1:3:A:CYS:CA	1:3:A:CYS:C	1:4:A:ALA:N	17	2.35
(1,64)	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	1:50:A:SER:N	19	2.34
(1,7)	1:5:A:GLU:C	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	15	2.33
(1,138)	1:100:A:ARG:N	1:100:A:ARG:CA	1:100:A:ARG:C	1:101:A:ASN:N	8	2.31
(1,50)	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	1:36:A:PRO:N	3	2.29
(1,9)	1:7:A:ASP:C	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:C	9	2.29
(1,109)	1:82:A:ASN:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	20	2.28
(1,42)	1:27:A:ASP:N	1:27:A:ASP:CA	1:27:A:ASP:C	1:28:A:CYS:N	16	2.28
(1,44)	1:29:A:GLU:N	1:29:A:GLU:CA	1:29:A:GLU:C	1:30:A:ASP:N	20	2.27
(1,127)	1:94:A:SER:C	1:95:A:GLY:N	1:95:A:GLY:CA	1:95:A:GLY:C	10	2.26
(1,64)	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	1:50:A:SER:N	20	2.25
(1,159)	1:115:A:ASP:C	1:116:A:GLU:N	1:116:A:GLU:CA	1:116:A:GLU:C	9	2.24
(1,106)	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	1:78:A:GLU:N	8	2.24
(1,5)	1:4:A:ALA:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	4	2.24
(1,113)	1:84:A:THR:C	1:85:A:CYS:N	1:85:A:CYS:CA	1:85:A:CYS:C	4	2.23
(1,80)	1:60:A:PRO:N	1:60:A:PRO:CA	1:60:A:PRO:C	1:61:A:VAL:N	20	2.23
(1,13)	1:9:A:VAL:C	1:10:A:CYS:N	1:10:A:CYS:CA	1:10:A:CYS:C	3	2.23
(1,151)	1:109:A:ASP:C	1:110:A:CYS:N	1:110:A:CYS:CA	1:110:A:CYS:C	17	2.22
(1,138)	1:100:A:ARG:N	1:100:A:ARG:CA	1:100:A:ARG:C	1:101:A:ASN:N	11	2.22
(1,26)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:PRO:N	4	2.21
(1,138)	1:100:A:ARG:N	1:100:A:ARG:CA	1:100:A:ARG:C	1:101:A:ASN:N	1	2.2
(1,88)	1:65:A:CYS:N	1:65:A:CYS:CA	1:65:A:CYS:C	1:66:A:ASP:N	10	2.2
(1,98)	1:71:A:CYS:N	1:71:A:CYS:CA	1:71:A:CYS:C	1:72:A:ASP:N	1	2.19
(1,81)	1:60:A:PRO:C	1:61:A:VAL:N	1:61:A:VAL:CA	1:61:A:VAL:C	1	2.18
(1,159)	1:115:A:ASP:C	1:116:A:GLU:N	1:116:A:GLU:CA	1:116:A:GLU:C	10	2.17
(1,124)	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	1:94:A:SER:N	12	2.17
(1,141)	1:101:A:ASN:C	1:102:A:PHE:N	1:102:A:PHE:CA	1:102:A:PHE:C	9	2.13
(1,67)	1:52:A:GLY:C	1:53:A:ALA:N	1:53:A:ALA:CA	1:53:A:ALA:C	8	2.13
(1,10)	1:8:A:PHE:N	1:8:A:PHE:CA	1:8:A:PHE:C	1:9:A:VAL:N	14	2.13
(1,160)	1:116:A:GLU:N	1:116:A:GLU:CA	1:116:A:GLU:C	1:117:A:LEU:N	9	2.12
(1,50)	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	1:36:A:PRO:N	7	2.11
(1,32)	1:19:A:ARG:N	1:19:A:ARG:CA	1:19:A:ARG:C	1:20:A:TRP:N	18	2.11
(1,30)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:ARG:N	2	2.11
(1,182)	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	1:113:A:GLY:N	1	2.1
(1,149)	1:107:A:GLN:C	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	7	2.1
(1,103)	1:75:A:GLU:C	1:76:A:ASP:N	1:76:A:ASP:CA	1:76:A:ASP:C	13	2.1
(1,98)	1:71:A:CYS:N	1:71:A:CYS:CA	1:71:A:CYS:C	1:72:A:ASP:N	8	2.09
(1,136)	1:99:A:SER:N	1:99:A:SER:CA	1:99:A:SER:C	1:100:A:ARG:N	13	2.08
(1,107)	1:77:A:GLU:C	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	20	2.08
(1,23)	1:14:A:GLN:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	17	2.08
(1,161)	1:116:A:GLU:C	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	12	2.07
(1,130)	1:96:A:ARG:N	1:96:A:ARG:CA	1:96:A:ARG:C	1:97:A:CYS:N	20	2.07
(1,31)	1:18:A:SER:C	1:19:A:ARG:N	1:19:A:ARG:CA	1:19:A:ARG:C	11	2.07
(1,30)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:ARG:N	6	2.04
(1,177)	1:91:A:THR:C	1:92:A:CYS:N	1:92:A:CYS:CA	1:92:A:CYS:C	9	2.02

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,131)	1:96:A:ARG:C	1:97:A:CYS:N	1:97:A:CYS:CA	1:97:A:CYS:C	13	2.02
(1,14)	1:10:A:CYS:N	1:10:A:CYS:CA	1:10:A:CYS:C	1:11:A:ASN:N	8	2.02
(1,5)	1:4:A:ALA:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	19	2.02
(1,103)	1:75:A:GLU:C	1:76:A:ASP:N	1:76:A:ASP:CA	1:76:A:ASP:C	17	2.01
(1,50)	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	1:36:A:PRO:N	4	2.01
(1,50)	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	1:36:A:PRO:N	12	2.0
(1,114)	1:85:A:CYS:N	1:85:A:CYS:CA	1:85:A:CYS:C	1:86:A:SER:N	15	1.99
(1,55)	1:37:A:GLU:C	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	8	1.97
(1,30)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:ARG:N	17	1.97
(1,30)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:ARG:N	18	1.97
(1,160)	1:116:A:GLU:N	1:116:A:GLU:CA	1:116:A:GLU:C	1:117:A:LEU:N	7	1.96
(1,50)	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	1:36:A:PRO:N	2	1.96
(1,157)	1:114:A:SER:C	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	9	1.95
(1,143)	1:102:A:PHE:C	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	5	1.95
(1,35)	1:21:A:LYS:C	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	13	1.95
(1,3)	1:2:A:THR:C	1:3:A:CYS:N	1:3:A:CYS:CA	1:3:A:CYS:C	20	1.95
(1,161)	1:116:A:GLU:C	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	18	1.94
(1,138)	1:100:A:ARG:N	1:100:A:ARG:CA	1:100:A:ARG:C	1:101:A:ASN:N	4	1.94
(1,125)	1:93:A:SER:C	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	8	1.94
(1,114)	1:85:A:CYS:N	1:85:A:CYS:CA	1:85:A:CYS:C	1:86:A:SER:N	6	1.94
(1,136)	1:99:A:SER:N	1:99:A:SER:CA	1:99:A:SER:C	1:100:A:ARG:N	15	1.93
(1,128)	1:95:A:GLY:N	1:95:A:GLY:CA	1:95:A:GLY:C	1:96:A:ARG:N	20	1.93
(1,80)	1:60:A:PRO:N	1:60:A:PRO:CA	1:60:A:PRO:C	1:61:A:VAL:N	1	1.93
(1,49)	1:34:A:GLU:C	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	1	1.93
(1,153)	1:110:A:CYS:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	15	1.92
(1,35)	1:21:A:LYS:C	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	7	1.92
(1,5)	1:4:A:ALA:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	5	1.92
(1,138)	1:100:A:ARG:N	1:100:A:ARG:CA	1:100:A:ARG:C	1:101:A:ASN:N	18	1.9
(1,130)	1:96:A:ARG:N	1:96:A:ARG:CA	1:96:A:ARG:C	1:97:A:CYS:N	8	1.9
(1,81)	1:60:A:PRO:C	1:61:A:VAL:N	1:61:A:VAL:CA	1:61:A:VAL:C	16	1.89
(1,49)	1:34:A:GLU:C	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	17	1.89
(1,2)	1:2:A:THR:N	1:2:A:THR:CA	1:2:A:THR:C	1:3:A:CYS:N	20	1.89
(1,144)	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	1:104:A:CYS:N	16	1.88
(1,35)	1:21:A:LYS:C	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	20	1.88
(1,13)	1:9:A:VAL:C	1:10:A:CYS:N	1:10:A:CYS:CA	1:10:A:CYS:C	18	1.88
(1,44)	1:29:A:GLU:N	1:29:A:GLU:CA	1:29:A:GLU:C	1:30:A:ASP:N	11	1.87
(1,138)	1:100:A:ARG:N	1:100:A:ARG:CA	1:100:A:ARG:C	1:101:A:ASN:N	13	1.86
(1,153)	1:110:A:CYS:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	14	1.84
(1,145)	1:105:A:ASN:C	1:106:A:GLY:N	1:106:A:GLY:CA	1:106:A:GLY:C	11	1.84
(1,13)	1:9:A:VAL:C	1:10:A:CYS:N	1:10:A:CYS:CA	1:10:A:CYS:C	19	1.84
(1,55)	1:37:A:GLU:C	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	9	1.83
(1,7)	1:5:A:GLU:C	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	14	1.83
(1,151)	1:109:A:ASP:C	1:110:A:CYS:N	1:110:A:CYS:CA	1:110:A:CYS:C	9	1.81
(1,80)	1:60:A:PRO:N	1:60:A:PRO:CA	1:60:A:PRO:C	1:61:A:VAL:N	6	1.81
(1,70)	1:54:A:HIS:N	1:54:A:HIS:CA	1:54:A:HIS:C	1:55:A:SER:N	4	1.81
(1,23)	1:14:A:GLN:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	5	1.81
(1,122)	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	1:91:A:THR:N	6	1.8
(1,95)	1:68:A:GLU:C	1:69:A:ASN:N	1:69:A:ASN:CA	1:69:A:ASN:C	4	1.8
(1,54)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:GLN:N	18	1.8
(1,51)	1:35:A:SER:C	1:36:A:PRO:N	1:36:A:PRO:CA	1:36:A:PRO:C	10	1.8
(1,149)	1:107:A:GLN:C	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	18	1.79

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,150)	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	1:109:A:ASP:N	11	1.78
(1,97)	1:70:A:ASP:C	1:71:A:CYS:N	1:71:A:CYS:CA	1:71:A:CYS:C	18	1.78
(1,55)	1:37:A:GLU:C	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	20	1.77
(1,32)	1:19:A:ARG:N	1:19:A:ARG:CA	1:19:A:ARG:C	1:20:A:TRP:N	3	1.77
(1,30)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:ARG:N	10	1.77
(1,23)	1:14:A:GLN:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	14	1.77
(1,107)	1:77:A:GLU:C	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	10	1.76
(1,32)	1:19:A:ARG:N	1:19:A:ARG:CA	1:19:A:ARG:C	1:20:A:TRP:N	10	1.76
(1,181)	1:111:A:SER:C	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	6	1.75
(1,143)	1:102:A:PHE:C	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	19	1.75
(1,99)	1:71:A:CYS:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	19	1.75
(1,54)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:GLN:N	6	1.75
(1,49)	1:34:A:GLU:C	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	6	1.73
(1,54)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:GLN:N	9	1.71
(1,50)	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	1:36:A:PRO:N	8	1.71
(1,3)	1:2:A:THR:C	1:3:A:CYS:N	1:3:A:CYS:CA	1:3:A:CYS:C	8	1.71
(1,26)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:PRO:N	8	1.7
(1,145)	1:105:A:ASN:C	1:106:A:GLY:N	1:106:A:GLY:CA	1:106:A:GLY:C	14	1.69
(1,44)	1:29:A:GLU:N	1:29:A:GLU:CA	1:29:A:GLU:C	1:30:A:ASP:N	16	1.69
(1,31)	1:18:A:SER:C	1:19:A:ARG:N	1:19:A:ARG:CA	1:19:A:ARG:C	6	1.69
(1,128)	1:95:A:GLY:N	1:95:A:GLY:CA	1:95:A:GLY:C	1:96:A:ARG:N	15	1.68
(1,150)	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	1:109:A:ASP:N	13	1.67
(1,128)	1:95:A:GLY:N	1:95:A:GLY:CA	1:95:A:GLY:C	1:96:A:ARG:N	12	1.67
(1,149)	1:107:A:GLN:C	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	12	1.66
(1,49)	1:34:A:GLU:C	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	20	1.66
(1,122)	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	1:91:A:THR:N	9	1.65
(1,80)	1:60:A:PRO:N	1:60:A:PRO:CA	1:60:A:PRO:C	1:61:A:VAL:N	15	1.65
(1,49)	1:34:A:GLU:C	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	16	1.65
(1,15)	1:10:A:CYS:C	1:11:A:ASN:N	1:11:A:ASN:CA	1:11:A:ASN:C	5	1.64
(1,13)	1:9:A:VAL:C	1:10:A:CYS:N	1:10:A:CYS:CA	1:10:A:CYS:C	7	1.64
(1,181)	1:111:A:SER:C	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	14	1.63
(1,133)	1:97:A:CYS:C	1:98:A:ILE:N	1:98:A:ILE:CA	1:98:A:ILE:C	11	1.63
(1,103)	1:75:A:GLU:C	1:76:A:ASP:N	1:76:A:ASP:CA	1:76:A:ASP:C	15	1.63
(1,63)	1:48:A:GLU:C	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	15	1.63
(1,31)	1:18:A:SER:C	1:19:A:ARG:N	1:19:A:ARG:CA	1:19:A:ARG:C	13	1.63
(1,157)	1:114:A:SER:C	1:115:A:ASP:N	1:115:A:ASP:CA	1:115:A:ASP:C	16	1.62
(1,138)	1:100:A:ARG:N	1:100:A:ARG:CA	1:100:A:ARG:C	1:101:A:ASN:N	6	1.62
(1,161)	1:116:A:GLU:C	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	11	1.61
(1,6)	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	1:6:A:SER:N	3	1.6
(1,23)	1:14:A:GLN:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	8	1.59
(1,23)	1:14:A:GLN:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	9	1.59
(1,134)	1:98:A:ILE:N	1:98:A:ILE:CA	1:98:A:ILE:C	1:99:A:SER:N	10	1.57
(1,23)	1:14:A:GLN:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	13	1.57
(1,5)	1:4:A:ALA:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	1	1.57
(1,161)	1:116:A:GLU:C	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	14	1.56
(1,138)	1:100:A:ARG:N	1:100:A:ARG:CA	1:100:A:ARG:C	1:101:A:ASN:N	2	1.56
(1,19)	1:12:A:ASN:C	1:13:A:GLY:N	1:13:A:GLY:CA	1:13:A:GLY:C	12	1.56
(1,7)	1:5:A:GLU:C	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	20	1.56
(1,23)	1:14:A:GLN:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	10	1.55
(1,83)	1:61:A:VAL:C	1:62:A:SER:N	1:62:A:SER:CA	1:62:A:SER:C	15	1.54
(1,54)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:GLN:N	13	1.54

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,127)	1:94:A:SER:C	1:95:A:GLY:N	1:95:A:GLY:CA	1:95:A:GLY:C	15	1.53
(1,42)	1:27:A:ASP:N	1:27:A:ASP:CA	1:27:A:ASP:C	1:28:A:CYS:N	4	1.52
(1,149)	1:107:A:GLN:C	1:108:A:ASP:N	1:108:A:ASP:CA	1:108:A:ASP:C	9	1.51
(1,32)	1:19:A:ARG:N	1:19:A:ARG:CA	1:19:A:ARG:C	1:20:A:TRP:N	19	1.51
(1,136)	1:99:A:SER:N	1:99:A:SER:CA	1:99:A:SER:C	1:100:A:ARG:N	11	1.5
(1,97)	1:70:A:ASP:C	1:71:A:CYS:N	1:71:A:CYS:CA	1:71:A:CYS:C	14	1.5
(1,5)	1:4:A:ALA:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	2	1.5
(1,138)	1:100:A:ARG:N	1:100:A:ARG:CA	1:100:A:ARG:C	1:101:A:ASN:N	19	1.49
(1,132)	1:97:A:CYS:N	1:97:A:CYS:CA	1:97:A:CYS:C	1:98:A:ILE:N	9	1.49
(1,30)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:ARG:N	20	1.49
(1,5)	1:4:A:ALA:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	17	1.49
(1,120)	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	1:90:A:PHE:N	19	1.48
(1,30)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:ARG:N	3	1.48
(1,109)	1:82:A:ASN:C	1:83:A:ILE:N	1:83:A:ILE:CA	1:83:A:ILE:C	10	1.47
(1,55)	1:37:A:GLU:C	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	10	1.47
(1,132)	1:97:A:CYS:N	1:97:A:CYS:CA	1:97:A:CYS:C	1:98:A:ILE:N	15	1.46
(1,128)	1:95:A:GLY:N	1:95:A:GLY:CA	1:95:A:GLY:C	1:96:A:ARG:N	13	1.46
(1,90)	1:66:A:ASP:N	1:66:A:ASP:CA	1:66:A:ASP:C	1:67:A:GLY:N	8	1.46
(1,55)	1:37:A:GLU:C	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	11	1.46
(1,153)	1:110:A:CYS:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	13	1.45
(1,161)	1:116:A:GLU:C	1:117:A:LEU:N	1:117:A:LEU:CA	1:117:A:LEU:C	15	1.44
(1,5)	1:4:A:ALA:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	8	1.43
(1,113)	1:84:A:THR:C	1:85:A:CYS:N	1:85:A:CYS:CA	1:85:A:CYS:C	10	1.42
(1,49)	1:34:A:GLU:C	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	8	1.42
(1,31)	1:18:A:SER:C	1:19:A:ARG:N	1:19:A:ARG:CA	1:19:A:ARG:C	17	1.41
(1,130)	1:96:A:ARG:N	1:96:A:ARG:CA	1:96:A:ARG:C	1:97:A:CYS:N	4	1.39
(1,125)	1:93:A:SER:C	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	1	1.39
(1,177)	1:91:A:THR:C	1:92:A:CYS:N	1:92:A:CYS:CA	1:92:A:CYS:C	16	1.37
(1,70)	1:54:A:HIS:N	1:54:A:HIS:CA	1:54:A:HIS:C	1:55:A:SER:N	13	1.36
(1,50)	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	1:36:A:PRO:N	14	1.36
(1,35)	1:21:A:LYS:C	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	9	1.36
(1,19)	1:12:A:ASN:C	1:13:A:GLY:N	1:13:A:GLY:CA	1:13:A:GLY:C	18	1.36
(1,88)	1:65:A:CYS:N	1:65:A:CYS:CA	1:65:A:CYS:C	1:66:A:ASP:N	3	1.34
(1,182)	1:112:A:ASP:N	1:112:A:ASP:CA	1:112:A:ASP:C	1:113:A:GLY:N	15	1.32
(1,27)	1:16:A:VAL:C	1:17:A:PRO:N	1:17:A:PRO:CA	1:17:A:PRO:C	6	1.32
(1,21)	1:13:A:GLY:C	1:14:A:GLN:N	1:14:A:GLN:CA	1:14:A:GLN:C	4	1.31
(1,144)	1:103:A:VAL:N	1:103:A:VAL:CA	1:103:A:VAL:C	1:104:A:CYS:N	20	1.3
(1,30)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:ARG:N	16	1.3
(1,66)	1:50:A:SER:N	1:50:A:SER:CA	1:50:A:SER:C	1:51:A:CYS:N	8	1.29
(1,61)	1:47:A:HIS:C	1:48:A:GLU:N	1:48:A:GLU:CA	1:48:A:GLU:C	6	1.29
(1,32)	1:19:A:ARG:N	1:19:A:ARG:CA	1:19:A:ARG:C	1:20:A:TRP:N	17	1.29
(1,31)	1:18:A:SER:C	1:19:A:ARG:N	1:19:A:ARG:CA	1:19:A:ARG:C	2	1.29
(1,23)	1:14:A:GLN:C	1:15:A:CYS:N	1:15:A:CYS:CA	1:15:A:CYS:C	6	1.29
(1,112)	1:84:A:THR:N	1:84:A:THR:CA	1:84:A:THR:C	1:85:A:CYS:N	1	1.28
(1,72)	1:55:A:SER:N	1:55:A:SER:CA	1:55:A:SER:C	1:56:A:THR:N	10	1.28
(1,21)	1:13:A:GLY:C	1:14:A:GLN:N	1:14:A:GLN:CA	1:14:A:GLN:C	17	1.28
(1,135)	1:98:A:ILE:C	1:99:A:SER:N	1:99:A:SER:CA	1:99:A:SER:C	16	1.27
(1,131)	1:96:A:ARG:C	1:97:A:CYS:N	1:97:A:CYS:CA	1:97:A:CYS:C	12	1.27
(1,32)	1:19:A:ARG:N	1:19:A:ARG:CA	1:19:A:ARG:C	1:20:A:TRP:N	20	1.27
(1,8)	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	1:7:A:ASP:N	15	1.27
(1,2)	1:2:A:THR:N	1:2:A:THR:CA	1:2:A:THR:C	1:3:A:CYS:N	1	1.27

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,160)	1:116:A:GLU:N	1:116:A:GLU:CA	1:116:A:GLU:C	1:117:A:LEU:N	4	1.26
(1,30)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:ARG:N	7	1.26
(1,18)	1:12:A:ASN:N	1:12:A:ASN:CA	1:12:A:ASN:C	1:13:A:GLY:N	17	1.26
(1,27)	1:16:A:VAL:C	1:17:A:PRO:N	1:17:A:PRO:CA	1:17:A:PRO:C	8	1.25
(1,132)	1:97:A:CYS:N	1:97:A:CYS:CA	1:97:A:CYS:C	1:98:A:ILE:N	16	1.24
(1,131)	1:96:A:ARG:C	1:97:A:CYS:N	1:97:A:CYS:CA	1:97:A:CYS:C	11	1.24
(1,101)	1:74:A:GLY:C	1:75:A:GLU:N	1:75:A:GLU:CA	1:75:A:GLU:C	1	1.24
(1,42)	1:27:A:ASP:N	1:27:A:ASP:CA	1:27:A:ASP:C	1:28:A:CYS:N	5	1.24
(1,16)	1:11:A:ASN:N	1:11:A:ASN:CA	1:11:A:ASN:C	1:12:A:ASN:N	10	1.24
(1,2)	1:2:A:THR:N	1:2:A:THR:CA	1:2:A:THR:C	1:3:A:CYS:N	8	1.24
(1,7)	1:5:A:GLU:C	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	10	1.23
(1,126)	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	1:95:A:GLY:N	17	1.22
(1,116)	1:87:A:PRO:N	1:87:A:PRO:CA	1:87:A:PRO:C	1:88:A:ASP:N	10	1.22
(1,99)	1:71:A:CYS:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	12	1.22
(1,49)	1:34:A:GLU:C	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	5	1.22
(1,50)	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	1:36:A:PRO:N	11	1.21
(1,121)	1:89:A:GLU:C	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	2	1.2
(1,55)	1:37:A:GLU:C	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	16	1.2
(1,153)	1:110:A:CYS:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	12	1.19
(1,120)	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	1:90:A:PHE:N	1	1.19
(1,120)	1:89:A:GLU:N	1:89:A:GLU:CA	1:89:A:GLU:C	1:90:A:PHE:N	2	1.19
(1,54)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:GLN:N	7	1.19
(1,32)	1:19:A:ARG:N	1:19:A:ARG:CA	1:19:A:ARG:C	1:20:A:TRP:N	1	1.19
(1,4)	1:3:A:CYS:N	1:3:A:CYS:CA	1:3:A:CYS:C	1:4:A:ALA:N	10	1.19
(1,113)	1:84:A:THR:C	1:85:A:CYS:N	1:85:A:CYS:CA	1:85:A:CYS:C	8	1.18
(1,64)	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	1:50:A:SER:N	7	1.18
(1,107)	1:77:A:GLU:C	1:78:A:GLU:N	1:78:A:GLU:CA	1:78:A:GLU:C	8	1.16
(1,45)	1:29:A:GLU:C	1:30:A:ASP:N	1:30:A:ASP:CA	1:30:A:ASP:C	12	1.16
(1,7)	1:5:A:GLU:C	1:6:A:SER:N	1:6:A:SER:CA	1:6:A:SER:C	12	1.16
(1,175)	1:90:A:PHE:C	1:91:A:THR:N	1:91:A:THR:CA	1:91:A:THR:C	20	1.15
(1,153)	1:110:A:CYS:C	1:111:A:SER:N	1:111:A:SER:CA	1:111:A:SER:C	20	1.15
(1,113)	1:84:A:THR:C	1:85:A:CYS:N	1:85:A:CYS:CA	1:85:A:CYS:C	19	1.15
(1,104)	1:76:A:ASP:N	1:76:A:ASP:CA	1:76:A:ASP:C	1:77:A:GLU:N	17	1.15
(1,54)	1:37:A:GLU:N	1:37:A:GLU:CA	1:37:A:GLU:C	1:38:A:GLN:N	11	1.15
(1,35)	1:21:A:LYS:C	1:22:A:CYS:N	1:22:A:CYS:CA	1:22:A:CYS:C	5	1.13
(1,30)	1:18:A:SER:N	1:18:A:SER:CA	1:18:A:SER:C	1:19:A:ARG:N	13	1.13
(1,12)	1:9:A:VAL:N	1:9:A:VAL:CA	1:9:A:VAL:C	1:10:A:CYS:N	2	1.11
(1,5)	1:4:A:ALA:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	20	1.11
(1,4)	1:3:A:CYS:N	1:3:A:CYS:CA	1:3:A:CYS:C	1:4:A:ALA:N	16	1.11
(1,133)	1:97:A:CYS:C	1:98:A:ILE:N	1:98:A:ILE:CA	1:98:A:ILE:C	13	1.1
(1,116)	1:87:A:PRO:N	1:87:A:PRO:CA	1:87:A:PRO:C	1:88:A:ASP:N	15	1.1
(1,99)	1:71:A:CYS:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	15	1.1
(1,61)	1:47:A:HIS:C	1:48:A:GLU:N	1:48:A:GLU:CA	1:48:A:GLU:C	2	1.1
(1,26)	1:16:A:VAL:N	1:16:A:VAL:CA	1:16:A:VAL:C	1:17:A:PRO:N	1	1.1
(1,68)	1:53:A:ALA:N	1:53:A:ALA:CA	1:53:A:ALA:C	1:54:A:HIS:N	7	1.08
(1,55)	1:37:A:GLU:C	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	5	1.08
(1,49)	1:34:A:GLU:C	1:35:A:SER:N	1:35:A:SER:CA	1:35:A:SER:C	19	1.08
(1,127)	1:94:A:SER:C	1:95:A:GLY:N	1:95:A:GLY:CA	1:95:A:GLY:C	19	1.07
(1,123)	1:92:A:CYS:C	1:93:A:SER:N	1:93:A:SER:CA	1:93:A:SER:C	18	1.07
(1,122)	1:90:A:PHE:N	1:90:A:PHE:CA	1:90:A:PHE:C	1:91:A:THR:N	2	1.06
(1,146)	1:106:A:GLY:N	1:106:A:GLY:CA	1:106:A:GLY:C	1:107:A:GLN:N	3	1.04

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,82)	1:61:A:VAL:N	1:61:A:VAL:CA	1:61:A:VAL:C	1:62:A:SER:N	10	1.04
(1,64)	1:49:A:ILE:N	1:49:A:ILE:CA	1:49:A:ILE:C	1:50:A:SER:N	10	1.04
(1,55)	1:37:A:GLU:C	1:38:A:GLN:N	1:38:A:GLN:CA	1:38:A:GLN:C	7	1.04
(1,2)	1:2:A:THR:N	1:2:A:THR:CA	1:2:A:THR:C	1:3:A:CYS:N	17	1.04
(1,125)	1:93:A:SER:C	1:94:A:SER:N	1:94:A:SER:CA	1:94:A:SER:C	6	1.03
(1,80)	1:60:A:PRO:N	1:60:A:PRO:CA	1:60:A:PRO:C	1:61:A:VAL:N	19	1.02
(1,79)	1:59:A:ILE:C	1:60:A:PRO:N	1:60:A:PRO:CA	1:60:A:PRO:C	15	1.02
(1,70)	1:54:A:HIS:N	1:54:A:HIS:CA	1:54:A:HIS:C	1:55:A:SER:N	7	1.02
(1,32)	1:19:A:ARG:N	1:19:A:ARG:CA	1:19:A:ARG:C	1:20:A:TRP:N	2	1.02
(1,5)	1:4:A:ALA:C	1:5:A:GLU:N	1:5:A:GLU:CA	1:5:A:GLU:C	10	1.02
(1,3)	1:2:A:THR:C	1:3:A:CYS:N	1:3:A:CYS:CA	1:3:A:CYS:C	6	1.02
(1,79)	1:59:A:ILE:C	1:60:A:PRO:N	1:60:A:PRO:CA	1:60:A:PRO:C	14	1.01
(1,2)	1:2:A:THR:N	1:2:A:THR:CA	1:2:A:THR:C	1:3:A:CYS:N	5	1.01
(1,2)	1:2:A:THR:N	1:2:A:THR:CA	1:2:A:THR:C	1:3:A:CYS:N	6	1.01
(1,114)	1:85:A:CYS:N	1:85:A:CYS:CA	1:85:A:CYS:C	1:86:A:SER:N	7	1.0
(1,114)	1:85:A:CYS:N	1:85:A:CYS:CA	1:85:A:CYS:C	1:86:A:SER:N	18	1.0
(1,106)	1:77:A:GLU:N	1:77:A:GLU:CA	1:77:A:GLU:C	1:78:A:GLU:N	17	1.0
(1,32)	1:19:A:ARG:N	1:19:A:ARG:CA	1:19:A:ARG:C	1:20:A:TRP:N	8	1.0