



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 04:29 PM UTC

PDB ID : 7PRD / pdb_00007prd
BMRB ID : 34668
Title : Solution structure of the chimeric Nrd1-Nab3 heterodimerization domains
Authors : Chaves-Arquero, B.; Martinez-Lumbreras, S.; Perez-Canadillas, J.M.
Deposited on : 2021-09-21

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

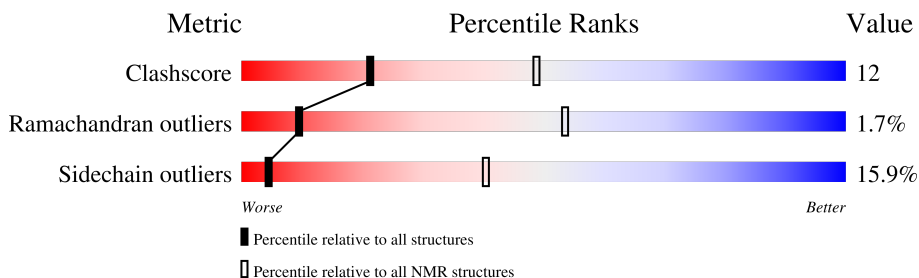
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 94%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	125	

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:167-A:274 (108)	1.01	1

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 2 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1968 atoms, of which 993 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein NRD1,HLJ1_G0022400.mRNA.1.CDS.1.

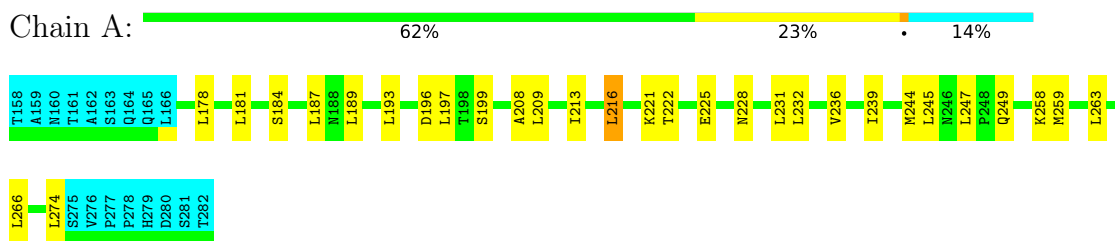
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	125	1968	610	993	168	192	5	0

4 Residue-property plots [\(i\)](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Protein NRD1,HLJ1_G0022400.mRNA.1.CDS.1

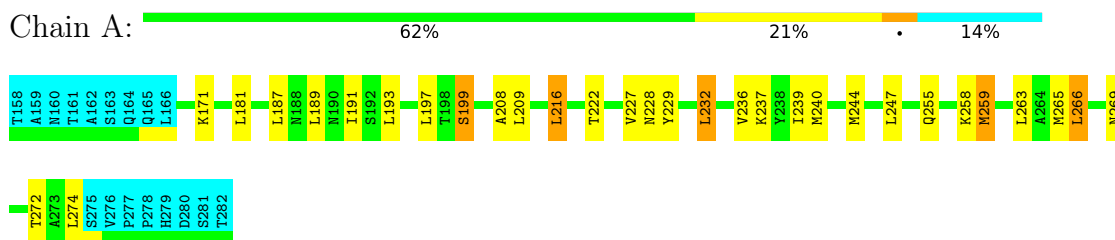


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

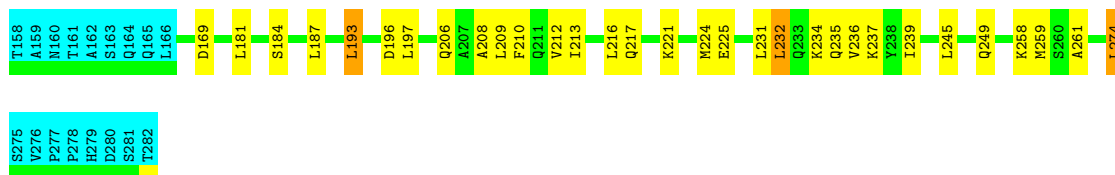
- Molecule 1: Protein NRD1,HLJ1_G0022400.mRNA.1.CDS.1



4.2.2 Score per residue for model 2

- Molecule 1: Protein NRD1,HLJ1_G0022400.mRNA.1.CDS.1

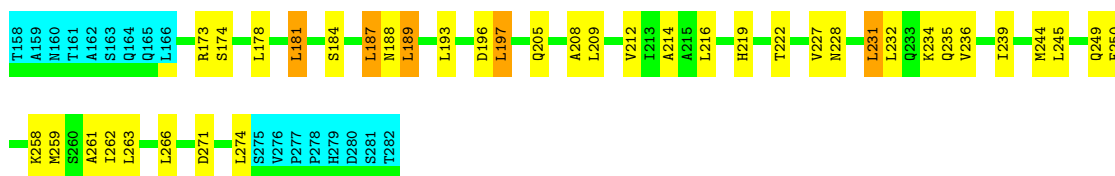




4.2.3 Score per residue for model 3

- Molecule 1: Protein NRD1,HLJ1_G0022400.mRNA.1.CDS.1

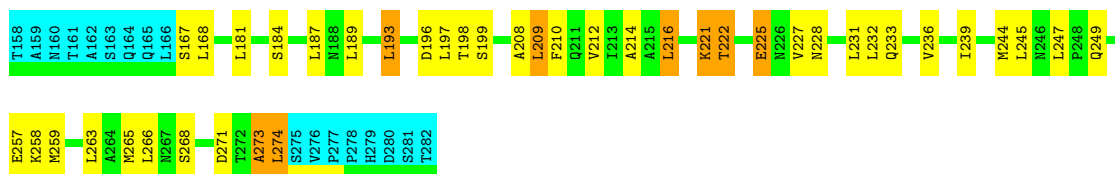
Chain A: 55% 27% 14%



4.2.4 Score per residue for model 4

- Molecule 1: Protein NRD1,HLJ1_G0022400.mRNA.1.CDS.1

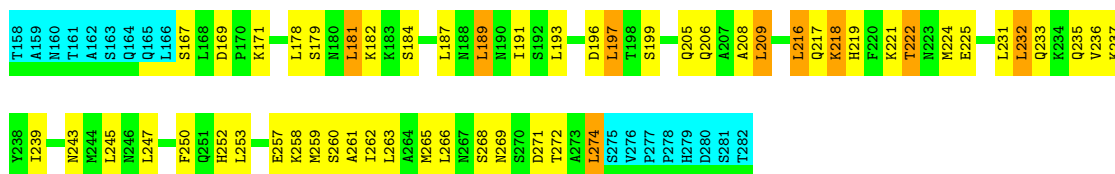
Chain A: 54% 26% 6% 14%



4.2.5 Score per residue for model 5

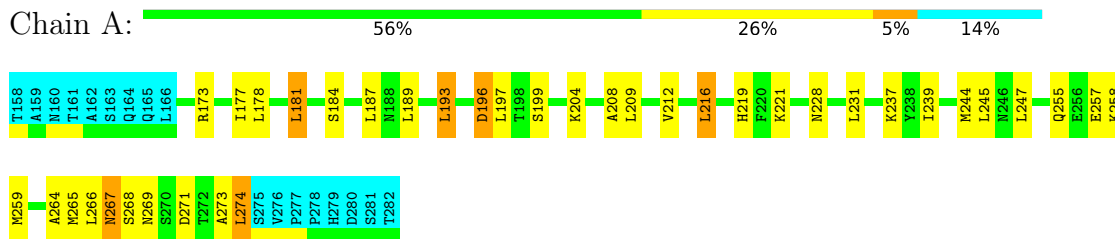
- Molecule 1: Protein NRD1,HLJ1_G0022400.mRNA.1.CDS.1

Chain A: 43% 36% 7% 14%



4.2.6 Score per residue for model 6

- Molecule 1: Protein NRD1,HLJ1_G0022400.mRNA.1.CDS.1



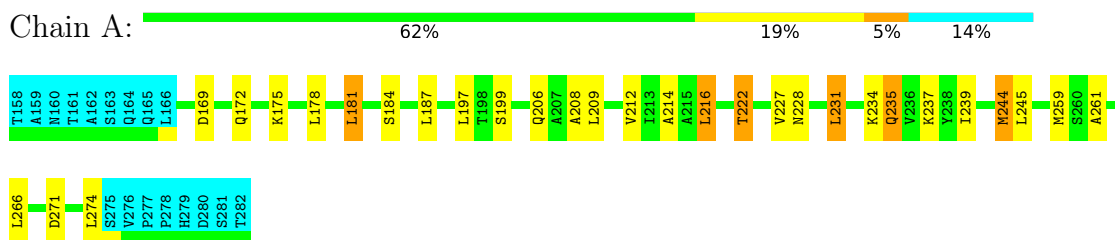
4.2.7 Score per residue for model 7

- Molecule 1: Protein NRD1,HLJ1_G0022400.mRNA.1.CDS.1



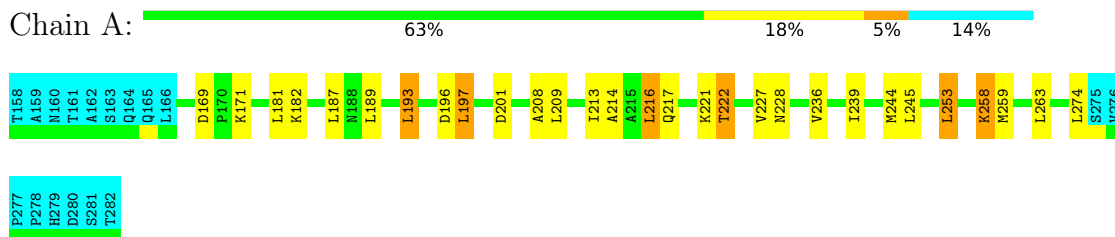
4.2.8 Score per residue for model 8

- Molecule 1: Protein NRD1,HLJ1_G0022400.mRNA.1.CDS.1



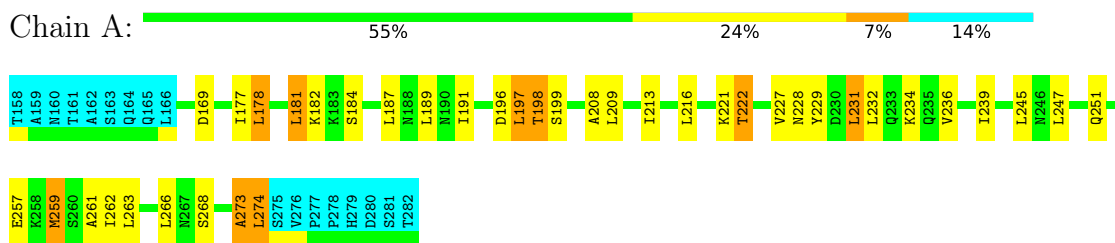
4.2.9 Score per residue for model 9

- Molecule 1: Protein NRD1,HLJ1_G0022400.mRNA.1.CDS.1



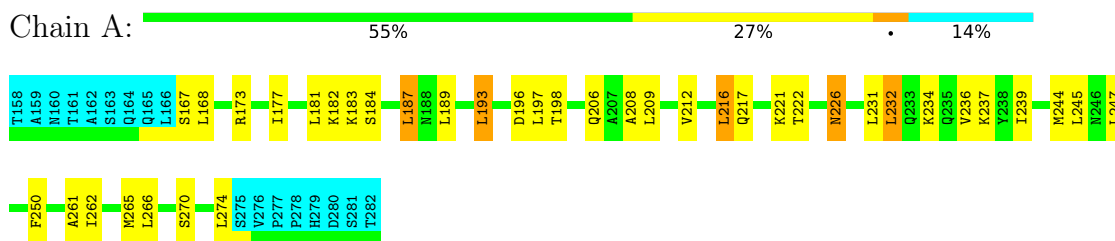
4.2.10 Score per residue for model 10

- Molecule 1: Protein NRD1,HLJ1_G0022400.mRNA.1.CDS.1



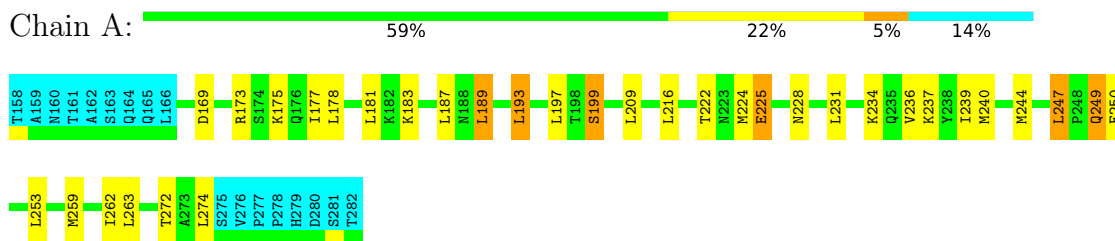
4.2.11 Score per residue for model 11

- Molecule 1: Protein NRD1,HLJ1_G0022400.mRNA.1.CDS.1



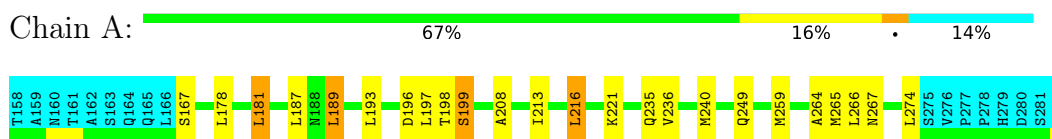
4.2.12 Score per residue for model 12

- Molecule 1: Protein NRD1,HLJ1_G0022400.mRNA.1.CDS.1



4.2.13 Score per residue for model 13

- Molecule 1: Protein NRD1,HLJ1_G0022400.mRNA.1.CDS.1





4.2.18 Score per residue for model 18

- Molecule 1: Protein NRD1,HLJ1_G0022400.mRNA.1.CDS.1

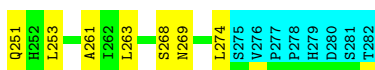
Chain A: 58% 24% 14%



4.2.19 Score per residue for model 19

- Molecule 1: Protein NRD1,HLJ1_G0022400.mRNA.1.CDS.1

Chain A: 57% 25% 5% 14%



4.2.20 Score per residue for model 20

- Molecule 1: Protein NRD1,HLJ1_G0022400.mRNA.1.CDS.1

Chain A: 51% 30% 5% 14%



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure calculation	

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	1603
Number of shifts mapped to atoms	1603
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	94%

6 Model quality i

6.1 Standard geometry i

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts 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	853	880	880	20±5
All	All	17060	17600	17600	408

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:209:LEU:HD23	1:A:236:VAL:HG13	0.98	1.30	1	6
1:A:189:LEU:HD11	1:A:263:LEU:HD22	0.90	1.42	4	3
1:A:187:LEU:HD21	1:A:189:LEU:HD12	0.84	1.49	6	3
1:A:214:ALA:HB1	1:A:227:VAL:HG21	0.82	1.50	9	4
1:A:187:LEU:HD21	1:A:263:LEU:HD23	0.82	1.49	18	2
1:A:209:LEU:HD12	1:A:245:LEU:HD11	0.79	1.53	14	1
1:A:189:LEU:HD23	1:A:191:ILE:HD12	0.79	1.55	14	1
1:A:197:LEU:HD12	1:A:212:VAL:HG21	0.78	1.53	20	5
1:A:212:VAL:HG22	1:A:259:MET:HE1	0.74	1.59	16	1
1:A:187:LEU:HD12	1:A:189:LEU:HD11	0.72	1.61	3	1
1:A:197:LEU:HD21	1:A:245:LEU:HD22	0.71	1.61	20	3
1:A:187:LEU:HD11	1:A:263:LEU:HD23	0.71	1.60	14	4
1:A:193:LEU:HD11	1:A:197:LEU:HD13	0.68	1.64	6	1
1:A:193:LEU:HD21	1:A:197:LEU:HD13	0.68	1.66	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:210:PHE:CE2	1:A:236:VAL:HG11	0.67	2.24	17	5
1:A:197:LEU:HD13	1:A:245:LEU:HD22	0.67	1.67	10	2
1:A:209:LEU:HD21	1:A:245:LEU:HD11	0.67	1.67	11	1
1:A:196:ASP:CB	1:A:208:ALA:HB2	0.64	2.22	13	8
1:A:197:LEU:CD2	1:A:245:LEU:HD22	0.64	2.22	11	4
1:A:209:LEU:HD11	1:A:245:LEU:HD11	0.64	1.69	18	4
1:A:239:ILE:HD11	1:A:266:LEU:CD2	0.64	2.22	11	1
1:A:197:LEU:HD22	1:A:212:VAL:HG21	0.63	1.70	8	1
1:A:231:LEU:HD13	1:A:274:LEU:HD22	0.63	1.69	8	1
1:A:249:GLN:O	1:A:253:LEU:HD13	0.63	1.94	19	3
1:A:178:LEU:HD13	1:A:249:GLN:CB	0.62	2.24	3	2
1:A:187:LEU:HD22	1:A:263:LEU:HD23	0.62	1.71	17	1
1:A:193:LEU:HD13	1:A:193:LEU:N	0.62	2.10	12	1
1:A:187:LEU:HG	1:A:263:LEU:HD23	0.62	1.72	3	1
1:A:197:LEU:CD1	1:A:212:VAL:HG21	0.61	2.25	20	4
1:A:191:ILE:HG13	1:A:259:MET:HE2	0.61	1.70	16	1
1:A:187:LEU:HD12	1:A:189:LEU:CD1	0.61	2.26	3	1
1:A:181:LEU:HD21	1:A:264:ALA:HB3	0.61	1.73	13	3
1:A:231:LEU:HD23	1:A:271:ASP:O	0.60	1.95	8	1
1:A:274:LEU:O	1:A:274:LEU:HD13	0.60	1.97	12	2
1:A:209:LEU:HD12	1:A:245:LEU:CD2	0.60	2.26	4	1
1:A:205:GLN:HG2	1:A:245:LEU:HD23	0.60	1.74	3	2
1:A:274:LEU:HD13	1:A:274:LEU:O	0.60	1.96	14	3
1:A:235:GLN:NE2	1:A:266:LEU:HD23	0.60	2.12	5	2
1:A:187:LEU:HD13	1:A:263:LEU:HD22	0.60	1.73	19	1
1:A:193:LEU:CD2	1:A:197:LEU:HD13	0.59	2.28	11	1
1:A:239:ILE:HD11	1:A:266:LEU:HG	0.59	1.73	15	1
1:A:208:ALA:O	1:A:212:VAL:HG23	0.59	1.97	17	1
1:A:187:LEU:HD11	1:A:263:LEU:CD2	0.59	2.26	9	2
1:A:239:ILE:HD11	1:A:266:LEU:HB2	0.59	1.73	10	1
1:A:174:SER:O	1:A:178:LEU:HD12	0.59	1.98	3	1
1:A:193:LEU:HB2	1:A:197:LEU:HD23	0.59	1.74	16	2
1:A:181:LEU:HD13	1:A:261:ALA:CB	0.58	2.27	5	1
1:A:173:ARG:O	1:A:177:ILE:HG23	0.58	1.97	6	4
1:A:191:ILE:HD12	1:A:259:MET:HE3	0.58	1.76	10	1
1:A:189:LEU:HD23	1:A:219:HIS:CD2	0.58	2.33	3	2
1:A:198:THR:HG21	1:A:258:LYS:NZ	0.58	2.14	4	2
1:A:239:ILE:HG23	1:A:244:MET:CG	0.58	2.28	8	3
1:A:178:LEU:HD13	1:A:249:GLN:HB2	0.58	1.76	3	1
1:A:209:LEU:CD1	1:A:245:LEU:HD11	0.57	2.29	14	4
1:A:239:ILE:HD12	1:A:244:MET:HE3	0.57	1.76	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:181:LEU:HD11	1:A:261:ALA:HA	0.57	1.74	8	6
1:A:213:ILE:HD13	1:A:236:VAL:HG22	0.57	1.76	18	1
1:A:196:ASP:HB2	1:A:208:ALA:HB2	0.57	1.76	9	6
1:A:239:ILE:HD11	1:A:266:LEU:HD12	0.57	1.76	1	2
1:A:250:PHE:CZ	1:A:262:ILE:HD11	0.57	2.34	3	7
1:A:189:LEU:HD13	1:A:259:MET:HE2	0.56	1.76	4	2
1:A:189:LEU:HD23	1:A:191:ILE:CD1	0.56	2.29	14	2
1:A:231:LEU:HD23	1:A:274:LEU:HB2	0.56	1.75	20	4
1:A:209:LEU:HD21	1:A:239:ILE:HB	0.56	1.74	3	5
1:A:196:ASP:HB3	1:A:208:ALA:HB2	0.56	1.77	14	6
1:A:197:LEU:HD12	1:A:197:LEU:O	0.56	2.01	1	4
1:A:209:LEU:HD23	1:A:236:VAL:CG1	0.56	2.30	3	1
1:A:178:LEU:HD21	1:A:250:PHE:HB2	0.56	1.76	19	1
1:A:214:ALA:CB	1:A:227:VAL:HG21	0.55	2.30	9	2
1:A:187:LEU:CD2	1:A:189:LEU:HD12	0.55	2.27	6	2
1:A:212:VAL:CG2	1:A:259:MET:HE1	0.55	2.32	16	1
1:A:197:LEU:HD13	1:A:245:LEU:HG	0.55	1.78	7	2
1:A:210:PHE:CE1	1:A:236:VAL:HG21	0.55	2.37	4	2
1:A:216:LEU:HD12	1:A:216:LEU:O	0.55	2.02	16	1
1:A:213:ILE:HD13	1:A:266:LEU:HD21	0.55	1.79	17	1
1:A:239:ILE:HG23	1:A:244:MET:HG3	0.54	1.79	8	1
1:A:244:MET:HE1	1:A:262:ILE:HA	0.54	1.79	3	3
1:A:193:LEU:CD1	1:A:197:LEU:HD13	0.54	2.31	6	1
1:A:181:LEU:HD21	1:A:261:ALA:HA	0.54	1.80	19	2
1:A:189:LEU:HD13	1:A:259:MET:HE3	0.54	1.80	13	1
1:A:216:LEU:CD2	1:A:259:MET:HE1	0.53	2.34	13	2
1:A:197:LEU:O	1:A:197:LEU:HD13	0.53	2.04	12	1
1:A:209:LEU:HD11	1:A:239:ILE:CG2	0.53	2.33	5	2
1:A:232:LEU:O	1:A:236:VAL:HG23	0.53	2.03	3	7
1:A:231:LEU:O	1:A:231:LEU:HD13	0.53	2.03	15	2
1:A:193:LEU:HD11	1:A:258:LYS:HD3	0.53	1.81	16	1
1:A:269:ASN:HB3	1:A:272:THR:HG22	0.52	1.80	16	4
1:A:266:LEU:O	1:A:272:THR:HG23	0.52	2.04	5	3
1:A:197:LEU:HA	1:A:208:ALA:HB3	0.52	1.81	8	4
1:A:209:LEU:HD12	1:A:245:LEU:HD21	0.52	1.81	4	1
1:A:181:LEU:HD13	1:A:261:ALA:HB1	0.52	1.81	5	1
1:A:244:MET:HE2	1:A:265:MET:SD	0.52	2.44	1	1
1:A:217:GLN:NE2	1:A:231:LEU:HD11	0.52	2.20	7	1
1:A:197:LEU:HD12	1:A:250:PHE:CE2	0.52	2.40	5	1
1:A:213:ILE:HB	1:A:232:LEU:HD21	0.51	1.81	20	3
1:A:197:LEU:HD23	1:A:197:LEU:O	0.51	2.04	6	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:193:LEU:HD11	1:A:258:LYS:HG2	0.51	1.81	9	1
1:A:227:VAL:HG12	1:A:232:LEU:HD11	0.51	1.82	10	1
1:A:187:LEU:CD1	1:A:263:LEU:HD22	0.51	2.35	19	1
1:A:193:LEU:HD23	1:A:197:LEU:HG	0.51	1.82	5	1
1:A:231:LEU:HD12	1:A:235:GLN:HG3	0.51	1.82	7	1
1:A:231:LEU:CD2	1:A:274:LEU:HD13	0.51	2.35	11	1
1:A:217:GLN:NE2	1:A:274:LEU:HD13	0.51	2.20	19	3
1:A:273:ALA:O	1:A:274:LEU:HD22	0.50	2.06	6	3
1:A:229:TYR:HA	1:A:232:LEU:HD12	0.50	1.82	10	1
1:A:239:ILE:HD12	1:A:244:MET:CE	0.50	2.36	6	2
1:A:193:LEU:CD2	1:A:197:LEU:HD23	0.50	2.36	17	1
1:A:197:LEU:HD23	1:A:245:LEU:HG	0.50	1.83	4	2
1:A:227:VAL:CG1	1:A:232:LEU:HD11	0.50	2.37	10	1
1:A:193:LEU:HD22	1:A:258:LYS:HB3	0.50	1.83	15	1
1:A:220:PHE:CD1	1:A:274:LEU:HD11	0.50	2.42	7	2
1:A:209:LEU:HD11	1:A:245:LEU:CD1	0.50	2.36	8	2
1:A:231:LEU:HD22	1:A:274:LEU:HB2	0.50	1.84	8	1
1:A:178:LEU:CD1	1:A:247:LEU:HD23	0.50	2.36	10	1
1:A:209:LEU:HD22	1:A:236:VAL:HG13	0.50	1.82	14	2
1:A:216:LEU:O	1:A:216:LEU:HD12	0.49	2.07	1	2
1:A:239:ILE:CG2	1:A:245:LEU:HD21	0.49	2.37	20	1
1:A:191:ILE:CG1	1:A:259:MET:HE2	0.49	2.36	16	1
1:A:205:GLN:HG3	1:A:245:LEU:HD23	0.49	1.84	5	1
1:A:216:LEU:C	1:A:274:LEU:HD11	0.49	2.33	6	1
1:A:274:LEU:HD12	1:A:274:LEU:O	0.49	2.08	3	1
1:A:187:LEU:HD12	1:A:189:LEU:HG	0.49	1.83	11	2
1:A:193:LEU:CG	1:A:197:LEU:HD13	0.49	2.37	4	1
1:A:181:LEU:HD21	1:A:264:ALA:CB	0.49	2.37	7	2
1:A:178:LEU:HD11	1:A:253:LEU:HD22	0.49	1.85	7	1
1:A:235:GLN:HG3	1:A:266:LEU:HD12	0.49	1.85	8	1
1:A:178:LEU:HA	1:A:181:LEU:HD13	0.48	1.85	8	1
1:A:259:MET:HA	1:A:262:ILE:HD12	0.48	1.85	10	1
1:A:198:THR:HG22	1:A:251:GLN:NE2	0.48	2.24	10	1
1:A:189:LEU:HD12	1:A:259:MET:HG3	0.48	1.84	20	1
1:A:216:LEU:CB	1:A:274:LEU:HD21	0.48	2.38	6	2
1:A:232:LEU:HD23	1:A:236:VAL:HG23	0.48	1.85	11	4
1:A:178:LEU:HD23	1:A:181:LEU:HD13	0.48	1.85	15	1
1:A:252:HIS:O	1:A:253:LEU:HD12	0.48	2.09	17	1
1:A:216:LEU:HB3	1:A:274:LEU:HD21	0.47	1.84	6	1
1:A:253:LEU:HD22	1:A:257:GLU:HG2	0.47	1.86	18	2
1:A:231:LEU:HD23	1:A:274:LEU:HD13	0.47	1.84	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:189:LEU:CD2	1:A:263:LEU:HD22	0.47	2.39	17	1
1:A:274:LEU:HD13	1:A:274:LEU:C	0.47	2.34	13	6
1:A:239:ILE:HD11	1:A:266:LEU:HD22	0.47	1.85	11	1
1:A:244:MET:HE3	1:A:265:MET:HG2	0.47	1.86	11	1
1:A:221:LYS:O	1:A:222:THR:HG23	0.47	2.10	4	6
1:A:189:LEU:HD12	1:A:191:ILE:H	0.46	1.71	18	1
1:A:214:ALA:HB1	1:A:227:VAL:CG2	0.46	2.40	3	1
1:A:175:LYS:HG2	1:A:247:LEU:HD21	0.46	1.85	12	1
1:A:187:LEU:O	1:A:187:LEU:HD12	0.46	2.10	1	1
1:A:178:LEU:HA	1:A:181:LEU:HD23	0.46	1.87	19	1
1:A:231:LEU:HD13	1:A:231:LEU:C	0.46	2.36	15	1
1:A:209:LEU:CD2	1:A:245:LEU:HD11	0.46	2.41	17	1
1:A:209:LEU:HD11	1:A:239:ILE:HG21	0.46	1.85	3	2
1:A:198:THR:HG21	1:A:258:LYS:CE	0.46	2.41	16	1
1:A:182:LYS:HE3	1:A:253:LEU:HD21	0.46	1.88	5	1
1:A:178:LEU:HA	1:A:181:LEU:HD12	0.45	1.88	5	1
1:A:231:LEU:HD11	1:A:271:ASP:O	0.45	2.10	6	1
1:A:239:ILE:HD12	1:A:244:MET:SD	0.45	2.51	19	5
1:A:239:ILE:HD11	1:A:266:LEU:HB3	0.45	1.88	7	1
1:A:239:ILE:CG2	1:A:245:LEU:HD13	0.45	2.41	5	1
1:A:232:LEU:HD23	1:A:236:VAL:CG2	0.45	2.41	11	1
1:A:267:ASN:HA	1:A:273:ALA:HB2	0.45	1.86	6	1
1:A:197:LEU:HD21	1:A:209:LEU:HD12	0.45	1.87	12	1
1:A:247:LEU:HD23	1:A:248:PRO:HD2	0.45	1.88	18	1
1:A:189:LEU:CD1	1:A:263:LEU:HD22	0.45	2.29	4	1
1:A:216:LEU:HD23	1:A:216:LEU:N	0.45	2.26	9	9
1:A:209:LEU:HD23	1:A:213:ILE:HG13	0.45	1.87	14	1
1:A:209:LEU:HD23	1:A:245:LEU:HD11	0.45	1.87	17	1
1:A:197:LEU:HD12	1:A:245:LEU:HD13	0.45	1.88	18	1
1:A:274:LEU:O	1:A:274:LEU:HD12	0.45	2.12	8	2
1:A:221:LYS:O	1:A:222:THR:C	0.45	2.59	19	1
1:A:227:VAL:HG12	1:A:232:LEU:CD1	0.45	2.42	1	1
1:A:193:LEU:HG	1:A:197:LEU:HD13	0.45	1.89	4	1
1:A:224:MET:O	1:A:225:GLU:C	0.44	2.58	5	1
1:A:262:ILE:O	1:A:266:LEU:HD23	0.44	2.11	11	1
1:A:239:ILE:HD11	1:A:266:LEU:CD1	0.44	2.41	16	1
1:A:213:ILE:CD1	1:A:266:LEU:HD11	0.44	2.42	20	1
1:A:197:LEU:HD12	1:A:250:PHE:HE2	0.44	1.72	5	1
1:A:199:SER:O	1:A:200:THR:C	0.44	2.60	18	1
1:A:253:LEU:HD22	1:A:257:GLU:CD	0.44	2.37	5	1
1:A:231:LEU:HD23	1:A:231:LEU:O	0.44	2.12	14	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:250:PHE:HZ	1:A:262:ILE:HD11	0.44	1.73	12	4
1:A:181:LEU:CD1	1:A:261:ALA:HB2	0.44	2.43	11	1
1:A:209:LEU:HD13	1:A:213:ILE:HG13	0.44	1.90	17	1
1:A:231:LEU:HD23	1:A:235:GLN:CG	0.44	2.43	3	1
1:A:210:PHE:CD2	1:A:236:VAL:HG11	0.44	2.48	18	1
1:A:213:ILE:HG13	1:A:236:VAL:HG22	0.43	1.90	9	2
1:A:216:LEU:HD22	1:A:259:MET:HE1	0.43	1.89	13	1
1:A:242:SER:HB2	1:A:265:MET:HE2	0.43	1.90	18	1
1:A:193:LEU:HD13	1:A:193:LEU:H	0.43	1.72	12	1
1:A:187:LEU:HD13	1:A:263:LEU:HD23	0.43	1.90	17	1
1:A:197:LEU:CD2	1:A:212:VAL:HG21	0.43	2.42	3	1
1:A:220:PHE:HB3	1:A:274:LEU:HD11	0.43	1.89	15	1
1:A:212:VAL:CG1	1:A:213:ILE:N	0.43	2.81	16	1
1:A:193:LEU:HD22	1:A:258:LYS:HD2	0.43	1.90	2	1
1:A:209:LEU:HD11	1:A:239:ILE:HG22	0.43	1.91	5	1
1:A:174:SER:HA	1:A:177:ILE:CG1	0.43	2.44	7	1
1:A:274:LEU:C	1:A:274:LEU:HD13	0.43	2.38	18	1
1:A:181:LEU:CD1	1:A:253:LEU:HD21	0.43	2.44	9	1
1:A:209:LEU:HD21	1:A:239:ILE:CG2	0.42	2.44	15	1
1:A:224:MET:O	1:A:225:GLU:CB	0.42	2.67	2	1
1:A:205:GLN:CG	1:A:245:LEU:HD23	0.42	2.42	3	1
1:A:189:LEU:O	1:A:190:ASN:C	0.42	2.63	18	1
1:A:218:LYS:O	1:A:222:THR:HG23	0.42	2.14	5	1
1:A:239:ILE:HD11	1:A:266:LEU:CG	0.42	2.45	15	1
1:A:227:VAL:HG12	1:A:232:LEU:HD12	0.42	1.91	20	1
1:A:187:LEU:CG	1:A:263:LEU:HD23	0.42	2.44	3	1
1:A:253:LEU:HD13	1:A:257:GLU:OE1	0.42	2.14	5	1
1:A:232:LEU:HD13	1:A:236:VAL:HG23	0.42	1.92	17	1
1:A:217:GLN:HG2	1:A:274:LEU:HD12	0.42	1.92	9	1
1:A:193:LEU:HG	1:A:197:LEU:HD23	0.41	1.91	1	1
1:A:239:ILE:HG21	1:A:245:LEU:HD21	0.41	1.91	11	1
1:A:187:LEU:HG	1:A:189:LEU:HD13	0.41	1.91	14	1
1:A:209:LEU:HD12	1:A:245:LEU:CD1	0.41	2.34	14	1
1:A:244:MET:HE2	1:A:265:MET:HG2	0.41	1.93	6	1
1:A:206:GLN:HA	1:A:209:LEU:HD12	0.41	1.90	11	1
1:A:193:LEU:HD21	1:A:258:LYS:HB2	0.41	1.92	16	1
1:A:174:SER:OG	1:A:265:MET:HE1	0.41	2.15	20	1
1:A:189:LEU:HD21	1:A:263:LEU:CD2	0.41	2.46	1	1
1:A:191:ILE:CG2	1:A:259:MET:HE3	0.41	2.46	1	1
1:A:177:ILE:C	1:A:177:ILE:HD12	0.41	2.41	20	1
1:A:189:LEU:HD21	1:A:263:LEU:HD22	0.41	1.93	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:193:LEU:HD22	1:A:193:LEU:O	0.41	2.15	12	1
1:A:216:LEU:N	1:A:216:LEU:HD23	0.41	2.31	13	1
1:A:209:LEU:HD23	1:A:245:LEU:CD1	0.41	2.46	17	1
1:A:206:GLN:OE1	1:A:240:MET:HE2	0.41	2.14	18	1
1:A:227:VAL:HG11	1:A:229:TYR:CZ	0.41	2.51	19	1
1:A:167:SER:C	1:A:168:LEU:HD12	0.41	2.40	11	1
1:A:217:GLN:HG2	1:A:274:LEU:HD23	0.41	1.92	11	1
1:A:187:LEU:CD1	1:A:263:LEU:HD23	0.41	2.39	14	1
1:A:262:ILE:O	1:A:266:LEU:HD13	0.40	2.16	17	1
1:A:235:GLN:OE1	1:A:274:LEU:HD22	0.40	2.16	2	1
1:A:244:MET:HE3	1:A:265:MET:SD	0.40	2.56	4	1
1:A:187:LEU:HD23	1:A:189:LEU:HB2	0.40	1.93	5	1
1:A:178:LEU:HD22	1:A:249:GLN:HB3	0.40	1.93	13	1
1:A:213:ILE:HG13	1:A:236:VAL:HG12	0.40	1.91	13	1
1:A:189:LEU:HD23	1:A:216:LEU:HD22	0.40	1.92	17	1
1:A:187:LEU:HD13	1:A:263:LEU:CD2	0.40	2.45	19	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	108/125 (86%)	99±2 (92±2%)	7±2 (6±2%)	2±1 (2±1%)	9	53
All	All	2160/2500 (86%)	1986 (92%)	137 (6%)	37 (2%)	9	53

All 10 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	199	SER	12
1	A	228	ASN	9
1	A	225	GLU	5
1	A	268	SER	3
1	A	273	ALA	2
1	A	226	ASN	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	222	THR	1
1	A	189	LEU	1
1	A	182	LYS	1
1	A	183	LYS	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	100/115 (87%)	84±4 (84±4%)	16±4 (16±4%)	4	40
All	All	2000/2300 (87%)	1682 (84%)	318 (16%)	4	40

All 69 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	216	LEU	15
1	A	181	LEU	14
1	A	222	THR	13
1	A	184	SER	13
1	A	193	LEU	13
1	A	247	LEU	11
1	A	259	MET	11
1	A	187	LEU	11
1	A	232	LEU	10
1	A	169	ASP	9
1	A	221	LYS	9
1	A	237	LYS	8
1	A	231	LEU	8
1	A	234	LYS	8
1	A	189	LEU	7
1	A	209	LEU	7
1	A	171	LYS	6
1	A	240	MET	6
1	A	258	LYS	6
1	A	274	LEU	6
1	A	197	LEU	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	257	GLU	6
1	A	199	SER	5
1	A	249	GLN	5
1	A	267	ASN	5
1	A	266	LEU	4
1	A	206	GLN	4
1	A	173	ARG	4
1	A	167	SER	4
1	A	225	GLU	4
1	A	178	LEU	4
1	A	204	LYS	4
1	A	182	LYS	4
1	A	177	ILE	4
1	A	183	LYS	4
1	A	271	ASP	3
1	A	268	SER	3
1	A	265	MET	3
1	A	196	ASP	3
1	A	201	ASP	3
1	A	198	THR	3
1	A	229	TYR	2
1	A	255	GLN	2
1	A	168	LEU	2
1	A	228	ASN	2
1	A	233	GLN	2
1	A	218	LYS	2
1	A	219	HIS	2
1	A	243	ASN	2
1	A	269	ASN	2
1	A	172	GLN	2
1	A	175	LYS	2
1	A	244	MET	2
1	A	213	ILE	2
1	A	226	ASN	2
1	A	188	ASN	1
1	A	179	SER	1
1	A	252	HIS	1
1	A	260	SER	1
1	A	235	GLN	1
1	A	253	LEU	1
1	A	270	SER	1
1	A	224	MET	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	272	THR	1
1	A	241	ASP	1
1	A	192	SER	1
1	A	212	VAL	1
1	A	220	PHE	1
1	A	251	GLN	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

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

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_1*

7.1.1 Bookkeeping [i](#)

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	1603
Number of shifts mapped to atoms	1603
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	125	-0.35 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	122	0.19 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	115	-0.29 ± 0.09	None needed (< 0.5 ppm)
^{15}N	116	-0.12 ± 0.27	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 94%, i.e. 1414 atoms were assigned a chemical shift out of a possible 1503. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	519/526 (99%)	209/209 (100%)	209/216 (97%)	101/101 (100%)
Sidechain	865/915 (95%)	574/595 (96%)	270/286 (94%)	21/34 (62%)

Continued on next page...

Continued from previous page...

	Total	¹H	¹³C	¹⁵N
Aromatic	30/62 (48%)	25/31 (81%)	5/29 (17%)	0/2 (0%)
Overall	1414/1503 (94%)	808/835 (97%)	484/531 (91%)	122/137 (89%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 94%, i.e. 1598 atoms were assigned a chemical shift out of a possible 1701. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	596/607 (98%)	240/241 (100%)	240/250 (96%)	116/116 (100%)
Sidechain	970/1025 (95%)	645/667 (97%)	301/321 (94%)	24/37 (65%)
Aromatic	32/69 (46%)	26/35 (74%)	6/31 (19%)	0/3 (0%)
Overall	1598/1701 (94%)	911/943 (97%)	547/602 (91%)	140/156 (90%)

7.1.4 Statistically unusual chemical shifts [i](#)

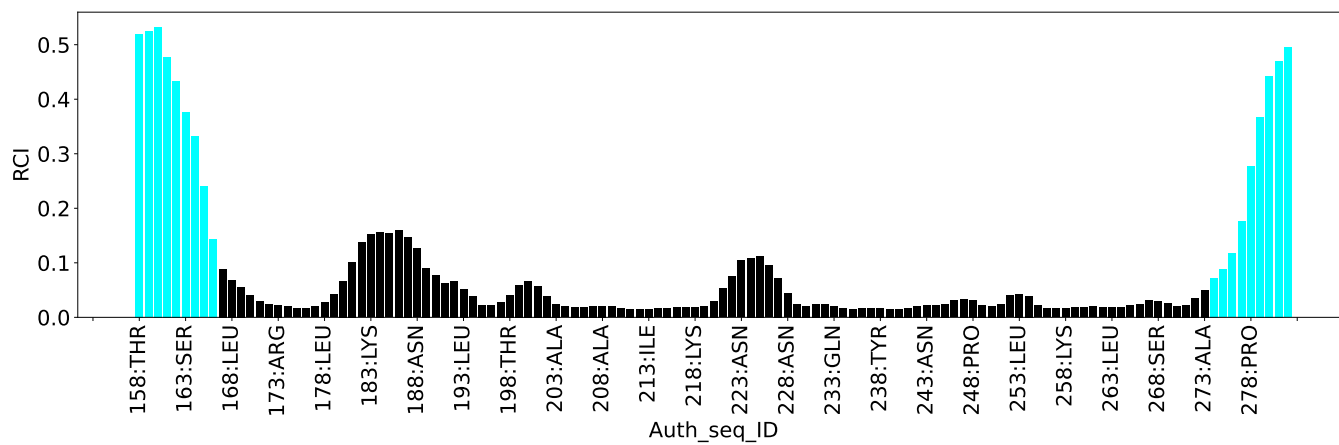
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	272	THR	HG1	5.12	0.08 – 2.19	18.9
1	A	258	LYS	HG2	-0.10	0.13 – 2.61	-5.9
1	A	235	GLN	HE22	4.88	4.88 – 9.19	-5.0

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	1801
Intra-residue ($ i-j =0$)	310
Sequential ($ i-j =1$)	366
Medium range ($ i-j >1$ and $ i-j <5$)	501
Long range ($ i-j \geq 5$)	548
Inter-chain	0
Hydrogen bond restraints	76
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	14.4
Number of long range restraints per residue ¹	4.4

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)	11.3	0.2
0.2-0.5 (Medium)	2.4	0.48
>0.5 (Large)	0.2	0.57

8.2.2 Average number of dihedral-angle violations per model

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

9 Distance violation analysis [i](#)

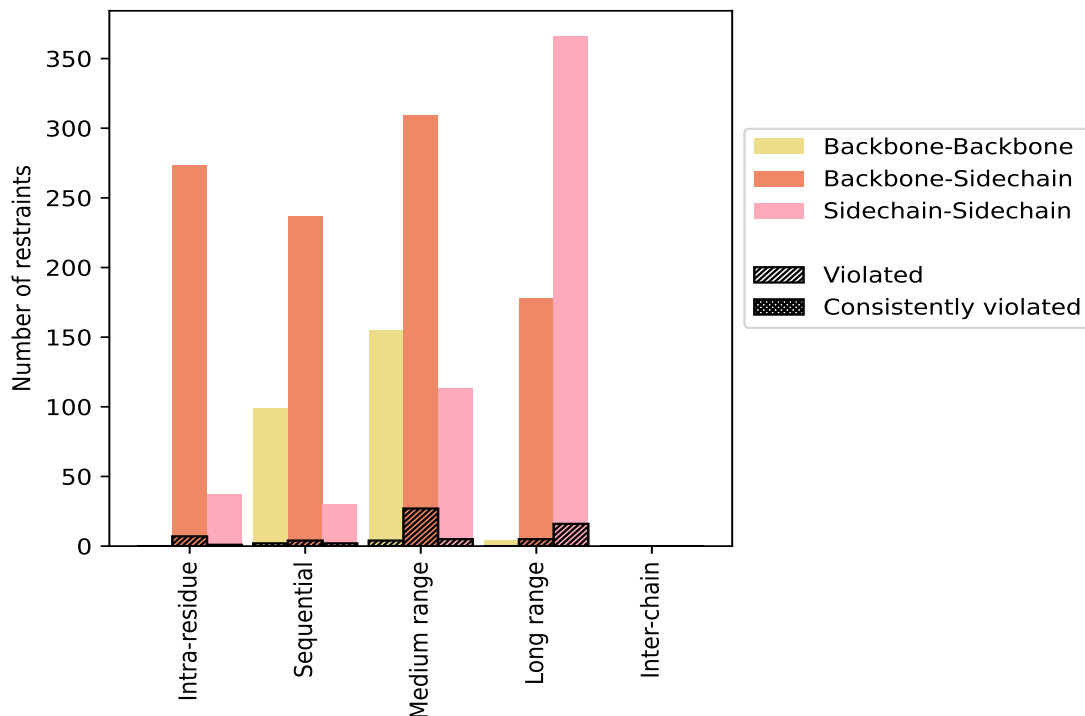
9.1 Summary of distance violations [i](#)

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 ($i-j =0$)	310	17.2	8	2.6	0.4	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	273	15.2	7	2.6	0.4	0	0.0	0.0
Sidechain-Sidechain	37	2.1	1	2.7	0.1	0	0.0	0.0
Sequential ($i-j =1$)	366	20.3	8	2.2	0.4	0	0.0	0.0
Backbone-Backbone	99	5.5	2	2.0	0.1	0	0.0	0.0
Backbone-Sidechain	237	13.2	4	1.7	0.2	0	0.0	0.0
Sidechain-Sidechain	30	1.7	2	6.7	0.1	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	501	27.8	17	3.4	0.9	0	0.0	0.0
Backbone-Backbone	155	8.6	4	2.6	0.2	0	0.0	0.0
Backbone-Sidechain	233	12.9	8	3.4	0.4	0	0.0	0.0
Sidechain-Sidechain	113	6.3	5	4.4	0.3	0	0.0	0.0
Long range ($i-j \geq 5$)	548	30.4	21	3.8	1.2	0	0.0	0.0
Backbone-Backbone	4	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	178	9.9	5	2.8	0.3	0	0.0	0.0
Sidechain-Sidechain	366	20.3	16	4.4	0.9	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	76	4.2	19	25.0	1.1	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1801	100.0	73	4.1	4.1	0	0.0	0.0
Backbone-Backbone	258	14.3	6	2.3	0.3	0	0.0	0.0
Backbone-Sidechain	997	55.4	43	4.3	2.4	0	0.0	0.0
Sidechain-Sidechain	546	30.3	24	4.4	1.3	0	0.0	0.0

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

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



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfid 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	1	2	7	3	0	13	0.16	0.27	0.05	0.14
2	0	4	6	2	0	12	0.14	0.2	0.02	0.13
3	1	2	9	5	0	17	0.16	0.34	0.06	0.13
4	0	1	5	4	0	10	0.14	0.18	0.03	0.14
5	1	3	7	2	0	13	0.15	0.24	0.04	0.13
6	1	2	5	3	0	11	0.19	0.55	0.13	0.14
7	1	1	8	3	0	13	0.18	0.56	0.12	0.14
8	1	2	8	5	0	16	0.16	0.29	0.05	0.14
9	2	4	10	3	0	19	0.16	0.3	0.05	0.14
10	2	2	11	5	0	20	0.15	0.35	0.06	0.13

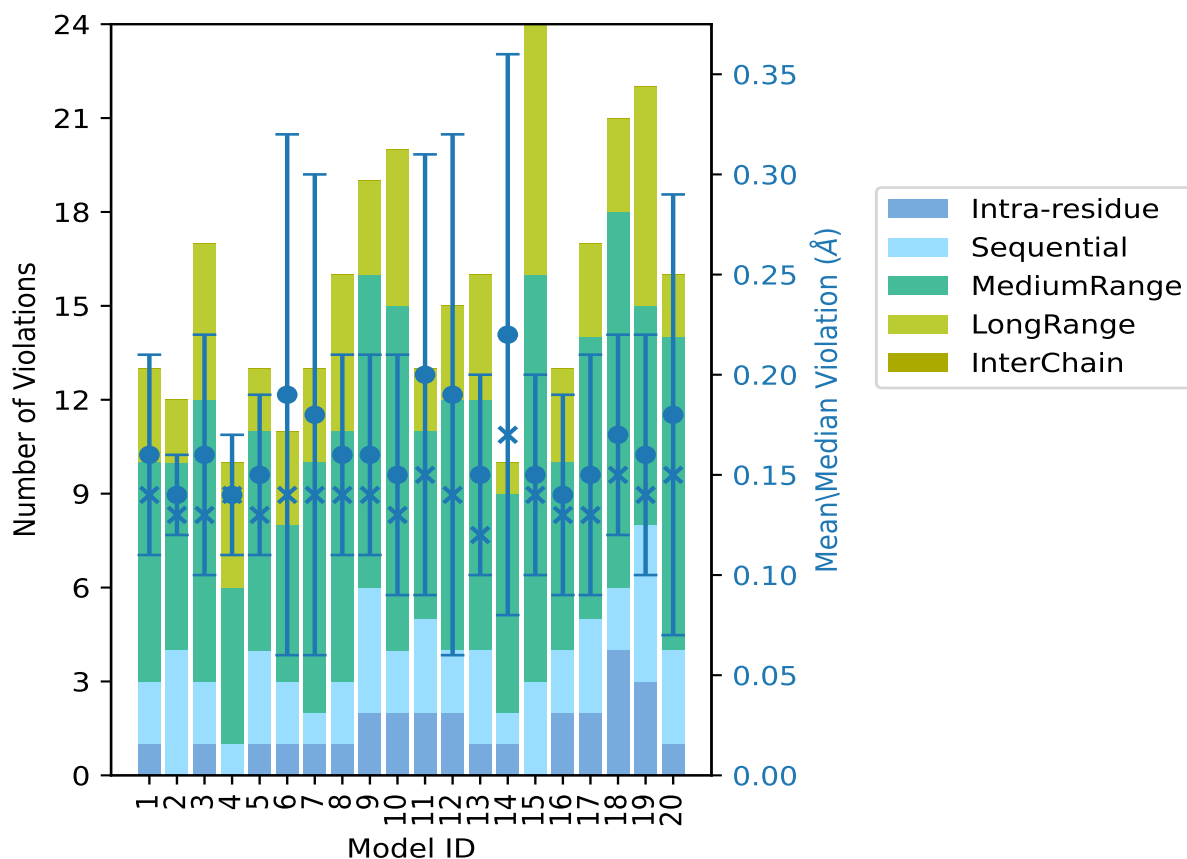
Continued on next page...

Continued from previous page...

Model ID	Number of violations					Total	Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵					
11	2	3	6	2	0	13	0.2	0.48	0.11	0.15
12	2	2	8	3	0	15	0.19	0.56	0.13	0.14
13	1	3	8	4	0	16	0.15	0.32	0.05	0.12
14	1	1	7	1	0	10	0.22	0.57	0.14	0.17
15	0	3	13	8	0	24	0.15	0.29	0.05	0.14
16	2	2	6	3	0	13	0.14	0.29	0.05	0.13
17	2	3	9	3	0	17	0.15	0.3	0.06	0.13
18	4	2	12	3	0	21	0.17	0.28	0.05	0.15
19	3	5	7	7	0	22	0.16	0.32	0.06	0.14
20	1	3	10	2	0	16	0.18	0.57	0.11	0.15

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

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



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

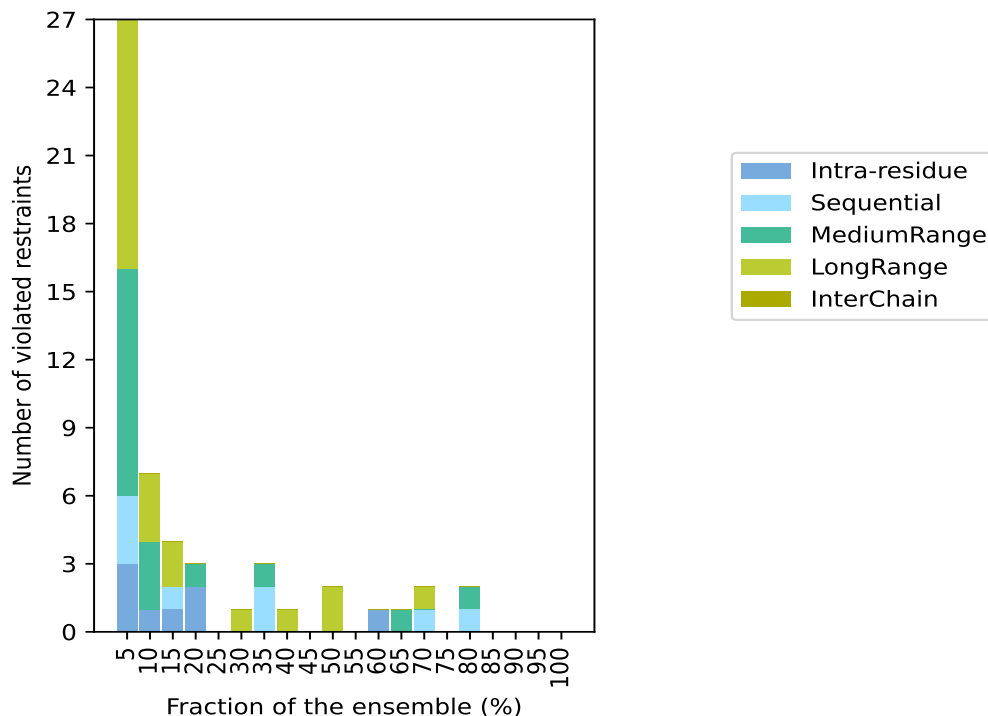
9.3 Distance violation statistics for the ensemble

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, 1671(IR:302, SQ:358, MR:484, LR:527, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
3	3	10	11	0	27	1	5.0
1	0	3	3	0	7	2	10.0
1	1	0	2	0	4	3	15.0
2	0	1	0	0	3	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	1	0	1	6	30.0
0	2	1	0	0	3	7	35.0
0	0	0	1	0	1	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	2	0	2	10	50.0
0	0	0	0	0	0	11	55.0
1	0	0	0	0	1	12	60.0
0	0	1	0	0	1	13	65.0
0	1	0	1	0	2	14	70.0
0	0	0	0	0	0	15	75.0
0	1	1	0	0	2	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	20	100.0

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

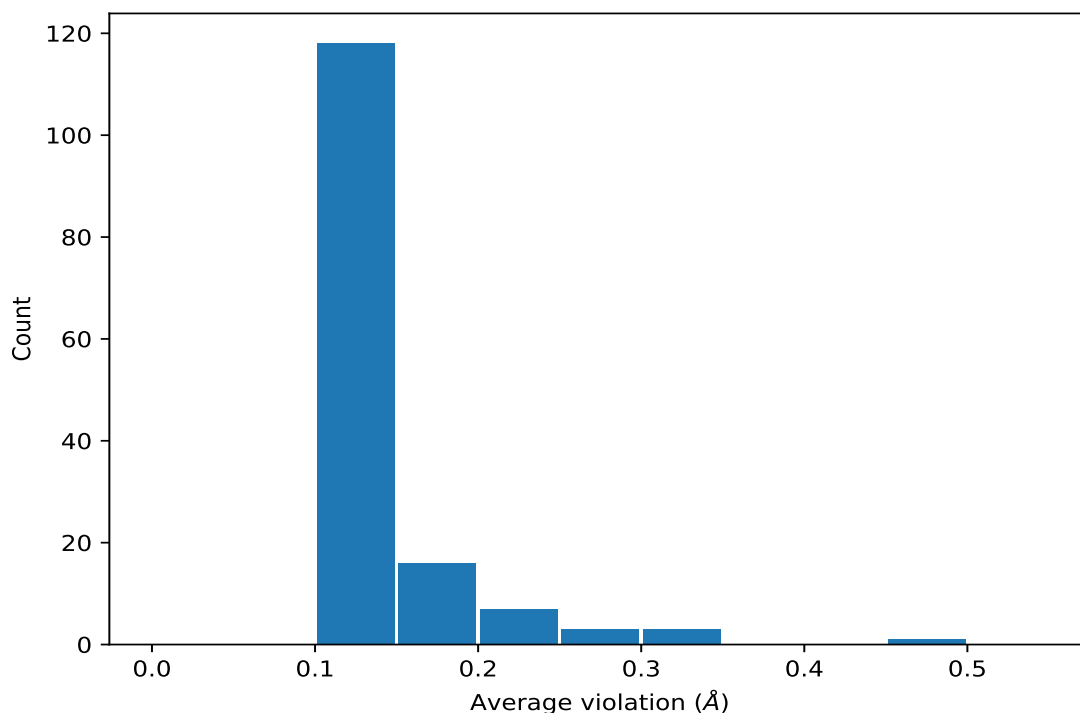
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(3,35)	1:212:A:VAL:O	1:216:A:LEU:H	18	0.21	0.05	0.2
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG21	16	0.15	0.03	0.15
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG22	16	0.15	0.03	0.15
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG23	16	0.15	0.03	0.15
(3,15)	1:201:A:ASP:O	1:205:A:GLN:H	16	0.14	0.02	0.14
(1,58)	1:203:A:ALA:HB1	1:205:A:GLN:H	16	0.12	0.02	0.12
(1,58)	1:203:A:ALA:HB2	1:205:A:GLN:H	16	0.12	0.02	0.12
(1,58)	1:203:A:ALA:HB3	1:205:A:GLN:H	16	0.12	0.02	0.12
(1,1134)	1:231:A:LEU:HD11	1:276:A:VAL:HB	14	0.23	0.05	0.24
(1,1134)	1:231:A:LEU:HD12	1:276:A:VAL:HB	14	0.23	0.05	0.24
(1,1134)	1:231:A:LEU:HD13	1:276:A:VAL:HB	14	0.23	0.05	0.24
(1,1134)	1:231:A:LEU:HD21	1:276:A:VAL:HB	14	0.23	0.05	0.24
(1,1134)	1:231:A:LEU:HD22	1:276:A:VAL:HB	14	0.23	0.05	0.24
(1,1134)	1:231:A:LEU:HD23	1:276:A:VAL:HB	14	0.23	0.05	0.24
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD1	14	0.19	0.07	0.15
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD2	14	0.19	0.07	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,36)	1:212:A:VAL:O	1:216:A:LEU:N	14	0.13	0.03	0.12
(1,453)	1:213:A:ILE:HG21	1:216:A:LEU:HG	13	0.14	0.02	0.13
(1,453)	1:213:A:ILE:HG22	1:216:A:LEU:HG	13	0.14	0.02	0.13
(1,453)	1:213:A:ILE:HG23	1:216:A:LEU:HG	13	0.14	0.02	0.13
(1,24)	1:197:A:LEU:H	1:197:A:LEU:HG	12	0.25	0.07	0.22
(3,33)	1:211:A:GLN:O	1:215:A:ALA:H	11	0.13	0.02	0.12
(1,1067)	1:217:A:GLN:HE21	1:226:A:ASN:HD21	10	0.17	0.05	0.16
(1,1067)	1:217:A:GLN:HE21	1:226:A:ASN:HD22	10	0.17	0.05	0.16
(1,1067)	1:217:A:GLN:HE22	1:226:A:ASN:HD21	10	0.17	0.05	0.16
(1,1067)	1:217:A:GLN:HE22	1:226:A:ASN:HD22	10	0.17	0.05	0.16
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD11	10	0.14	0.02	0.13
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD12	10	0.14	0.02	0.13
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD13	10	0.14	0.02	0.13
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD21	10	0.14	0.02	0.13
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD22	10	0.14	0.02	0.13
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD23	10	0.14	0.02	0.13
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD11	10	0.14	0.02	0.13
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD12	10	0.14	0.02	0.13
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD13	10	0.14	0.02	0.13
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD21	10	0.14	0.02	0.13
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD22	10	0.14	0.02	0.13
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD23	10	0.14	0.02	0.13
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD11	10	0.14	0.02	0.13
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD12	10	0.14	0.02	0.13
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD13	10	0.14	0.02	0.13
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD21	10	0.14	0.02	0.13
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD22	10	0.14	0.02	0.13
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD23	10	0.14	0.02	0.13
(3,39)	1:214:A:ALA:O	1:218:A:LYS:H	10	0.12	0.01	0.12
(1,1233)	1:247:A:LEU:HD11	1:265:A:MET:HE1	8	0.15	0.05	0.13
(1,1233)	1:247:A:LEU:HD11	1:265:A:MET:HE2	8	0.15	0.05	0.13
(1,1233)	1:247:A:LEU:HD11	1:265:A:MET:HE3	8	0.15	0.05	0.13
(1,1233)	1:247:A:LEU:HD12	1:265:A:MET:HE1	8	0.15	0.05	0.13
(1,1233)	1:247:A:LEU:HD12	1:265:A:MET:HE2	8	0.15	0.05	0.13
(1,1233)	1:247:A:LEU:HD12	1:265:A:MET:HE3	8	0.15	0.05	0.13
(1,1233)	1:247:A:LEU:HD13	1:265:A:MET:HE1	8	0.15	0.05	0.13
(1,1233)	1:247:A:LEU:HD13	1:265:A:MET:HE2	8	0.15	0.05	0.13
(1,1233)	1:247:A:LEU:HD13	1:265:A:MET:HE3	8	0.15	0.05	0.13
(1,1233)	1:247:A:LEU:HD21	1:265:A:MET:HE1	8	0.15	0.05	0.13
(1,1233)	1:247:A:LEU:HD21	1:265:A:MET:HE2	8	0.15	0.05	0.13
(1,1233)	1:247:A:LEU:HD21	1:265:A:MET:HE3	8	0.15	0.05	0.13
(1,1233)	1:247:A:LEU:HD22	1:265:A:MET:HE1	8	0.15	0.05	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1233)	1:247:A:LEU:HD22	1:265:A:MET:HE2	8	0.15	0.05	0.13
(1,1233)	1:247:A:LEU:HD22	1:265:A:MET:HE3	8	0.15	0.05	0.13
(1,1233)	1:247:A:LEU:HD23	1:265:A:MET:HE1	8	0.15	0.05	0.13
(1,1233)	1:247:A:LEU:HD23	1:265:A:MET:HE2	8	0.15	0.05	0.13
(1,1233)	1:247:A:LEU:HD23	1:265:A:MET:HE3	8	0.15	0.05	0.13
(1,450)	1:174:A:SER:HA	1:177:A:ILE:HB	7	0.48	0.16	0.56
(1,63)	1:180:A:ASN:H	1:181:A:LEU:HA	7	0.13	0.03	0.13
(1,376)	1:177:A:ILE:HD11	1:178:A:LEU:HA	7	0.11	0.01	0.11
(1,376)	1:177:A:ILE:HD12	1:178:A:LEU:HA	7	0.11	0.01	0.11
(1,376)	1:177:A:ILE:HD13	1:178:A:LEU:HA	7	0.11	0.01	0.11
(1,217)	1:195:A:THR:HG21	1:200:A:THR:HB	6	0.19	0.06	0.18
(1,217)	1:195:A:THR:HG22	1:200:A:THR:HB	6	0.19	0.06	0.18
(1,217)	1:195:A:THR:HG23	1:200:A:THR:HB	6	0.19	0.06	0.18
(3,43)	1:216:A:LEU:O	1:220:A:PHE:H	5	0.15	0.06	0.13
(3,37)	1:213:A:ILE:O	1:217:A:GLN:H	5	0.13	0.02	0.13
(1,123)	1:177:A:ILE:HA	1:177:A:ILE:HD11	4	0.34	0.0	0.34
(1,123)	1:177:A:ILE:HA	1:177:A:ILE:HD12	4	0.34	0.0	0.34
(1,123)	1:177:A:ILE:HA	1:177:A:ILE:HD13	4	0.34	0.0	0.34
(2,170)	1:221:A:LYS:H	1:223:A:ASN:H	4	0.16	0.04	0.15
(1,526)	1:197:A:LEU:HA	1:197:A:LEU:HD21	4	0.14	0.04	0.13
(1,526)	1:197:A:LEU:HA	1:197:A:LEU:HD22	4	0.14	0.04	0.13
(1,526)	1:197:A:LEU:HA	1:197:A:LEU:HD23	4	0.14	0.04	0.13
(3,40)	1:214:A:ALA:O	1:218:A:LYS:N	4	0.11	0.01	0.11
(3,1)	1:169:A:ASP:O	1:173:A:ARG:H	4	0.1	0.0	0.1
(1,900)	1:193:A:LEU:HB2	1:194:A:PRO:HD2	3	0.16	0.0	0.16
(1,900)	1:193:A:LEU:HB2	1:194:A:PRO:HD3	3	0.16	0.0	0.16
(1,900)	1:193:A:LEU:HB3	1:194:A:PRO:HD2	3	0.16	0.0	0.16
(1,900)	1:193:A:LEU:HB3	1:194:A:PRO:HD3	3	0.16	0.0	0.16
(1,1052)	1:216:A:LEU:HB2	1:259:A:MET:HE1	3	0.15	0.01	0.15
(1,1052)	1:216:A:LEU:HB2	1:259:A:MET:HE2	3	0.15	0.01	0.15
(1,1052)	1:216:A:LEU:HB2	1:259:A:MET:HE3	3	0.15	0.01	0.15
(1,1052)	1:216:A:LEU:HB3	1:259:A:MET:HE1	3	0.15	0.01	0.15
(1,1052)	1:216:A:LEU:HB3	1:259:A:MET:HE2	3	0.15	0.01	0.15
(1,1052)	1:216:A:LEU:HB3	1:259:A:MET:HE3	3	0.15	0.01	0.15
(3,45)	1:217:A:GLN:O	1:221:A:LYS:H	3	0.14	0.01	0.13
(1,491)	1:181:A:LEU:HA	1:181:A:LEU:HD11	3	0.12	0.02	0.12
(1,491)	1:181:A:LEU:HA	1:181:A:LEU:HD12	3	0.12	0.02	0.12
(1,491)	1:181:A:LEU:HA	1:181:A:LEU:HD13	3	0.12	0.02	0.12
(1,1176)	1:238:A:TYR:HB2	1:265:A:MET:HE1	3	0.12	0.01	0.12
(1,1176)	1:238:A:TYR:HB2	1:265:A:MET:HE2	3	0.12	0.01	0.12
(1,1176)	1:238:A:TYR:HB2	1:265:A:MET:HE3	3	0.12	0.01	0.12
(1,1176)	1:238:A:TYR:HB3	1:265:A:MET:HE1	3	0.12	0.01	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1176)	1:238:A:TYR:HB3	1:265:A:MET:HE2	3	0.12	0.01	0.12
(1,1176)	1:238:A:TYR:HB3	1:265:A:MET:HE3	3	0.12	0.01	0.12
(3,53)	1:234:A:LYS:O	1:238:A:TYR:H	3	0.12	0.02	0.11
(3,46)	1:217:A:GLN:O	1:221:A:LYS:N	3	0.11	0.01	0.1
(1,792)	1:171:A:LYS:H	1:173:A:ARG:HD2	2	0.26	0.03	0.26
(1,792)	1:171:A:LYS:H	1:173:A:ARG:HD3	2	0.26	0.03	0.26
(1,1164)	1:235:A:GLN:HE21	1:274:A:LEU:HG	2	0.18	0.04	0.18
(1,1164)	1:235:A:GLN:HE22	1:274:A:LEU:HG	2	0.18	0.04	0.18
(1,538)	1:231:A:LEU:HD11	1:235:A:GLN:HE22	2	0.15	0.03	0.15
(1,538)	1:231:A:LEU:HD12	1:235:A:GLN:HE22	2	0.15	0.03	0.15
(1,538)	1:231:A:LEU:HD13	1:235:A:GLN:HE22	2	0.15	0.03	0.15
(1,1035)	1:213:A:ILE:HD11	1:216:A:LEU:HD11	2	0.13	0.0	0.13
(1,1035)	1:213:A:ILE:HD11	1:216:A:LEU:HD12	2	0.13	0.0	0.13
(1,1035)	1:213:A:ILE:HD11	1:216:A:LEU:HD13	2	0.13	0.0	0.13
(1,1035)	1:213:A:ILE:HD11	1:216:A:LEU:HD21	2	0.13	0.0	0.13
(1,1035)	1:213:A:ILE:HD11	1:216:A:LEU:HD22	2	0.13	0.0	0.13
(1,1035)	1:213:A:ILE:HD11	1:216:A:LEU:HD23	2	0.13	0.0	0.13
(1,1035)	1:213:A:ILE:HD12	1:216:A:LEU:HD11	2	0.13	0.0	0.13
(1,1035)	1:213:A:ILE:HD12	1:216:A:LEU:HD12	2	0.13	0.0	0.13
(1,1035)	1:213:A:ILE:HD12	1:216:A:LEU:HD13	2	0.13	0.0	0.13
(1,1035)	1:213:A:ILE:HD12	1:216:A:LEU:HD21	2	0.13	0.0	0.13
(1,1035)	1:213:A:ILE:HD12	1:216:A:LEU:HD22	2	0.13	0.0	0.13
(1,1035)	1:213:A:ILE:HD12	1:216:A:LEU:HD23	2	0.13	0.0	0.13
(1,1035)	1:213:A:ILE:HD13	1:216:A:LEU:HD11	2	0.13	0.0	0.13
(1,1035)	1:213:A:ILE:HD13	1:216:A:LEU:HD12	2	0.13	0.0	0.13
(1,1035)	1:213:A:ILE:HD13	1:216:A:LEU:HD13	2	0.13	0.0	0.13
(1,1035)	1:213:A:ILE:HD13	1:216:A:LEU:HD21	2	0.13	0.0	0.13
(1,1035)	1:213:A:ILE:HD13	1:216:A:LEU:HD22	2	0.13	0.0	0.13
(1,1035)	1:213:A:ILE:HD13	1:216:A:LEU:HD23	2	0.13	0.0	0.13
(1,689)	1:178:A:LEU:H	1:178:A:LEU:HG	2	0.12	0.02	0.12
(3,38)	1:213:A:ILE:O	1:217:A:GLN:N	2	0.12	0.0	0.12
(1,410)	1:177:A:ILE:HD11	1:244:A:MET:HE1	2	0.11	0.01	0.11
(1,410)	1:177:A:ILE:HD11	1:244:A:MET:HE2	2	0.11	0.01	0.11
(1,410)	1:177:A:ILE:HD11	1:244:A:MET:HE3	2	0.11	0.01	0.11
(1,410)	1:177:A:ILE:HD12	1:244:A:MET:HE1	2	0.11	0.01	0.11
(1,410)	1:177:A:ILE:HD12	1:244:A:MET:HE2	2	0.11	0.01	0.11
(1,410)	1:177:A:ILE:HD12	1:244:A:MET:HE3	2	0.11	0.01	0.11
(1,410)	1:177:A:ILE:HD13	1:244:A:MET:HE1	2	0.11	0.01	0.11
(1,410)	1:177:A:ILE:HD13	1:244:A:MET:HE2	2	0.11	0.01	0.11
(1,410)	1:177:A:ILE:HD13	1:244:A:MET:HE3	2	0.11	0.01	0.11
(3,75)	1:262:A:ILE:O	1:266:A:LEU:H	2	0.11	0.01	0.11
(1,920)	1:194:A:PRO:HB2	1:208:A:ALA:HB1	2	0.11	0.0	0.11

Continued on next page...

Continued from previous page...

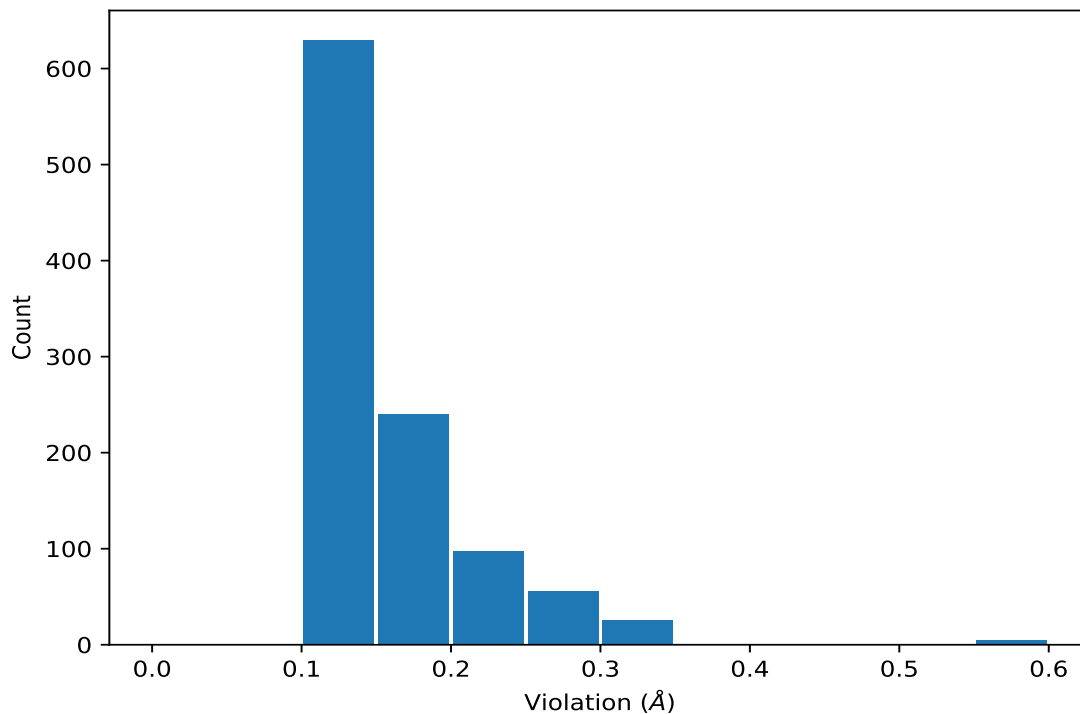
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,920)	1:194:A:PRO:HB2	1:208:A:ALA:HB2	2	0.11	0.0	0.11
(1,920)	1:194:A:PRO:HB2	1:208:A:ALA:HB3	2	0.11	0.0	0.11
(1,920)	1:194:A:PRO:HB3	1:208:A:ALA:HB1	2	0.11	0.0	0.11
(1,920)	1:194:A:PRO:HB3	1:208:A:ALA:HB2	2	0.11	0.0	0.11
(1,920)	1:194:A:PRO:HB3	1:208:A:ALA:HB3	2	0.11	0.0	0.11
(3,41)	1:215:A:ALA:O	1:219:A:HIS:H	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,450)	1:174:A:SER:HA	1:177:A:ILE:HB	14	0.57
(1,450)	1:174:A:SER:HA	1:177:A:ILE:HB	20	0.57
(1,450)	1:174:A:SER:HA	1:177:A:ILE:HB	7	0.56
(1,450)	1:174:A:SER:HA	1:177:A:ILE:HB	12	0.56
(1,450)	1:174:A:SER:HA	1:177:A:ILE:HB	6	0.55
(1,450)	1:174:A:SER:HA	1:177:A:ILE:HB	11	0.48
(1,24)	1:197:A:LEU:H	1:197:A:LEU:HG	12	0.4
(1,314)	1:266:A:LEU:H	1:266:A:LEU:HG	10	0.35
(1,123)	1:177:A:ILE:HA	1:177:A:ILE:HD11	6	0.34
(1,123)	1:177:A:ILE:HA	1:177:A:ILE:HD12	6	0.34
(1,123)	1:177:A:ILE:HA	1:177:A:ILE:HD13	6	0.34
(1,123)	1:177:A:ILE:HA	1:177:A:ILE:HD11	12	0.34
(1,123)	1:177:A:ILE:HA	1:177:A:ILE:HD12	12	0.34
(1,123)	1:177:A:ILE:HA	1:177:A:ILE:HD13	12	0.34
(1,123)	1:177:A:ILE:HA	1:177:A:ILE:HD11	14	0.34
(1,123)	1:177:A:ILE:HA	1:177:A:ILE:HD12	14	0.34
(1,123)	1:177:A:ILE:HA	1:177:A:ILE:HD13	14	0.34
(1,24)	1:197:A:LEU:H	1:197:A:LEU:HG	3	0.34
(1,123)	1:177:A:ILE:HA	1:177:A:ILE:HD11	11	0.33
(1,123)	1:177:A:ILE:HA	1:177:A:ILE:HD12	11	0.33
(1,123)	1:177:A:ILE:HA	1:177:A:ILE:HD13	11	0.33
(1,1134)	1:231:A:LEU:HD11	1:276:A:VAL:HB	19	0.32
(1,1134)	1:231:A:LEU:HD12	1:276:A:VAL:HB	19	0.32
(1,1134)	1:231:A:LEU:HD13	1:276:A:VAL:HB	19	0.32
(1,1134)	1:231:A:LEU:HD21	1:276:A:VAL:HB	19	0.32
(1,1134)	1:231:A:LEU:HD22	1:276:A:VAL:HB	19	0.32
(1,1134)	1:231:A:LEU:HD23	1:276:A:VAL:HB	19	0.32
(1,24)	1:197:A:LEU:H	1:197:A:LEU:HG	13	0.32
(1,1067)	1:217:A:GLN:HE21	1:226:A:ASN:HD21	17	0.3
(1,1067)	1:217:A:GLN:HE21	1:226:A:ASN:HD22	17	0.3
(1,1067)	1:217:A:GLN:HE22	1:226:A:ASN:HD21	17	0.3
(1,1067)	1:217:A:GLN:HE22	1:226:A:ASN:HD22	17	0.3
(1,24)	1:197:A:LEU:H	1:197:A:LEU:HG	9	0.3
(3,35)	1:212:A:VAL:O	1:216:A:LEU:H	11	0.29
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD1	8	0.29
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD2	8	0.29
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD1	16	0.29
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD2	16	0.29
(1,1229)	1:247:A:LEU:HD11	1:249:A:GLN:HA	15	0.29
(1,1229)	1:247:A:LEU:HD12	1:249:A:GLN:HA	15	0.29
(1,1229)	1:247:A:LEU:HD13	1:249:A:GLN:HA	15	0.29
(1,1229)	1:247:A:LEU:HD21	1:249:A:GLN:HA	15	0.29
(1,1229)	1:247:A:LEU:HD22	1:249:A:GLN:HA	15	0.29

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1229)	1:247:A:LEU:HD23	1:249:A:GLN:HA	15	0.29
(1,1134)	1:231:A:LEU:HD11	1:276:A:VAL:HB	14	0.29
(1,1134)	1:231:A:LEU:HD12	1:276:A:VAL:HB	14	0.29
(1,1134)	1:231:A:LEU:HD13	1:276:A:VAL:HB	14	0.29
(1,1134)	1:231:A:LEU:HD21	1:276:A:VAL:HB	14	0.29
(1,1134)	1:231:A:LEU:HD22	1:276:A:VAL:HB	14	0.29
(1,1134)	1:231:A:LEU:HD23	1:276:A:VAL:HB	14	0.29
(1,1134)	1:231:A:LEU:HD11	1:276:A:VAL:HB	17	0.29
(1,1134)	1:231:A:LEU:HD12	1:276:A:VAL:HB	17	0.29
(1,1134)	1:231:A:LEU:HD13	1:276:A:VAL:HB	17	0.29
(1,1134)	1:231:A:LEU:HD21	1:276:A:VAL:HB	17	0.29
(1,1134)	1:231:A:LEU:HD22	1:276:A:VAL:HB	17	0.29
(1,1134)	1:231:A:LEU:HD23	1:276:A:VAL:HB	17	0.29
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD1	19	0.28
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD2	19	0.28
(1,792)	1:171:A:LYS:H	1:173:A:ARG:HD2	18	0.28
(1,792)	1:171:A:LYS:H	1:173:A:ARG:HD3	18	0.28
(3,35)	1:212:A:VAL:O	1:216:A:LEU:H	3	0.27
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD1	1	0.27
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD2	1	0.27
(1,24)	1:197:A:LEU:H	1:197:A:LEU:HG	10	0.27
(3,43)	1:216:A:LEU:O	1:220:A:PHE:H	19	0.26
(3,35)	1:212:A:VAL:O	1:216:A:LEU:H	9	0.26
(3,35)	1:212:A:VAL:O	1:216:A:LEU:H	10	0.26
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD1	15	0.26
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD2	15	0.26
(1,1134)	1:231:A:LEU:HD11	1:276:A:VAL:HB	20	0.26
(1,1134)	1:231:A:LEU:HD12	1:276:A:VAL:HB	20	0.26
(1,1134)	1:231:A:LEU:HD13	1:276:A:VAL:HB	20	0.26
(1,1134)	1:231:A:LEU:HD21	1:276:A:VAL:HB	20	0.26
(1,1134)	1:231:A:LEU:HD22	1:276:A:VAL:HB	20	0.26
(1,1134)	1:231:A:LEU:HD23	1:276:A:VAL:HB	20	0.26
(1,217)	1:195:A:THR:HG21	1:200:A:THR:HB	7	0.26
(1,217)	1:195:A:THR:HG22	1:200:A:THR:HB	7	0.26
(1,217)	1:195:A:THR:HG23	1:200:A:THR:HB	7	0.26
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD1	18	0.25
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD2	18	0.25
(1,1134)	1:231:A:LEU:HD11	1:276:A:VAL:HB	1	0.25
(1,1134)	1:231:A:LEU:HD12	1:276:A:VAL:HB	1	0.25
(1,1134)	1:231:A:LEU:HD13	1:276:A:VAL:HB	1	0.25
(1,1134)	1:231:A:LEU:HD21	1:276:A:VAL:HB	1	0.25
(1,1134)	1:231:A:LEU:HD22	1:276:A:VAL:HB	1	0.25

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1134)	1:231:A:LEU:HD23	1:276:A:VAL:HB	1	0.25
(1,217)	1:195:A:THR:HG21	1:200:A:THR:HB	18	0.25
(1,217)	1:195:A:THR:HG22	1:200:A:THR:HB	18	0.25
(1,217)	1:195:A:THR:HG23	1:200:A:THR:HB	18	0.25
(3,35)	1:212:A:VAL:O	1:216:A:LEU:H	15	0.24
(3,35)	1:212:A:VAL:O	1:216:A:LEU:H	18	0.24
(1,1233)	1:247:A:LEU:HD11	1:265:A:MET:HE1	15	0.24
(1,1233)	1:247:A:LEU:HD11	1:265:A:MET:HE2	15	0.24
(1,1233)	1:247:A:LEU:HD11	1:265:A:MET:HE3	15	0.24
(1,1233)	1:247:A:LEU:HD12	1:265:A:MET:HE1	15	0.24
(1,1233)	1:247:A:LEU:HD12	1:265:A:MET:HE2	15	0.24
(1,1233)	1:247:A:LEU:HD12	1:265:A:MET:HE3	15	0.24
(1,1233)	1:247:A:LEU:HD13	1:265:A:MET:HE1	15	0.24
(1,1233)	1:247:A:LEU:HD13	1:265:A:MET:HE2	15	0.24
(1,1233)	1:247:A:LEU:HD13	1:265:A:MET:HE3	15	0.24
(1,1233)	1:247:A:LEU:HD21	1:265:A:MET:HE1	15	0.24
(1,1233)	1:247:A:LEU:HD21	1:265:A:MET:HE2	15	0.24
(1,1233)	1:247:A:LEU:HD21	1:265:A:MET:HE3	15	0.24
(1,1233)	1:247:A:LEU:HD22	1:265:A:MET:HE1	15	0.24
(1,1233)	1:247:A:LEU:HD22	1:265:A:MET:HE2	15	0.24
(1,1233)	1:247:A:LEU:HD22	1:265:A:MET:HE3	15	0.24
(1,1233)	1:247:A:LEU:HD23	1:265:A:MET:HE1	15	0.24
(1,1233)	1:247:A:LEU:HD23	1:265:A:MET:HE2	15	0.24
(1,1233)	1:247:A:LEU:HD23	1:265:A:MET:HE3	15	0.24
(1,1134)	1:231:A:LEU:HD11	1:276:A:VAL:HB	5	0.24
(1,1134)	1:231:A:LEU:HD12	1:276:A:VAL:HB	5	0.24
(1,1134)	1:231:A:LEU:HD13	1:276:A:VAL:HB	5	0.24
(1,1134)	1:231:A:LEU:HD21	1:276:A:VAL:HB	5	0.24
(1,1134)	1:231:A:LEU:HD22	1:276:A:VAL:HB	5	0.24
(1,1134)	1:231:A:LEU:HD23	1:276:A:VAL:HB	5	0.24
(1,1134)	1:231:A:LEU:HD11	1:276:A:VAL:HB	8	0.24
(1,1134)	1:231:A:LEU:HD12	1:276:A:VAL:HB	8	0.24
(1,1134)	1:231:A:LEU:HD13	1:276:A:VAL:HB	8	0.24
(1,1134)	1:231:A:LEU:HD21	1:276:A:VAL:HB	8	0.24
(1,1134)	1:231:A:LEU:HD22	1:276:A:VAL:HB	8	0.24
(1,1134)	1:231:A:LEU:HD23	1:276:A:VAL:HB	8	0.24
(1,1134)	1:231:A:LEU:HD11	1:276:A:VAL:HB	11	0.24
(1,1134)	1:231:A:LEU:HD12	1:276:A:VAL:HB	11	0.24
(1,1134)	1:231:A:LEU:HD13	1:276:A:VAL:HB	11	0.24
(1,1134)	1:231:A:LEU:HD21	1:276:A:VAL:HB	11	0.24
(1,1134)	1:231:A:LEU:HD22	1:276:A:VAL:HB	11	0.24
(1,1134)	1:231:A:LEU:HD23	1:276:A:VAL:HB	11	0.24

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1164)	1:235:A:GLN:HE21	1:274:A:LEU:HG	7	0.23
(1,1164)	1:235:A:GLN:HE22	1:274:A:LEU:HG	7	0.23
(1,1134)	1:231:A:LEU:HD11	1:276:A:VAL:HB	3	0.23
(1,1134)	1:231:A:LEU:HD12	1:276:A:VAL:HB	3	0.23
(1,1134)	1:231:A:LEU:HD13	1:276:A:VAL:HB	3	0.23
(1,1134)	1:231:A:LEU:HD21	1:276:A:VAL:HB	3	0.23
(1,1134)	1:231:A:LEU:HD22	1:276:A:VAL:HB	3	0.23
(1,1134)	1:231:A:LEU:HD23	1:276:A:VAL:HB	3	0.23
(1,792)	1:171:A:LYS:H	1:173:A:ARG:HD2	20	0.23
(1,792)	1:171:A:LYS:H	1:173:A:ARG:HD3	20	0.23
(1,24)	1:197:A:LEU:H	1:197:A:LEU:HG	18	0.23
(3,35)	1:212:A:VAL:O	1:216:A:LEU:H	8	0.22
(3,35)	1:212:A:VAL:O	1:216:A:LEU:H	14	0.22
(2,170)	1:221:A:LYS:H	1:223:A:ASN:H	16	0.22
(1,1134)	1:231:A:LEU:HD11	1:276:A:VAL:HB	9	0.22
(1,1134)	1:231:A:LEU:HD12	1:276:A:VAL:HB	9	0.22
(1,1134)	1:231:A:LEU:HD13	1:276:A:VAL:HB	9	0.22
(1,1134)	1:231:A:LEU:HD21	1:276:A:VAL:HB	9	0.22
(1,1134)	1:231:A:LEU:HD22	1:276:A:VAL:HB	9	0.22
(1,1134)	1:231:A:LEU:HD23	1:276:A:VAL:HB	9	0.22
(1,1233)	1:247:A:LEU:HD11	1:265:A:MET:HE1	10	0.21
(1,1233)	1:247:A:LEU:HD11	1:265:A:MET:HE2	10	0.21
(1,1233)	1:247:A:LEU:HD11	1:265:A:MET:HE3	10	0.21
(1,1233)	1:247:A:LEU:HD12	1:265:A:MET:HE1	10	0.21
(1,1233)	1:247:A:LEU:HD12	1:265:A:MET:HE2	10	0.21
(1,1233)	1:247:A:LEU:HD12	1:265:A:MET:HE3	10	0.21
(1,1233)	1:247:A:LEU:HD13	1:265:A:MET:HE1	10	0.21
(1,1233)	1:247:A:LEU:HD13	1:265:A:MET:HE2	10	0.21
(1,1233)	1:247:A:LEU:HD13	1:265:A:MET:HE3	10	0.21
(1,1233)	1:247:A:LEU:HD21	1:265:A:MET:HE1	10	0.21
(1,1233)	1:247:A:LEU:HD21	1:265:A:MET:HE2	10	0.21
(1,1233)	1:247:A:LEU:HD21	1:265:A:MET:HE3	10	0.21
(1,1233)	1:247:A:LEU:HD22	1:265:A:MET:HE1	10	0.21
(1,1233)	1:247:A:LEU:HD22	1:265:A:MET:HE2	10	0.21
(1,1233)	1:247:A:LEU:HD22	1:265:A:MET:HE3	10	0.21
(1,1233)	1:247:A:LEU:HD23	1:265:A:MET:HE1	10	0.21
(1,1233)	1:247:A:LEU:HD23	1:265:A:MET:HE2	10	0.21
(1,1233)	1:247:A:LEU:HD23	1:265:A:MET:HE3	10	0.21
(1,24)	1:197:A:LEU:H	1:197:A:LEU:HG	5	0.21
(3,35)	1:212:A:VAL:O	1:216:A:LEU:H	5	0.2
(3,35)	1:212:A:VAL:O	1:216:A:LEU:H	12	0.2
(3,35)	1:212:A:VAL:O	1:216:A:LEU:H	20	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,34)	1:177:A:ILE:HA	1:180:A:ASN:HA	18	0.2
(1,1134)	1:231:A:LEU:HD11	1:276:A:VAL:HB	2	0.2
(1,1134)	1:231:A:LEU:HD12	1:276:A:VAL:HB	2	0.2
(1,1134)	1:231:A:LEU:HD13	1:276:A:VAL:HB	2	0.2
(1,1134)	1:231:A:LEU:HD21	1:276:A:VAL:HB	2	0.2
(1,1134)	1:231:A:LEU:HD22	1:276:A:VAL:HB	2	0.2
(1,1134)	1:231:A:LEU:HD23	1:276:A:VAL:HB	2	0.2
(1,1067)	1:217:A:GLN:HE21	1:226:A:ASN:HD21	9	0.2
(1,1067)	1:217:A:GLN:HE21	1:226:A:ASN:HD22	9	0.2
(1,1067)	1:217:A:GLN:HE22	1:226:A:ASN:HD21	9	0.2
(1,1067)	1:217:A:GLN:HE22	1:226:A:ASN:HD22	9	0.2
(1,671)	1:181:A:LEU:HD21	1:182:A:LYS:H	18	0.2
(1,671)	1:181:A:LEU:HD22	1:182:A:LYS:H	18	0.2
(1,671)	1:181:A:LEU:HD23	1:182:A:LYS:H	18	0.2
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG21	9	0.2
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG22	9	0.2
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG23	9	0.2
(3,36)	1:212:A:VAL:O	1:216:A:LEU:N	3	0.19
(3,35)	1:212:A:VAL:O	1:216:A:LEU:H	7	0.19
(3,15)	1:201:A:ASP:O	1:205:A:GLN:H	1	0.19
(1,1258)	1:253:A:LEU:HB2	1:258:A:LYS:HA	13	0.19
(1,1258)	1:253:A:LEU:HB3	1:258:A:LYS:HA	13	0.19
(1,1067)	1:217:A:GLN:HE21	1:226:A:ASN:HD21	20	0.19
(1,1067)	1:217:A:GLN:HE21	1:226:A:ASN:HD22	20	0.19
(1,1067)	1:217:A:GLN:HE22	1:226:A:ASN:HD21	20	0.19
(1,1067)	1:217:A:GLN:HE22	1:226:A:ASN:HD22	20	0.19
(1,526)	1:197:A:LEU:HA	1:197:A:LEU:HD21	18	0.19
(1,526)	1:197:A:LEU:HA	1:197:A:LEU:HD22	18	0.19
(1,526)	1:197:A:LEU:HA	1:197:A:LEU:HD23	18	0.19
(1,453)	1:213:A:ILE:HG21	1:216:A:LEU:HG	9	0.19
(1,453)	1:213:A:ILE:HG22	1:216:A:LEU:HG	9	0.19
(1,453)	1:213:A:ILE:HG23	1:216:A:LEU:HG	9	0.19
(1,217)	1:195:A:THR:HG21	1:200:A:THR:HB	15	0.19
(1,217)	1:195:A:THR:HG22	1:200:A:THR:HB	15	0.19
(1,217)	1:195:A:THR:HG23	1:200:A:THR:HB	15	0.19
(1,24)	1:197:A:LEU:H	1:197:A:LEU:HG	1	0.19
(1,24)	1:197:A:LEU:H	1:197:A:LEU:HG	8	0.19
(3,35)	1:212:A:VAL:O	1:216:A:LEU:H	4	0.18
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD11	19	0.18
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD12	19	0.18
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD13	19	0.18
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD21	19	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD22	19	0.18
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD23	19	0.18
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD11	19	0.18
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD12	19	0.18
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD13	19	0.18
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD21	19	0.18
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD22	19	0.18
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD23	19	0.18
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD11	19	0.18
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD12	19	0.18
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD13	19	0.18
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD21	19	0.18
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD22	19	0.18
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD23	19	0.18
(1,538)	1:231:A:LEU:HD11	1:235:A:GLN:HE22	20	0.18
(1,538)	1:231:A:LEU:HD12	1:235:A:GLN:HE22	20	0.18
(1,538)	1:231:A:LEU:HD13	1:235:A:GLN:HE22	20	0.18
(1,453)	1:213:A:ILE:HG21	1:216:A:LEU:HG	8	0.18
(1,453)	1:213:A:ILE:HG22	1:216:A:LEU:HG	8	0.18
(1,453)	1:213:A:ILE:HG23	1:216:A:LEU:HG	8	0.18
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG21	4	0.18
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG22	4	0.18
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG23	4	0.18
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG21	12	0.18
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG22	12	0.18
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG23	12	0.18
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG21	14	0.18
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG22	14	0.18
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG23	14	0.18
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG21	15	0.18
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG22	15	0.18
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG23	15	0.18
(1,265)	1:219:A:HIS:HD2	1:220:A:PHE:HZ	19	0.18
(1,63)	1:180:A:ASN:H	1:181:A:LEU:HA	8	0.18
(1,24)	1:197:A:LEU:H	1:197:A:LEU:HG	17	0.18
(3,36)	1:212:A:VAL:O	1:216:A:LEU:N	9	0.17
(3,35)	1:212:A:VAL:O	1:216:A:LEU:H	6	0.17
(3,35)	1:212:A:VAL:O	1:216:A:LEU:H	13	0.17
(3,33)	1:211:A:GLN:O	1:215:A:ALA:H	15	0.17
(1,1233)	1:247:A:LEU:HD11	1:265:A:MET:HE1	3	0.17
(1,1233)	1:247:A:LEU:HD11	1:265:A:MET:HE2	3	0.17
(1,1233)	1:247:A:LEU:HD11	1:265:A:MET:HE3	3	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1233)	1:247:A:LEU:HD12	1:265:A:MET:HE1	3	0.17
(1,1233)	1:247:A:LEU:HD12	1:265:A:MET:HE2	3	0.17
(1,1233)	1:247:A:LEU:HD12	1:265:A:MET:HE3	3	0.17
(1,1233)	1:247:A:LEU:HD13	1:265:A:MET:HE1	3	0.17
(1,1233)	1:247:A:LEU:HD13	1:265:A:MET:HE2	3	0.17
(1,1233)	1:247:A:LEU:HD13	1:265:A:MET:HE3	3	0.17
(1,1233)	1:247:A:LEU:HD21	1:265:A:MET:HE1	3	0.17
(1,1233)	1:247:A:LEU:HD21	1:265:A:MET:HE2	3	0.17
(1,1233)	1:247:A:LEU:HD21	1:265:A:MET:HE3	3	0.17
(1,1233)	1:247:A:LEU:HD22	1:265:A:MET:HE1	3	0.17
(1,1233)	1:247:A:LEU:HD22	1:265:A:MET:HE2	3	0.17
(1,1233)	1:247:A:LEU:HD22	1:265:A:MET:HE3	3	0.17
(1,1233)	1:247:A:LEU:HD23	1:265:A:MET:HE1	3	0.17
(1,1233)	1:247:A:LEU:HD23	1:265:A:MET:HE2	3	0.17
(1,1233)	1:247:A:LEU:HD23	1:265:A:MET:HE3	3	0.17
(1,1067)	1:217:A:GLN:HE21	1:226:A:ASN:HD21	3	0.17
(1,1067)	1:217:A:GLN:HE21	1:226:A:ASN:HD22	3	0.17
(1,1067)	1:217:A:GLN:HE22	1:226:A:ASN:HD21	3	0.17
(1,1067)	1:217:A:GLN:HE22	1:226:A:ASN:HD22	3	0.17
(1,1067)	1:217:A:GLN:HE21	1:226:A:ASN:HD21	8	0.17
(1,1067)	1:217:A:GLN:HE21	1:226:A:ASN:HD22	8	0.17
(1,1067)	1:217:A:GLN:HE22	1:226:A:ASN:HD21	8	0.17
(1,1067)	1:217:A:GLN:HE22	1:226:A:ASN:HD22	8	0.17
(1,1052)	1:216:A:LEU:HB2	1:259:A:MET:HE1	4	0.17
(1,1052)	1:216:A:LEU:HB2	1:259:A:MET:HE2	4	0.17
(1,1052)	1:216:A:LEU:HB2	1:259:A:MET:HE3	4	0.17
(1,1052)	1:216:A:LEU:HB3	1:259:A:MET:HE1	4	0.17
(1,1052)	1:216:A:LEU:HB3	1:259:A:MET:HE2	4	0.17
(1,1052)	1:216:A:LEU:HB3	1:259:A:MET:HE3	4	0.17
(1,1042)	1:214:A:ALA:HA	1:217:A:GLN:HG2	19	0.17
(1,1042)	1:214:A:ALA:HA	1:217:A:GLN:HG3	19	0.17
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD11	4	0.17
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD12	4	0.17
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD13	4	0.17
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD21	4	0.17
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD22	4	0.17
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD23	4	0.17
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD11	4	0.17
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD12	4	0.17
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD13	4	0.17
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD21	4	0.17
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD22	4	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD23	4	0.17
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD11	4	0.17
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD12	4	0.17
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD13	4	0.17
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD21	4	0.17
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD22	4	0.17
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD23	4	0.17
(1,560)	1:213:A:ILE:HG21	1:213:A:ILE:HD11	18	0.17
(1,560)	1:213:A:ILE:HG21	1:213:A:ILE:HD12	18	0.17
(1,560)	1:213:A:ILE:HG21	1:213:A:ILE:HD13	18	0.17
(1,560)	1:213:A:ILE:HG22	1:213:A:ILE:HD11	18	0.17
(1,560)	1:213:A:ILE:HG22	1:213:A:ILE:HD12	18	0.17
(1,560)	1:213:A:ILE:HG22	1:213:A:ILE:HD13	18	0.17
(1,560)	1:213:A:ILE:HG23	1:213:A:ILE:HD11	18	0.17
(1,560)	1:213:A:ILE:HG23	1:213:A:ILE:HD12	18	0.17
(1,560)	1:213:A:ILE:HG23	1:213:A:ILE:HD13	18	0.17
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG21	19	0.17
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG22	19	0.17
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG23	19	0.17
(1,217)	1:195:A:THR:HG21	1:200:A:THR:HB	1	0.17
(1,217)	1:195:A:THR:HG22	1:200:A:THR:HB	1	0.17
(1,217)	1:195:A:THR:HG23	1:200:A:THR:HB	1	0.17
(1,24)	1:197:A:LEU:H	1:197:A:LEU:HG	16	0.17
(1,24)	1:197:A:LEU:H	1:197:A:LEU:HG	19	0.17
(3,45)	1:217:A:GLN:O	1:221:A:LYS:H	15	0.16
(3,37)	1:213:A:ILE:O	1:217:A:GLN:H	17	0.16
(3,33)	1:211:A:GLN:O	1:215:A:ALA:H	14	0.16
(3,15)	1:201:A:ASP:O	1:205:A:GLN:H	3	0.16
(3,15)	1:201:A:ASP:O	1:205:A:GLN:H	6	0.16
(3,15)	1:201:A:ASP:O	1:205:A:GLN:H	13	0.16
(1,1134)	1:231:A:LEU:HD11	1:276:A:VAL:HB	13	0.16
(1,1134)	1:231:A:LEU:HD12	1:276:A:VAL:HB	13	0.16
(1,1134)	1:231:A:LEU:HD13	1:276:A:VAL:HB	13	0.16
(1,1134)	1:231:A:LEU:HD21	1:276:A:VAL:HB	13	0.16
(1,1134)	1:231:A:LEU:HD22	1:276:A:VAL:HB	13	0.16
(1,1134)	1:231:A:LEU:HD23	1:276:A:VAL:HB	13	0.16
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD11	13	0.16
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD12	13	0.16
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD13	13	0.16
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD21	13	0.16
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD22	13	0.16
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD23	13	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD11	13	0.16
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD12	13	0.16
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD13	13	0.16
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD21	13	0.16
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD22	13	0.16
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD23	13	0.16
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD11	13	0.16
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD12	13	0.16
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD13	13	0.16
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD21	13	0.16
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD22	13	0.16
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD23	13	0.16
(1,900)	1:193:A:LEU:HB2	1:194:A:PRO:HD2	6	0.16
(1,900)	1:193:A:LEU:HB2	1:194:A:PRO:HD3	6	0.16
(1,900)	1:193:A:LEU:HB3	1:194:A:PRO:HD2	6	0.16
(1,900)	1:193:A:LEU:HB3	1:194:A:PRO:HD3	6	0.16
(1,900)	1:193:A:LEU:HB2	1:194:A:PRO:HD2	11	0.16
(1,900)	1:193:A:LEU:HB2	1:194:A:PRO:HD3	11	0.16
(1,900)	1:193:A:LEU:HB3	1:194:A:PRO:HD2	11	0.16
(1,900)	1:193:A:LEU:HB3	1:194:A:PRO:HD3	11	0.16
(1,900)	1:193:A:LEU:HB2	1:194:A:PRO:HD2	17	0.16
(1,900)	1:193:A:LEU:HB2	1:194:A:PRO:HD3	17	0.16
(1,900)	1:193:A:LEU:HB3	1:194:A:PRO:HD2	17	0.16
(1,900)	1:193:A:LEU:HB3	1:194:A:PRO:HD3	17	0.16
(1,460)	1:250:A:PHE:HD1	1:262:A:ILE:HG21	17	0.16
(1,460)	1:250:A:PHE:HD1	1:262:A:ILE:HG22	17	0.16
(1,460)	1:250:A:PHE:HD1	1:262:A:ILE:HG23	17	0.16
(1,460)	1:250:A:PHE:HD2	1:262:A:ILE:HG21	17	0.16
(1,460)	1:250:A:PHE:HD2	1:262:A:ILE:HG22	17	0.16
(1,460)	1:250:A:PHE:HD2	1:262:A:ILE:HG23	17	0.16
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG21	5	0.16
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG22	5	0.16
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG23	5	0.16
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG21	11	0.16
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG22	11	0.16
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG23	11	0.16
(1,127)	1:181:A:LEU:HA	1:181:A:LEU:HD21	18	0.16
(1,127)	1:181:A:LEU:HA	1:181:A:LEU:HD22	18	0.16
(1,127)	1:181:A:LEU:HA	1:181:A:LEU:HD23	18	0.16
(1,63)	1:180:A:ASN:H	1:181:A:LEU:HA	20	0.16
(1,58)	1:203:A:ALA:HB1	1:205:A:GLN:H	7	0.16
(1,58)	1:203:A:ALA:HB2	1:205:A:GLN:H	7	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:203:A:ALA:HB3	1:205:A:GLN:H	7	0.16
(3,53)	1:234:A:LYS:O	1:238:A:TYR:H	7	0.15
(3,39)	1:214:A:ALA:O	1:218:A:LYS:H	9	0.15
(3,37)	1:213:A:ILE:O	1:217:A:GLN:H	15	0.15
(3,36)	1:212:A:VAL:O	1:216:A:LEU:N	10	0.15
(3,36)	1:212:A:VAL:O	1:216:A:LEU:N	11	0.15
(3,33)	1:211:A:GLN:O	1:215:A:ALA:H	2	0.15
(3,33)	1:211:A:GLN:O	1:215:A:ALA:H	20	0.15
(2,170)	1:221:A:LYS:H	1:223:A:ASN:H	13	0.15
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD1	2	0.15
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD2	2	0.15
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD1	9	0.15
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD2	9	0.15
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD1	12	0.15
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD2	12	0.15
(1,1067)	1:217:A:GLN:HE21	1:226:A:ASN:HD21	1	0.15
(1,1067)	1:217:A:GLN:HE21	1:226:A:ASN:HD22	1	0.15
(1,1067)	1:217:A:GLN:HE22	1:226:A:ASN:HD21	1	0.15
(1,1067)	1:217:A:GLN:HE22	1:226:A:ASN:HD22	1	0.15
(1,1067)	1:217:A:GLN:HE21	1:226:A:ASN:HD21	15	0.15
(1,1067)	1:217:A:GLN:HE21	1:226:A:ASN:HD22	15	0.15
(1,1067)	1:217:A:GLN:HE22	1:226:A:ASN:HD21	15	0.15
(1,1067)	1:217:A:GLN:HE22	1:226:A:ASN:HD22	15	0.15
(1,1052)	1:216:A:LEU:HB2	1:259:A:MET:HE1	10	0.15
(1,1052)	1:216:A:LEU:HB2	1:259:A:MET:HE2	10	0.15
(1,1052)	1:216:A:LEU:HB2	1:259:A:MET:HE3	10	0.15
(1,1052)	1:216:A:LEU:HB3	1:259:A:MET:HE1	10	0.15
(1,1052)	1:216:A:LEU:HB3	1:259:A:MET:HE2	10	0.15
(1,1052)	1:216:A:LEU:HB3	1:259:A:MET:HE3	10	0.15
(1,526)	1:197:A:LEU:HA	1:197:A:LEU:HD21	19	0.15
(1,526)	1:197:A:LEU:HA	1:197:A:LEU:HD22	19	0.15
(1,526)	1:197:A:LEU:HA	1:197:A:LEU:HD23	19	0.15
(1,491)	1:181:A:LEU:HA	1:181:A:LEU:HD11	20	0.15
(1,491)	1:181:A:LEU:HA	1:181:A:LEU:HD12	20	0.15
(1,491)	1:181:A:LEU:HA	1:181:A:LEU:HD13	20	0.15
(1,453)	1:213:A:ILE:HG21	1:216:A:LEU:HG	18	0.15
(1,453)	1:213:A:ILE:HG22	1:216:A:LEU:HG	18	0.15
(1,453)	1:213:A:ILE:HG23	1:216:A:LEU:HG	18	0.15
(1,393)	1:197:A:LEU:HD21	1:245:A:LEU:HA	5	0.15
(1,393)	1:197:A:LEU:HD22	1:245:A:LEU:HA	5	0.15
(1,393)	1:197:A:LEU:HD23	1:245:A:LEU:HA	5	0.15
(1,58)	1:203:A:ALA:HB1	1:205:A:GLN:H	5	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:203:A:ALA:HB2	1:205:A:GLN:H	5	0.15
(1,58)	1:203:A:ALA:HB3	1:205:A:GLN:H	5	0.15
(1,58)	1:203:A:ALA:HB1	1:205:A:GLN:H	10	0.15
(1,58)	1:203:A:ALA:HB2	1:205:A:GLN:H	10	0.15
(1,58)	1:203:A:ALA:HB3	1:205:A:GLN:H	10	0.15
(3,43)	1:216:A:LEU:O	1:220:A:PHE:H	1	0.14
(3,39)	1:214:A:ALA:O	1:218:A:LYS:H	12	0.14
(3,36)	1:212:A:VAL:O	1:216:A:LEU:N	8	0.14
(3,36)	1:212:A:VAL:O	1:216:A:LEU:N	18	0.14
(3,35)	1:212:A:VAL:O	1:216:A:LEU:H	2	0.14
(3,35)	1:212:A:VAL:O	1:216:A:LEU:H	17	0.14
(3,15)	1:201:A:ASP:O	1:205:A:GLN:H	8	0.14
(3,15)	1:201:A:ASP:O	1:205:A:GLN:H	9	0.14
(3,15)	1:201:A:ASP:O	1:205:A:GLN:H	12	0.14
(3,15)	1:201:A:ASP:O	1:205:A:GLN:H	15	0.14
(3,15)	1:201:A:ASP:O	1:205:A:GLN:H	19	0.14
(2,170)	1:221:A:LYS:H	1:223:A:ASN:H	1	0.14
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD1	10	0.14
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD2	10	0.14
(1,1165)	1:235:A:GLN:HE21	1:274:A:LEU:HD11	15	0.14
(1,1165)	1:235:A:GLN:HE21	1:274:A:LEU:HD12	15	0.14
(1,1165)	1:235:A:GLN:HE21	1:274:A:LEU:HD13	15	0.14
(1,1165)	1:235:A:GLN:HE21	1:274:A:LEU:HD21	15	0.14
(1,1165)	1:235:A:GLN:HE21	1:274:A:LEU:HD22	15	0.14
(1,1165)	1:235:A:GLN:HE21	1:274:A:LEU:HD23	15	0.14
(1,1165)	1:235:A:GLN:HE22	1:274:A:LEU:HD11	15	0.14
(1,1165)	1:235:A:GLN:HE22	1:274:A:LEU:HD12	15	0.14
(1,1165)	1:235:A:GLN:HE22	1:274:A:LEU:HD13	15	0.14
(1,1165)	1:235:A:GLN:HE22	1:274:A:LEU:HD21	15	0.14
(1,1165)	1:235:A:GLN:HE22	1:274:A:LEU:HD22	15	0.14
(1,1165)	1:235:A:GLN:HE22	1:274:A:LEU:HD23	15	0.14
(1,1164)	1:235:A:GLN:HE21	1:274:A:LEU:HG	18	0.14
(1,1164)	1:235:A:GLN:HE22	1:274:A:LEU:HG	18	0.14
(1,1134)	1:231:A:LEU:HD11	1:276:A:VAL:HB	16	0.14
(1,1134)	1:231:A:LEU:HD12	1:276:A:VAL:HB	16	0.14
(1,1134)	1:231:A:LEU:HD13	1:276:A:VAL:HB	16	0.14
(1,1134)	1:231:A:LEU:HD21	1:276:A:VAL:HB	16	0.14
(1,1134)	1:231:A:LEU:HD22	1:276:A:VAL:HB	16	0.14
(1,1134)	1:231:A:LEU:HD23	1:276:A:VAL:HB	16	0.14
(1,1067)	1:217:A:GLN:HE21	1:226:A:ASN:HD21	19	0.14
(1,1067)	1:217:A:GLN:HE21	1:226:A:ASN:HD22	19	0.14
(1,1067)	1:217:A:GLN:HE22	1:226:A:ASN:HD21	19	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1067)	1:217:A:GLN:HE22	1:226:A:ASN:HD22	19	0.14
(1,1052)	1:216:A:LEU:HB2	1:259:A:MET:HE1	6	0.14
(1,1052)	1:216:A:LEU:HB2	1:259:A:MET:HE2	6	0.14
(1,1052)	1:216:A:LEU:HB2	1:259:A:MET:HE3	6	0.14
(1,1052)	1:216:A:LEU:HB3	1:259:A:MET:HE1	6	0.14
(1,1052)	1:216:A:LEU:HB3	1:259:A:MET:HE2	6	0.14
(1,1052)	1:216:A:LEU:HB3	1:259:A:MET:HE3	6	0.14
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD11	3	0.14
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD12	3	0.14
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD13	3	0.14
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD21	3	0.14
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD22	3	0.14
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD23	3	0.14
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD11	3	0.14
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD12	3	0.14
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD13	3	0.14
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD21	3	0.14
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD22	3	0.14
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD23	3	0.14
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD11	3	0.14
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD12	3	0.14
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD13	3	0.14
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD21	3	0.14
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD22	3	0.14
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD23	3	0.14
(1,689)	1:178:A:LEU:H	1:178:A:LEU:HG	7	0.14
(1,530)	1:197:A:LEU:HD11	1:245:A:LEU:HA	4	0.14
(1,530)	1:197:A:LEU:HD12	1:245:A:LEU:HA	4	0.14
(1,530)	1:197:A:LEU:HD13	1:245:A:LEU:HA	4	0.14
(1,453)	1:213:A:ILE:HG21	1:216:A:LEU:HG	2	0.14
(1,453)	1:213:A:ILE:HG22	1:216:A:LEU:HG	2	0.14
(1,453)	1:213:A:ILE:HG23	1:216:A:LEU:HG	2	0.14
(1,453)	1:213:A:ILE:HG21	1:216:A:LEU:HG	11	0.14
(1,453)	1:213:A:ILE:HG22	1:216:A:LEU:HG	11	0.14
(1,453)	1:213:A:ILE:HG23	1:216:A:LEU:HG	11	0.14
(1,453)	1:213:A:ILE:HG21	1:216:A:LEU:HG	16	0.14
(1,453)	1:213:A:ILE:HG22	1:216:A:LEU:HG	16	0.14
(1,453)	1:213:A:ILE:HG23	1:216:A:LEU:HG	16	0.14
(1,424)	1:177:A:ILE:HD11	1:265:A:MET:HE1	10	0.14
(1,424)	1:177:A:ILE:HD11	1:265:A:MET:HE2	10	0.14
(1,424)	1:177:A:ILE:HD11	1:265:A:MET:HE3	10	0.14
(1,424)	1:177:A:ILE:HD12	1:265:A:MET:HE1	10	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,424)	1:177:A:ILE:HD12	1:265:A:MET:HE2	10	0.14
(1,424)	1:177:A:ILE:HD12	1:265:A:MET:HE3	10	0.14
(1,424)	1:177:A:ILE:HD13	1:265:A:MET:HE1	10	0.14
(1,424)	1:177:A:ILE:HD13	1:265:A:MET:HE2	10	0.14
(1,424)	1:177:A:ILE:HD13	1:265:A:MET:HE3	10	0.14
(1,218)	1:222:A:THR:H	1:223:A:ASN:H	19	0.14
(1,217)	1:195:A:THR:HG21	1:200:A:THR:HB	8	0.14
(1,217)	1:195:A:THR:HG22	1:200:A:THR:HB	8	0.14
(1,217)	1:195:A:THR:HG23	1:200:A:THR:HB	8	0.14
(1,63)	1:180:A:ASN:H	1:181:A:LEU:HA	11	0.14
(3,45)	1:217:A:GLN:O	1:221:A:LYS:H	7	0.13
(3,45)	1:217:A:GLN:O	1:221:A:LYS:H	18	0.13
(3,43)	1:216:A:LEU:O	1:220:A:PHE:H	11	0.13
(3,40)	1:214:A:ALA:O	1:218:A:LYS:N	9	0.13
(3,39)	1:214:A:ALA:O	1:218:A:LYS:H	3	0.13
(3,39)	1:214:A:ALA:O	1:218:A:LYS:H	8	0.13
(3,37)	1:213:A:ILE:O	1:217:A:GLN:H	14	0.13
(3,35)	1:212:A:VAL:O	1:216:A:LEU:H	16	0.13
(3,33)	1:211:A:GLN:O	1:215:A:ALA:H	5	0.13
(3,15)	1:201:A:ASP:O	1:205:A:GLN:H	2	0.13
(3,15)	1:201:A:ASP:O	1:205:A:GLN:H	4	0.13
(3,15)	1:201:A:ASP:O	1:205:A:GLN:H	10	0.13
(3,15)	1:201:A:ASP:O	1:205:A:GLN:H	16	0.13
(3,15)	1:201:A:ASP:O	1:205:A:GLN:H	18	0.13
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD1	20	0.13
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD2	20	0.13
(1,1233)	1:247:A:LEU:HD11	1:265:A:MET:HE1	8	0.13
(1,1233)	1:247:A:LEU:HD11	1:265:A:MET:HE2	8	0.13
(1,1233)	1:247:A:LEU:HD11	1:265:A:MET:HE3	8	0.13
(1,1233)	1:247:A:LEU:HD12	1:265:A:MET:HE1	8	0.13
(1,1233)	1:247:A:LEU:HD12	1:265:A:MET:HE2	8	0.13
(1,1233)	1:247:A:LEU:HD12	1:265:A:MET:HE3	8	0.13
(1,1233)	1:247:A:LEU:HD13	1:265:A:MET:HE1	8	0.13
(1,1233)	1:247:A:LEU:HD13	1:265:A:MET:HE2	8	0.13
(1,1233)	1:247:A:LEU:HD13	1:265:A:MET:HE3	8	0.13
(1,1233)	1:247:A:LEU:HD21	1:265:A:MET:HE1	8	0.13
(1,1233)	1:247:A:LEU:HD21	1:265:A:MET:HE2	8	0.13
(1,1233)	1:247:A:LEU:HD21	1:265:A:MET:HE3	8	0.13
(1,1233)	1:247:A:LEU:HD22	1:265:A:MET:HE1	8	0.13
(1,1233)	1:247:A:LEU:HD22	1:265:A:MET:HE2	8	0.13
(1,1233)	1:247:A:LEU:HD22	1:265:A:MET:HE3	8	0.13
(1,1233)	1:247:A:LEU:HD23	1:265:A:MET:HE1	8	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1233)	1:247:A:LEU:HD23	1:265:A:MET:HE2	8	0.13
(1,1233)	1:247:A:LEU:HD23	1:265:A:MET:HE3	8	0.13
(1,1233)	1:247:A:LEU:HD11	1:265:A:MET:HE1	18	0.13
(1,1233)	1:247:A:LEU:HD11	1:265:A:MET:HE2	18	0.13
(1,1233)	1:247:A:LEU:HD11	1:265:A:MET:HE3	18	0.13
(1,1233)	1:247:A:LEU:HD12	1:265:A:MET:HE1	18	0.13
(1,1233)	1:247:A:LEU:HD12	1:265:A:MET:HE2	18	0.13
(1,1233)	1:247:A:LEU:HD12	1:265:A:MET:HE3	18	0.13
(1,1233)	1:247:A:LEU:HD13	1:265:A:MET:HE1	18	0.13
(1,1233)	1:247:A:LEU:HD13	1:265:A:MET:HE2	18	0.13
(1,1233)	1:247:A:LEU:HD13	1:265:A:MET:HE3	18	0.13
(1,1233)	1:247:A:LEU:HD21	1:265:A:MET:HE1	18	0.13
(1,1233)	1:247:A:LEU:HD21	1:265:A:MET:HE2	18	0.13
(1,1233)	1:247:A:LEU:HD21	1:265:A:MET:HE3	18	0.13
(1,1233)	1:247:A:LEU:HD22	1:265:A:MET:HE1	18	0.13
(1,1233)	1:247:A:LEU:HD22	1:265:A:MET:HE2	18	0.13
(1,1233)	1:247:A:LEU:HD22	1:265:A:MET:HE3	18	0.13
(1,1233)	1:247:A:LEU:HD23	1:265:A:MET:HE1	18	0.13
(1,1233)	1:247:A:LEU:HD23	1:265:A:MET:HE2	18	0.13
(1,1233)	1:247:A:LEU:HD23	1:265:A:MET:HE3	18	0.13
(1,1176)	1:238:A:TYR:HB2	1:265:A:MET:HE1	10	0.13
(1,1176)	1:238:A:TYR:HB2	1:265:A:MET:HE2	10	0.13
(1,1176)	1:238:A:TYR:HB2	1:265:A:MET:HE3	10	0.13
(1,1176)	1:238:A:TYR:HB3	1:265:A:MET:HE1	10	0.13
(1,1176)	1:238:A:TYR:HB3	1:265:A:MET:HE2	10	0.13
(1,1176)	1:238:A:TYR:HB3	1:265:A:MET:HE3	10	0.13
(1,1134)	1:231:A:LEU:HD11	1:276:A:VAL:HB	12	0.13
(1,1134)	1:231:A:LEU:HD12	1:276:A:VAL:HB	12	0.13
(1,1134)	1:231:A:LEU:HD13	1:276:A:VAL:HB	12	0.13
(1,1134)	1:231:A:LEU:HD21	1:276:A:VAL:HB	12	0.13
(1,1134)	1:231:A:LEU:HD22	1:276:A:VAL:HB	12	0.13
(1,1134)	1:231:A:LEU:HD23	1:276:A:VAL:HB	12	0.13
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD11	2	0.13
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD12	2	0.13
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD13	2	0.13
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD21	2	0.13
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD22	2	0.13
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD23	2	0.13
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD11	2	0.13
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD12	2	0.13
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD13	2	0.13
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD21	2	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD22	2	0.13
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD23	2	0.13
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD11	2	0.13
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD12	2	0.13
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD13	2	0.13
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD21	2	0.13
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD22	2	0.13
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD23	2	0.13
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD11	9	0.13
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD12	9	0.13
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD13	9	0.13
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD21	9	0.13
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD22	9	0.13
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD23	9	0.13
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD11	9	0.13
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD12	9	0.13
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD13	9	0.13
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD21	9	0.13
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD22	9	0.13
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD23	9	0.13
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD11	9	0.13
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD12	9	0.13
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD13	9	0.13
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD21	9	0.13
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD22	9	0.13
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD23	9	0.13
(1,1035)	1:213:A:ILE:HD11	1:216:A:LEU:HD11	10	0.13
(1,1035)	1:213:A:ILE:HD11	1:216:A:LEU:HD12	10	0.13
(1,1035)	1:213:A:ILE:HD11	1:216:A:LEU:HD13	10	0.13
(1,1035)	1:213:A:ILE:HD11	1:216:A:LEU:HD21	10	0.13
(1,1035)	1:213:A:ILE:HD11	1:216:A:LEU:HD22	10	0.13
(1,1035)	1:213:A:ILE:HD11	1:216:A:LEU:HD23	10	0.13
(1,1035)	1:213:A:ILE:HD12	1:216:A:LEU:HD11	10	0.13
(1,1035)	1:213:A:ILE:HD12	1:216:A:LEU:HD12	10	0.13
(1,1035)	1:213:A:ILE:HD12	1:216:A:LEU:HD13	10	0.13
(1,1035)	1:213:A:ILE:HD12	1:216:A:LEU:HD21	10	0.13
(1,1035)	1:213:A:ILE:HD12	1:216:A:LEU:HD22	10	0.13
(1,1035)	1:213:A:ILE:HD12	1:216:A:LEU:HD23	10	0.13
(1,1035)	1:213:A:ILE:HD13	1:216:A:LEU:HD11	10	0.13
(1,1035)	1:213:A:ILE:HD13	1:216:A:LEU:HD12	10	0.13
(1,1035)	1:213:A:ILE:HD13	1:216:A:LEU:HD13	10	0.13
(1,1035)	1:213:A:ILE:HD13	1:216:A:LEU:HD21	10	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1035)	1:213:A:ILE:HD13	1:216:A:LEU:HD22	10	0.13
(1,1035)	1:213:A:ILE:HD13	1:216:A:LEU:HD23	10	0.13
(1,1035)	1:213:A:ILE:HD11	1:216:A:LEU:HD11	17	0.13
(1,1035)	1:213:A:ILE:HD11	1:216:A:LEU:HD12	17	0.13
(1,1035)	1:213:A:ILE:HD11	1:216:A:LEU:HD13	17	0.13
(1,1035)	1:213:A:ILE:HD11	1:216:A:LEU:HD21	17	0.13
(1,1035)	1:213:A:ILE:HD11	1:216:A:LEU:HD22	17	0.13
(1,1035)	1:213:A:ILE:HD11	1:216:A:LEU:HD23	17	0.13
(1,1035)	1:213:A:ILE:HD12	1:216:A:LEU:HD11	17	0.13
(1,1035)	1:213:A:ILE:HD12	1:216:A:LEU:HD12	17	0.13
(1,1035)	1:213:A:ILE:HD12	1:216:A:LEU:HD13	17	0.13
(1,1035)	1:213:A:ILE:HD12	1:216:A:LEU:HD21	17	0.13
(1,1035)	1:213:A:ILE:HD12	1:216:A:LEU:HD22	17	0.13
(1,1035)	1:213:A:ILE:HD12	1:216:A:LEU:HD23	17	0.13
(1,1035)	1:213:A:ILE:HD13	1:216:A:LEU:HD11	17	0.13
(1,1035)	1:213:A:ILE:HD13	1:216:A:LEU:HD12	17	0.13
(1,1035)	1:213:A:ILE:HD13	1:216:A:LEU:HD13	17	0.13
(1,1035)	1:213:A:ILE:HD13	1:216:A:LEU:HD21	17	0.13
(1,1035)	1:213:A:ILE:HD13	1:216:A:LEU:HD22	17	0.13
(1,1035)	1:213:A:ILE:HD13	1:216:A:LEU:HD23	17	0.13
(1,754)	1:186:A:PRO:HA	1:188:A:ASN:H	18	0.13
(1,453)	1:213:A:ILE:HG21	1:216:A:LEU:HG	3	0.13
(1,453)	1:213:A:ILE:HG22	1:216:A:LEU:HG	3	0.13
(1,453)	1:213:A:ILE:HG23	1:216:A:LEU:HG	3	0.13
(1,453)	1:213:A:ILE:HG21	1:216:A:LEU:HG	5	0.13
(1,453)	1:213:A:ILE:HG22	1:216:A:LEU:HG	5	0.13
(1,453)	1:213:A:ILE:HG23	1:216:A:LEU:HG	5	0.13
(1,453)	1:213:A:ILE:HG21	1:216:A:LEU:HG	15	0.13
(1,453)	1:213:A:ILE:HG22	1:216:A:LEU:HG	15	0.13
(1,453)	1:213:A:ILE:HG23	1:216:A:LEU:HG	15	0.13
(1,453)	1:213:A:ILE:HG21	1:216:A:LEU:HG	17	0.13
(1,453)	1:213:A:ILE:HG22	1:216:A:LEU:HG	17	0.13
(1,453)	1:213:A:ILE:HG23	1:216:A:LEU:HG	17	0.13
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG21	7	0.13
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG22	7	0.13
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG23	7	0.13
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG21	10	0.13
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG22	10	0.13
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG23	10	0.13
(1,369)	1:220:A:PHE:HD1	1:274:A:LEU:HB2	13	0.13
(1,369)	1:220:A:PHE:HD2	1:274:A:LEU:HB2	13	0.13
(1,63)	1:180:A:ASN:H	1:181:A:LEU:HA	19	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:203:A:ALA:HB1	1:205:A:GLN:H	6	0.13
(1,58)	1:203:A:ALA:HB2	1:205:A:GLN:H	6	0.13
(1,58)	1:203:A:ALA:HB3	1:205:A:GLN:H	6	0.13
(1,58)	1:203:A:ALA:HB1	1:205:A:GLN:H	9	0.13
(1,58)	1:203:A:ALA:HB2	1:205:A:GLN:H	9	0.13
(1,58)	1:203:A:ALA:HB3	1:205:A:GLN:H	9	0.13
(3,75)	1:262:A:ILE:O	1:266:A:LEU:H	19	0.12
(3,46)	1:217:A:GLN:O	1:221:A:LYS:N	15	0.12
(3,40)	1:214:A:ALA:O	1:218:A:LYS:N	12	0.12
(3,39)	1:214:A:ALA:O	1:218:A:LYS:H	1	0.12
(3,39)	1:214:A:ALA:O	1:218:A:LYS:H	17	0.12
(3,38)	1:213:A:ILE:O	1:217:A:GLN:N	17	0.12
(3,36)	1:212:A:VAL:O	1:216:A:LEU:N	15	0.12
(3,33)	1:211:A:GLN:O	1:215:A:ALA:H	4	0.12
(3,33)	1:211:A:GLN:O	1:215:A:ALA:H	7	0.12
(3,25)	1:206:A:GLN:O	1:210:A:PHE:H	3	0.12
(3,19)	1:203:A:ALA:O	1:207:A:ALA:H	15	0.12
(3,15)	1:201:A:ASP:O	1:205:A:GLN:H	14	0.12
(2,257)	1:219:A:HIS:H	1:274:A:LEU:HD11	19	0.12
(2,257)	1:219:A:HIS:H	1:274:A:LEU:HD12	19	0.12
(2,257)	1:219:A:HIS:H	1:274:A:LEU:HD13	19	0.12
(2,257)	1:219:A:HIS:H	1:274:A:LEU:HD21	19	0.12
(2,257)	1:219:A:HIS:H	1:274:A:LEU:HD22	19	0.12
(2,257)	1:219:A:HIS:H	1:274:A:LEU:HD23	19	0.12
(2,170)	1:221:A:LYS:H	1:223:A:ASN:H	2	0.12
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD1	5	0.12
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD2	5	0.12
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD1	6	0.12
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD2	6	0.12
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD1	13	0.12
(2,123)	1:249:A:GLN:HA	1:250:A:PHE:HD2	13	0.12
(1,1273)	1:256:A:GLU:HA	1:259:A:MET:HG2	6	0.12
(1,1273)	1:256:A:GLU:HA	1:259:A:MET:HG3	6	0.12
(1,1233)	1:247:A:LEU:HD11	1:265:A:MET:HE1	4	0.12
(1,1233)	1:247:A:LEU:HD11	1:265:A:MET:HE2	4	0.12
(1,1233)	1:247:A:LEU:HD11	1:265:A:MET:HE3	4	0.12
(1,1233)	1:247:A:LEU:HD12	1:265:A:MET:HE1	4	0.12
(1,1233)	1:247:A:LEU:HD12	1:265:A:MET:HE2	4	0.12
(1,1233)	1:247:A:LEU:HD12	1:265:A:MET:HE3	4	0.12
(1,1233)	1:247:A:LEU:HD13	1:265:A:MET:HE1	4	0.12
(1,1233)	1:247:A:LEU:HD13	1:265:A:MET:HE2	4	0.12
(1,1233)	1:247:A:LEU:HD13	1:265:A:MET:HE3	4	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1233)	1:247:A:LEU:HD21	1:265:A:MET:HE1	4	0.12
(1,1233)	1:247:A:LEU:HD21	1:265:A:MET:HE2	4	0.12
(1,1233)	1:247:A:LEU:HD21	1:265:A:MET:HE3	4	0.12
(1,1233)	1:247:A:LEU:HD22	1:265:A:MET:HE1	4	0.12
(1,1233)	1:247:A:LEU:HD22	1:265:A:MET:HE2	4	0.12
(1,1233)	1:247:A:LEU:HD22	1:265:A:MET:HE3	4	0.12
(1,1233)	1:247:A:LEU:HD23	1:265:A:MET:HE1	4	0.12
(1,1233)	1:247:A:LEU:HD23	1:265:A:MET:HE2	4	0.12
(1,1233)	1:247:A:LEU:HD23	1:265:A:MET:HE3	4	0.12
(1,1233)	1:247:A:LEU:HD11	1:265:A:MET:HE1	6	0.12
(1,1233)	1:247:A:LEU:HD11	1:265:A:MET:HE2	6	0.12
(1,1233)	1:247:A:LEU:HD11	1:265:A:MET:HE3	6	0.12
(1,1233)	1:247:A:LEU:HD12	1:265:A:MET:HE1	6	0.12
(1,1233)	1:247:A:LEU:HD12	1:265:A:MET:HE2	6	0.12
(1,1233)	1:247:A:LEU:HD12	1:265:A:MET:HE3	6	0.12
(1,1233)	1:247:A:LEU:HD13	1:265:A:MET:HE1	6	0.12
(1,1233)	1:247:A:LEU:HD13	1:265:A:MET:HE2	6	0.12
(1,1233)	1:247:A:LEU:HD13	1:265:A:MET:HE3	6	0.12
(1,1233)	1:247:A:LEU:HD21	1:265:A:MET:HE1	6	0.12
(1,1233)	1:247:A:LEU:HD21	1:265:A:MET:HE2	6	0.12
(1,1233)	1:247:A:LEU:HD21	1:265:A:MET:HE3	6	0.12
(1,1233)	1:247:A:LEU:HD22	1:265:A:MET:HE1	6	0.12
(1,1233)	1:247:A:LEU:HD22	1:265:A:MET:HE2	6	0.12
(1,1233)	1:247:A:LEU:HD22	1:265:A:MET:HE3	6	0.12
(1,1233)	1:247:A:LEU:HD23	1:265:A:MET:HE1	6	0.12
(1,1233)	1:247:A:LEU:HD23	1:265:A:MET:HE2	6	0.12
(1,1233)	1:247:A:LEU:HD23	1:265:A:MET:HE3	6	0.12
(1,1182)	1:238:A:TYR:HE1	1:265:A:MET:HG2	15	0.12
(1,1182)	1:238:A:TYR:HE1	1:265:A:MET:HG3	15	0.12
(1,1182)	1:238:A:TYR:HE2	1:265:A:MET:HG2	15	0.12
(1,1182)	1:238:A:TYR:HE2	1:265:A:MET:HG3	15	0.12
(1,1176)	1:238:A:TYR:HB2	1:265:A:MET:HE1	15	0.12
(1,1176)	1:238:A:TYR:HB2	1:265:A:MET:HE2	15	0.12
(1,1176)	1:238:A:TYR:HB2	1:265:A:MET:HE3	15	0.12
(1,1176)	1:238:A:TYR:HB3	1:265:A:MET:HE1	15	0.12
(1,1176)	1:238:A:TYR:HB3	1:265:A:MET:HE2	15	0.12
(1,1176)	1:238:A:TYR:HB3	1:265:A:MET:HE3	15	0.12
(1,1067)	1:217:A:GLN:HE21	1:226:A:ASN:HD21	12	0.12
(1,1067)	1:217:A:GLN:HE21	1:226:A:ASN:HD22	12	0.12
(1,1067)	1:217:A:GLN:HE22	1:226:A:ASN:HD21	12	0.12
(1,1067)	1:217:A:GLN:HE22	1:226:A:ASN:HD22	12	0.12
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD11	8	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD12	8	0.12
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD13	8	0.12
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD21	8	0.12
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD22	8	0.12
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD23	8	0.12
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD11	8	0.12
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD12	8	0.12
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD13	8	0.12
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD21	8	0.12
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD22	8	0.12
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD23	8	0.12
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD11	8	0.12
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD12	8	0.12
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD13	8	0.12
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD21	8	0.12
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD22	8	0.12
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD23	8	0.12
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD11	11	0.12
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD12	11	0.12
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD13	11	0.12
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD21	11	0.12
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD22	11	0.12
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD23	11	0.12
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD11	11	0.12
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD12	11	0.12
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD13	11	0.12
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD21	11	0.12
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD22	11	0.12
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD23	11	0.12
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD11	11	0.12
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD12	11	0.12
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD13	11	0.12
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD21	11	0.12
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD22	11	0.12
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD23	11	0.12
(1,1031)	1:213:A:ILE:HG21	1:216:A:LEU:HB2	1	0.12
(1,1031)	1:213:A:ILE:HG21	1:216:A:LEU:HB3	1	0.12
(1,1031)	1:213:A:ILE:HG22	1:216:A:LEU:HB2	1	0.12
(1,1031)	1:213:A:ILE:HG22	1:216:A:LEU:HB3	1	0.12
(1,1031)	1:213:A:ILE:HG23	1:216:A:LEU:HB2	1	0.12
(1,1031)	1:213:A:ILE:HG23	1:216:A:LEU:HB3	1	0.12
(1,720)	1:273:A:ALA:HA	1:275:A:SER:H	18	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,538)	1:231:A:LEU:HD11	1:235:A:GLN:HE22	1	0.12
(1,538)	1:231:A:LEU:HD12	1:235:A:GLN:HE22	1	0.12
(1,538)	1:231:A:LEU:HD13	1:235:A:GLN:HE22	1	0.12
(1,491)	1:181:A:LEU:HA	1:181:A:LEU:HD11	11	0.12
(1,491)	1:181:A:LEU:HA	1:181:A:LEU:HD12	11	0.12
(1,491)	1:181:A:LEU:HA	1:181:A:LEU:HD13	11	0.12
(1,453)	1:213:A:ILE:HG21	1:216:A:LEU:HG	12	0.12
(1,453)	1:213:A:ILE:HG22	1:216:A:LEU:HG	12	0.12
(1,453)	1:213:A:ILE:HG23	1:216:A:LEU:HG	12	0.12
(1,453)	1:213:A:ILE:HG21	1:216:A:LEU:HG	13	0.12
(1,453)	1:213:A:ILE:HG22	1:216:A:LEU:HG	13	0.12
(1,453)	1:213:A:ILE:HG23	1:216:A:LEU:HG	13	0.12
(1,410)	1:177:A:ILE:HD11	1:244:A:MET:HE1	15	0.12
(1,410)	1:177:A:ILE:HD11	1:244:A:MET:HE2	15	0.12
(1,410)	1:177:A:ILE:HD11	1:244:A:MET:HE3	15	0.12
(1,410)	1:177:A:ILE:HD12	1:244:A:MET:HE1	15	0.12
(1,410)	1:177:A:ILE:HD12	1:244:A:MET:HE2	15	0.12
(1,410)	1:177:A:ILE:HD12	1:244:A:MET:HE3	15	0.12
(1,410)	1:177:A:ILE:HD13	1:244:A:MET:HE1	15	0.12
(1,410)	1:177:A:ILE:HD13	1:244:A:MET:HE2	15	0.12
(1,410)	1:177:A:ILE:HD13	1:244:A:MET:HE3	15	0.12
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG21	1	0.12
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG22	1	0.12
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG23	1	0.12
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG21	2	0.12
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG22	2	0.12
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG23	2	0.12
(1,376)	1:177:A:ILE:HD11	1:178:A:LEU:HA	2	0.12
(1,376)	1:177:A:ILE:HD12	1:178:A:LEU:HA	2	0.12
(1,376)	1:177:A:ILE:HD13	1:178:A:LEU:HA	2	0.12
(1,376)	1:177:A:ILE:HD11	1:178:A:LEU:HA	3	0.12
(1,376)	1:177:A:ILE:HD12	1:178:A:LEU:HA	3	0.12
(1,376)	1:177:A:ILE:HD13	1:178:A:LEU:HA	3	0.12
(1,63)	1:180:A:ASN:H	1:181:A:LEU:HA	9	0.12
(1,58)	1:203:A:ALA:HB1	1:205:A:GLN:H	2	0.12
(1,58)	1:203:A:ALA:HB2	1:205:A:GLN:H	2	0.12
(1,58)	1:203:A:ALA:HB3	1:205:A:GLN:H	2	0.12
(1,58)	1:203:A:ALA:HB1	1:205:A:GLN:H	13	0.12
(1,58)	1:203:A:ALA:HB2	1:205:A:GLN:H	13	0.12
(1,58)	1:203:A:ALA:HB3	1:205:A:GLN:H	13	0.12
(1,58)	1:203:A:ALA:HB1	1:205:A:GLN:H	14	0.12
(1,58)	1:203:A:ALA:HB2	1:205:A:GLN:H	14	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,58)	1:203:A:ALA:HB3	1:205:A:GLN:H	14	0.12
(1,58)	1:203:A:ALA:HB1	1:205:A:GLN:H	16	0.12
(1,58)	1:203:A:ALA:HB2	1:205:A:GLN:H	16	0.12
(1,58)	1:203:A:ALA:HB3	1:205:A:GLN:H	16	0.12
(1,58)	1:203:A:ALA:HB1	1:205:A:GLN:H	17	0.12
(1,58)	1:203:A:ALA:HB2	1:205:A:GLN:H	17	0.12
(1,58)	1:203:A:ALA:HB3	1:205:A:GLN:H	17	0.12
(1,58)	1:203:A:ALA:HB1	1:205:A:GLN:H	19	0.12
(1,58)	1:203:A:ALA:HB2	1:205:A:GLN:H	19	0.12
(1,58)	1:203:A:ALA:HB3	1:205:A:GLN:H	19	0.12
(3,53)	1:234:A:LYS:O	1:238:A:TYR:H	9	0.11
(3,47)	1:231:A:LEU:O	1:235:A:GLN:H	9	0.11
(3,43)	1:216:A:LEU:O	1:220:A:PHE:H	10	0.11
(3,41)	1:215:A:ALA:O	1:219:A:HIS:H	16	0.11
(3,39)	1:214:A:ALA:O	1:218:A:LYS:H	11	0.11
(3,39)	1:214:A:ALA:O	1:218:A:LYS:H	18	0.11
(3,39)	1:214:A:ALA:O	1:218:A:LYS:H	20	0.11
(3,38)	1:213:A:ILE:O	1:217:A:GLN:N	15	0.11
(3,37)	1:213:A:ILE:O	1:217:A:GLN:H	10	0.11
(3,36)	1:212:A:VAL:O	1:216:A:LEU:N	5	0.11
(3,36)	1:212:A:VAL:O	1:216:A:LEU:N	7	0.11
(3,36)	1:212:A:VAL:O	1:216:A:LEU:N	12	0.11
(3,36)	1:212:A:VAL:O	1:216:A:LEU:N	14	0.11
(3,36)	1:212:A:VAL:O	1:216:A:LEU:N	20	0.11
(3,33)	1:211:A:GLN:O	1:215:A:ALA:H	10	0.11
(3,33)	1:211:A:GLN:O	1:215:A:ALA:H	13	0.11
(3,15)	1:201:A:ASP:O	1:205:A:GLN:H	20	0.11
(3,1)	1:169:A:ASP:O	1:173:A:ARG:H	8	0.11
(1,1303)	1:265:A:MET:HE1	1:268:A:SER:HB2	10	0.11
(1,1303)	1:265:A:MET:HE1	1:268:A:SER:HB3	10	0.11
(1,1303)	1:265:A:MET:HE2	1:268:A:SER:HB2	10	0.11
(1,1303)	1:265:A:MET:HE2	1:268:A:SER:HB3	10	0.11
(1,1303)	1:265:A:MET:HE3	1:268:A:SER:HB2	10	0.11
(1,1303)	1:265:A:MET:HE3	1:268:A:SER:HB3	10	0.11
(1,1176)	1:238:A:TYR:HB2	1:265:A:MET:HE1	19	0.11
(1,1176)	1:238:A:TYR:HB2	1:265:A:MET:HE2	19	0.11
(1,1176)	1:238:A:TYR:HB2	1:265:A:MET:HE3	19	0.11
(1,1176)	1:238:A:TYR:HB3	1:265:A:MET:HE1	19	0.11
(1,1176)	1:238:A:TYR:HB3	1:265:A:MET:HE2	19	0.11
(1,1176)	1:238:A:TYR:HB3	1:265:A:MET:HE3	19	0.11
(1,1067)	1:217:A:GLN:HE21	1:226:A:ASN:HD21	16	0.11
(1,1067)	1:217:A:GLN:HE21	1:226:A:ASN:HD22	16	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1067)	1:217:A:GLN:HE22	1:226:A:ASN:HD21	16	0.11
(1,1067)	1:217:A:GLN:HE22	1:226:A:ASN:HD22	16	0.11
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD11	7	0.11
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD12	7	0.11
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD13	7	0.11
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD21	7	0.11
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD22	7	0.11
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD23	7	0.11
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD11	7	0.11
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD12	7	0.11
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD13	7	0.11
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD21	7	0.11
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD22	7	0.11
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD23	7	0.11
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD11	7	0.11
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD12	7	0.11
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD13	7	0.11
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD21	7	0.11
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD22	7	0.11
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD23	7	0.11
(1,920)	1:194:A:PRO:HB2	1:208:A:ALA:HB1	10	0.11
(1,920)	1:194:A:PRO:HB2	1:208:A:ALA:HB2	10	0.11
(1,920)	1:194:A:PRO:HB2	1:208:A:ALA:HB3	10	0.11
(1,920)	1:194:A:PRO:HB3	1:208:A:ALA:HB1	10	0.11
(1,920)	1:194:A:PRO:HB3	1:208:A:ALA:HB2	10	0.11
(1,920)	1:194:A:PRO:HB3	1:208:A:ALA:HB3	10	0.11
(1,689)	1:178:A:LEU:H	1:178:A:LEU:HG	19	0.11
(1,526)	1:197:A:LEU:HA	1:197:A:LEU:HD21	17	0.11
(1,526)	1:197:A:LEU:HA	1:197:A:LEU:HD22	17	0.11
(1,526)	1:197:A:LEU:HA	1:197:A:LEU:HD23	17	0.11
(1,453)	1:213:A:ILE:HG21	1:216:A:LEU:HG	20	0.11
(1,453)	1:213:A:ILE:HG22	1:216:A:LEU:HG	20	0.11
(1,453)	1:213:A:ILE:HG23	1:216:A:LEU:HG	20	0.11
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG21	3	0.11
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG22	3	0.11
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG23	3	0.11
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG21	13	0.11
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG22	13	0.11
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG23	13	0.11
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG21	17	0.11
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG22	17	0.11
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG23	17	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG21	20	0.11
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG22	20	0.11
(1,385)	1:190:A:ASN:H	1:191:A:ILE:HG23	20	0.11
(1,376)	1:177:A:ILE:HD11	1:178:A:LEU:HA	9	0.11
(1,376)	1:177:A:ILE:HD12	1:178:A:LEU:HA	9	0.11
(1,376)	1:177:A:ILE:HD13	1:178:A:LEU:HA	9	0.11
(1,376)	1:177:A:ILE:HD11	1:178:A:LEU:HA	13	0.11
(1,376)	1:177:A:ILE:HD12	1:178:A:LEU:HA	13	0.11
(1,376)	1:177:A:ILE:HD13	1:178:A:LEU:HA	13	0.11
(1,376)	1:177:A:ILE:HD11	1:178:A:LEU:HA	15	0.11
(1,376)	1:177:A:ILE:HD12	1:178:A:LEU:HA	15	0.11
(1,376)	1:177:A:ILE:HD13	1:178:A:LEU:HA	15	0.11
(1,376)	1:177:A:ILE:HD11	1:178:A:LEU:HA	17	0.11
(1,376)	1:177:A:ILE:HD12	1:178:A:LEU:HA	17	0.11
(1,376)	1:177:A:ILE:HD13	1:178:A:LEU:HA	17	0.11
(1,192)	1:197:A:LEU:HD21	1:209:A:LEU:H	19	0.11
(1,192)	1:197:A:LEU:HD22	1:209:A:LEU:H	19	0.11
(1,192)	1:197:A:LEU:HD23	1:209:A:LEU:H	19	0.11
(1,63)	1:180:A:ASN:H	1:181:A:LEU:HA	2	0.11
(1,58)	1:203:A:ALA:HB1	1:205:A:GLN:H	1	0.11
(1,58)	1:203:A:ALA:HB2	1:205:A:GLN:H	1	0.11
(1,58)	1:203:A:ALA:HB3	1:205:A:GLN:H	1	0.11
(1,58)	1:203:A:ALA:HB1	1:205:A:GLN:H	3	0.11
(1,58)	1:203:A:ALA:HB2	1:205:A:GLN:H	3	0.11
(1,58)	1:203:A:ALA:HB3	1:205:A:GLN:H	3	0.11
(1,58)	1:203:A:ALA:HB1	1:205:A:GLN:H	8	0.11
(1,58)	1:203:A:ALA:HB2	1:205:A:GLN:H	8	0.11
(1,58)	1:203:A:ALA:HB3	1:205:A:GLN:H	8	0.11
(1,58)	1:203:A:ALA:HB1	1:205:A:GLN:H	20	0.11
(1,58)	1:203:A:ALA:HB2	1:205:A:GLN:H	20	0.11
(1,58)	1:203:A:ALA:HB3	1:205:A:GLN:H	20	0.11
(3,75)	1:262:A:ILE:O	1:266:A:LEU:H	15	0.1
(3,53)	1:234:A:LYS:O	1:238:A:TYR:H	10	0.1
(3,46)	1:217:A:GLN:O	1:221:A:LYS:N	7	0.1
(3,46)	1:217:A:GLN:O	1:221:A:LYS:N	18	0.1
(3,43)	1:216:A:LEU:O	1:220:A:PHE:H	17	0.1
(3,41)	1:215:A:ALA:O	1:219:A:HIS:H	13	0.1
(3,40)	1:214:A:ALA:O	1:218:A:LYS:N	3	0.1
(3,40)	1:214:A:ALA:O	1:218:A:LYS:N	8	0.1
(3,39)	1:214:A:ALA:O	1:218:A:LYS:H	5	0.1
(3,37)	1:213:A:ILE:O	1:217:A:GLN:H	18	0.1
(3,36)	1:212:A:VAL:O	1:216:A:LEU:N	4	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,36)	1:212:A:VAL:O	1:216:A:LEU:N	13	0.1
(3,33)	1:211:A:GLN:O	1:215:A:ALA:H	3	0.1
(3,33)	1:211:A:GLN:O	1:215:A:ALA:H	12	0.1
(3,23)	1:205:A:GLN:O	1:209:A:LEU:H	9	0.1
(3,1)	1:169:A:ASP:O	1:173:A:ARG:H	5	0.1
(3,1)	1:169:A:ASP:O	1:173:A:ARG:H	15	0.1
(3,1)	1:169:A:ASP:O	1:173:A:ARG:H	17	0.1
(2,82)	1:216:A:LEU:HA	1:220:A:PHE:HZ	10	0.1
(1,1233)	1:247:A:LEU:HD11	1:265:A:MET:HE1	19	0.1
(1,1233)	1:247:A:LEU:HD11	1:265:A:MET:HE2	19	0.1
(1,1233)	1:247:A:LEU:HD11	1:265:A:MET:HE3	19	0.1
(1,1233)	1:247:A:LEU:HD12	1:265:A:MET:HE1	19	0.1
(1,1233)	1:247:A:LEU:HD12	1:265:A:MET:HE2	19	0.1
(1,1233)	1:247:A:LEU:HD12	1:265:A:MET:HE3	19	0.1
(1,1233)	1:247:A:LEU:HD13	1:265:A:MET:HE1	19	0.1
(1,1233)	1:247:A:LEU:HD13	1:265:A:MET:HE2	19	0.1
(1,1233)	1:247:A:LEU:HD13	1:265:A:MET:HE3	19	0.1
(1,1233)	1:247:A:LEU:HD21	1:265:A:MET:HE1	19	0.1
(1,1233)	1:247:A:LEU:HD21	1:265:A:MET:HE2	19	0.1
(1,1233)	1:247:A:LEU:HD21	1:265:A:MET:HE3	19	0.1
(1,1233)	1:247:A:LEU:HD22	1:265:A:MET:HE1	19	0.1
(1,1233)	1:247:A:LEU:HD22	1:265:A:MET:HE2	19	0.1
(1,1233)	1:247:A:LEU:HD22	1:265:A:MET:HE3	19	0.1
(1,1233)	1:247:A:LEU:HD23	1:265:A:MET:HE1	19	0.1
(1,1233)	1:247:A:LEU:HD23	1:265:A:MET:HE2	19	0.1
(1,1233)	1:247:A:LEU:HD23	1:265:A:MET:HE3	19	0.1
(1,1151)	1:234:A:LYS:HG2	1:272:A:THR:HG21	16	0.1
(1,1151)	1:234:A:LYS:HG2	1:272:A:THR:HG22	16	0.1
(1,1151)	1:234:A:LYS:HG2	1:272:A:THR:HG23	16	0.1
(1,1151)	1:234:A:LYS:HG3	1:272:A:THR:HG21	16	0.1
(1,1151)	1:234:A:LYS:HG3	1:272:A:THR:HG22	16	0.1
(1,1151)	1:234:A:LYS:HG3	1:272:A:THR:HG23	16	0.1
(1,1110)	1:228:A:ASN:H	1:231:A:LEU:HD11	19	0.1
(1,1110)	1:228:A:ASN:H	1:231:A:LEU:HD12	19	0.1
(1,1110)	1:228:A:ASN:H	1:231:A:LEU:HD13	19	0.1
(1,1110)	1:228:A:ASN:H	1:231:A:LEU:HD21	19	0.1
(1,1110)	1:228:A:ASN:H	1:231:A:LEU:HD22	19	0.1
(1,1110)	1:228:A:ASN:H	1:231:A:LEU:HD23	19	0.1
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD11	6	0.1
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD12	6	0.1
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD13	6	0.1
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD21	6	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD22	6	0.1
(1,1036)	1:213:A:ILE:HD11	1:232:A:LEU:HD23	6	0.1
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD11	6	0.1
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD12	6	0.1
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD13	6	0.1
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD21	6	0.1
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD22	6	0.1
(1,1036)	1:213:A:ILE:HD12	1:232:A:LEU:HD23	6	0.1
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD11	6	0.1
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD12	6	0.1
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD13	6	0.1
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD21	6	0.1
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD22	6	0.1
(1,1036)	1:213:A:ILE:HD13	1:232:A:LEU:HD23	6	0.1
(1,920)	1:194:A:PRO:HB2	1:208:A:ALA:HB1	15	0.1
(1,920)	1:194:A:PRO:HB2	1:208:A:ALA:HB2	15	0.1
(1,920)	1:194:A:PRO:HB2	1:208:A:ALA:HB3	15	0.1
(1,920)	1:194:A:PRO:HB3	1:208:A:ALA:HB1	15	0.1
(1,920)	1:194:A:PRO:HB3	1:208:A:ALA:HB2	15	0.1
(1,920)	1:194:A:PRO:HB3	1:208:A:ALA:HB3	15	0.1
(1,526)	1:197:A:LEU:HA	1:197:A:LEU:HD21	16	0.1
(1,526)	1:197:A:LEU:HA	1:197:A:LEU:HD22	16	0.1
(1,526)	1:197:A:LEU:HA	1:197:A:LEU:HD23	16	0.1
(1,491)	1:181:A:LEU:HA	1:181:A:LEU:HD11	9	0.1
(1,491)	1:181:A:LEU:HA	1:181:A:LEU:HD12	9	0.1
(1,491)	1:181:A:LEU:HA	1:181:A:LEU:HD13	9	0.1
(1,450)	1:174:A:SER:HA	1:177:A:ILE:HB	19	0.1
(1,410)	1:177:A:ILE:HD11	1:244:A:MET:HE1	3	0.1
(1,410)	1:177:A:ILE:HD11	1:244:A:MET:HE2	3	0.1
(1,410)	1:177:A:ILE:HD11	1:244:A:MET:HE3	3	0.1
(1,410)	1:177:A:ILE:HD12	1:244:A:MET:HE1	3	0.1
(1,410)	1:177:A:ILE:HD12	1:244:A:MET:HE2	3	0.1
(1,410)	1:177:A:ILE:HD12	1:244:A:MET:HE3	3	0.1
(1,410)	1:177:A:ILE:HD13	1:244:A:MET:HE1	3	0.1
(1,410)	1:177:A:ILE:HD13	1:244:A:MET:HE2	3	0.1
(1,410)	1:177:A:ILE:HD13	1:244:A:MET:HE3	3	0.1
(1,376)	1:177:A:ILE:HD11	1:178:A:LEU:HA	16	0.1
(1,376)	1:177:A:ILE:HD12	1:178:A:LEU:HA	16	0.1
(1,376)	1:177:A:ILE:HD13	1:178:A:LEU:HA	16	0.1
(1,217)	1:195:A:THR:HG21	1:200:A:THR:HB	12	0.1
(1,217)	1:195:A:THR:HG22	1:200:A:THR:HB	12	0.1
(1,217)	1:195:A:THR:HG23	1:200:A:THR:HB	12	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,63)	1:180:A:ASN:H	1:181:A:LEU:HA	5	0.1
(1,58)	1:203:A:ALA:HB1	1:205:A:GLN:H	4	0.1
(1,58)	1:203:A:ALA:HB2	1:205:A:GLN:H	4	0.1
(1,58)	1:203:A:ALA:HB3	1:205:A:GLN:H	4	0.1

10 Dihedral-angle violation analysis

No dihedral-angle restraints found