



Full wwPDB NMR Structure Validation Report ⓘ

Mar 29, 2026 – 09:26 PM UTC

PDB ID : 6XRG / pdb_00006xrg
BMRB ID : 30772
Title : Abl 1b isoform inactive2 state
Authors : Xie, T.; Saleh, T.; Rossi, P.; Kalodimos, C.G.
Deposited on : 2020-07-12

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

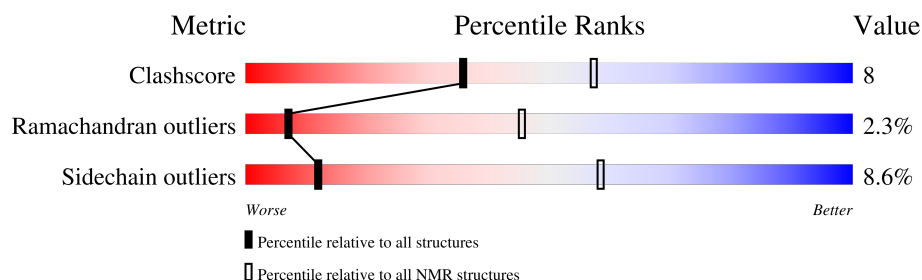
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 14%.

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	287	

2 Ensemble composition and analysis

This entry contains 20 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:254-A:406, A:422-A:517 (249)	0.93	6

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

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

The models can be grouped into 2 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4633 atoms, of which 2293 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tyrosine-protein kinase ABL1.

Mol	Chain	Residues	Atoms						Trace
1	A	287	Total	C	H	N	O	S	0
			4633	1504	2293	379	441	16	

There are 3 discrepancies between the modelled and reference sequences:

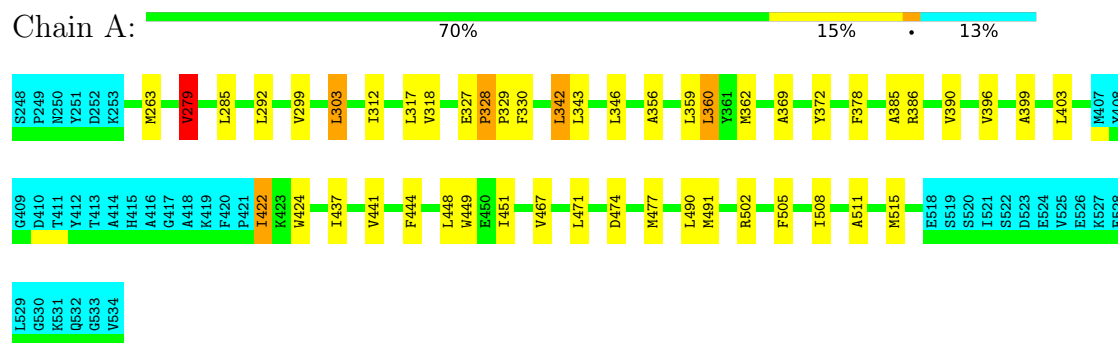
Chain	Residue	Modelled	Actual	Comment	Reference
A	269	GLU	GLY	engineered mutation	UNP P00519
A	309	LEU	MET	engineered mutation	UNP P00519
A	408	TYR	THR	engineered mutation	UNP P00519

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Tyrosine-protein kinase ABL1

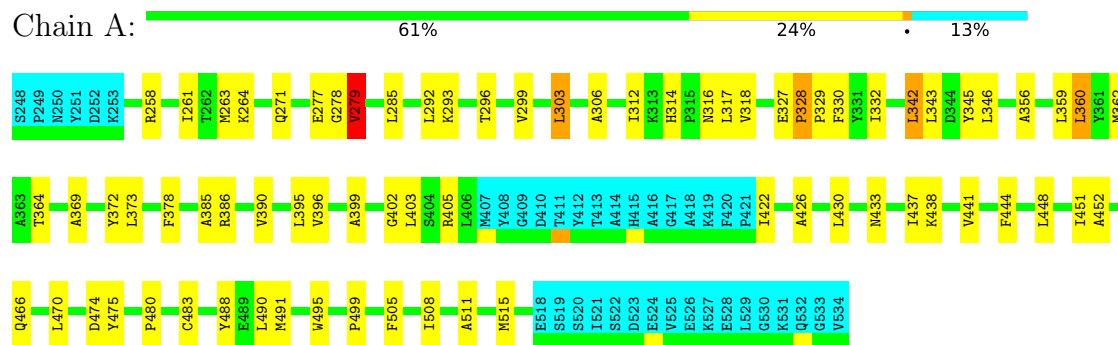


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

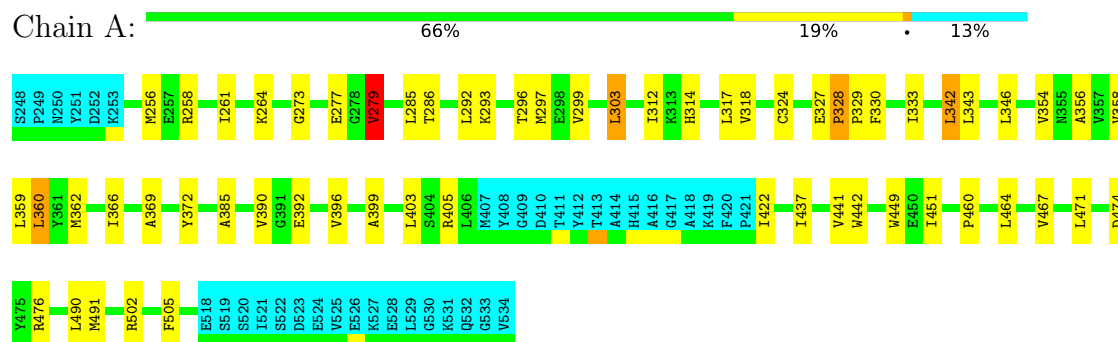
4.2.1 Score per residue for model 1

- Molecule 1: Tyrosine-protein kinase ABL1



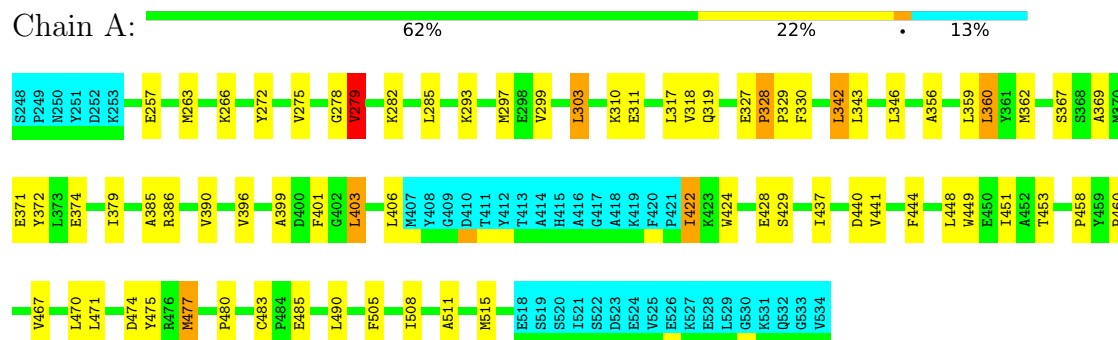
4.2.2 Score per residue for model 2

- Molecule 1: Tyrosine-protein kinase ABL1



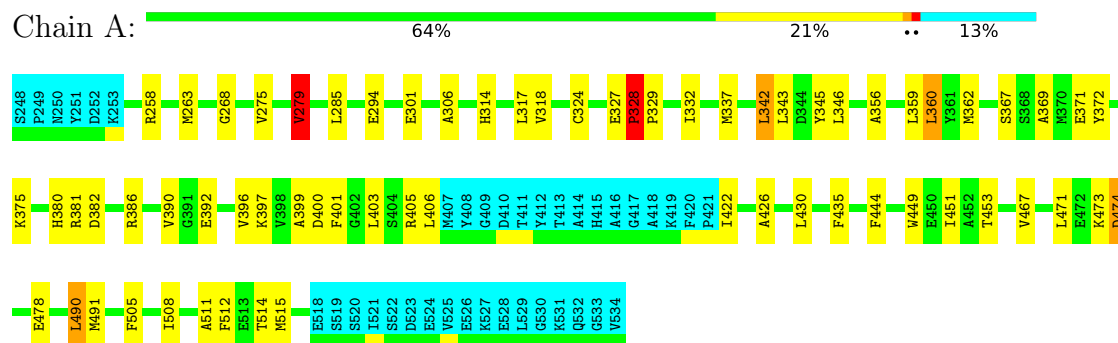
4.2.3 Score per residue for model 3

- Molecule 1: Tyrosine-protein kinase ABL1



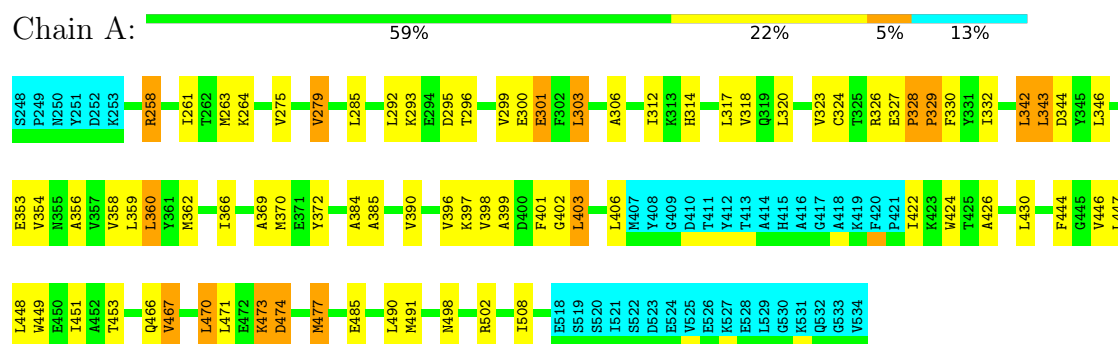
4.2.4 Score per residue for model 4

- Molecule 1: Tyrosine-protein kinase ABL1



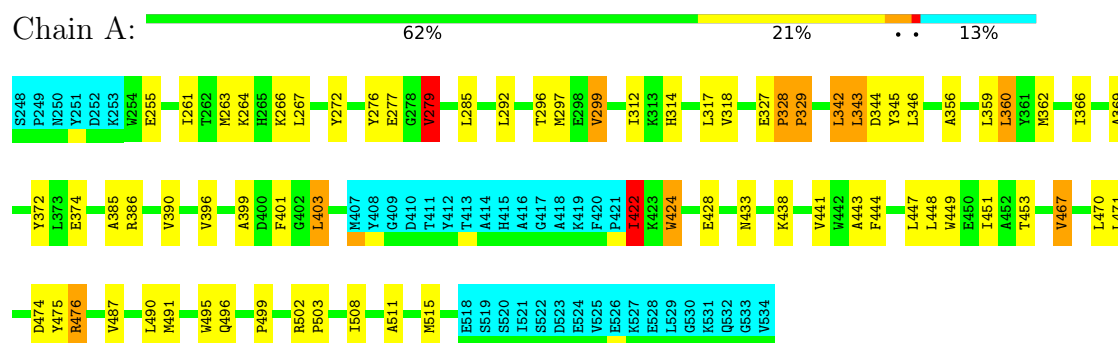
4.2.5 Score per residue for model 5

- Molecule 1: Tyrosine-protein kinase ABL1



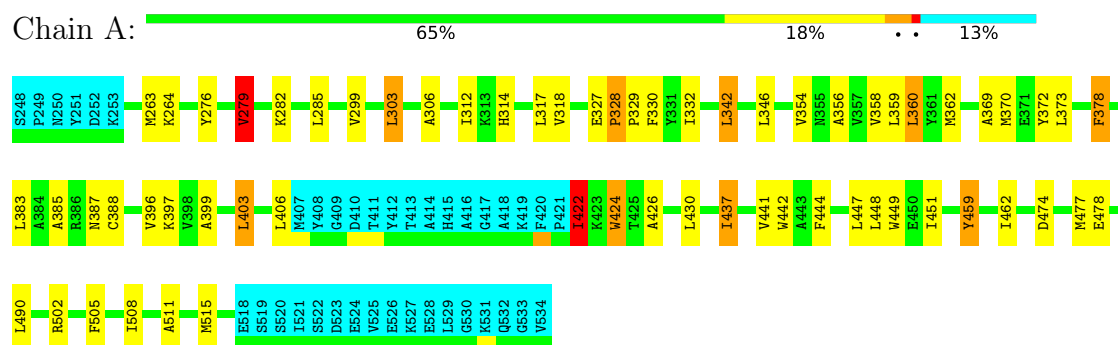
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Tyrosine-protein kinase ABL1



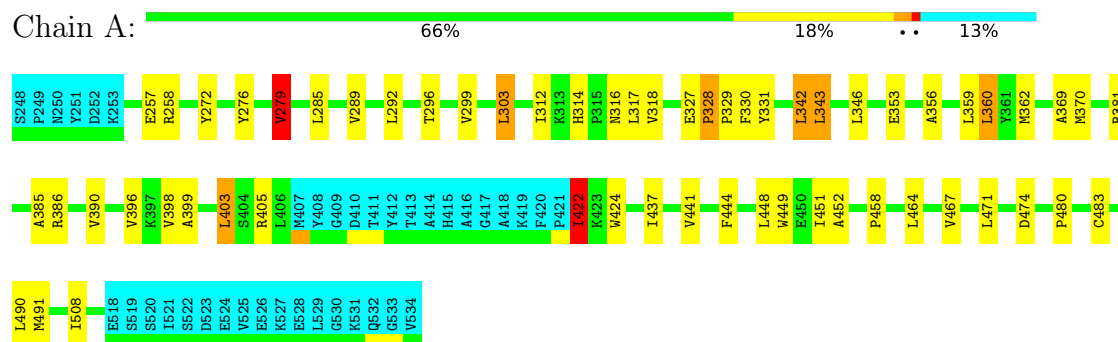
4.2.7 Score per residue for model 7

- Molecule 1: Tyrosine-protein kinase ABL1



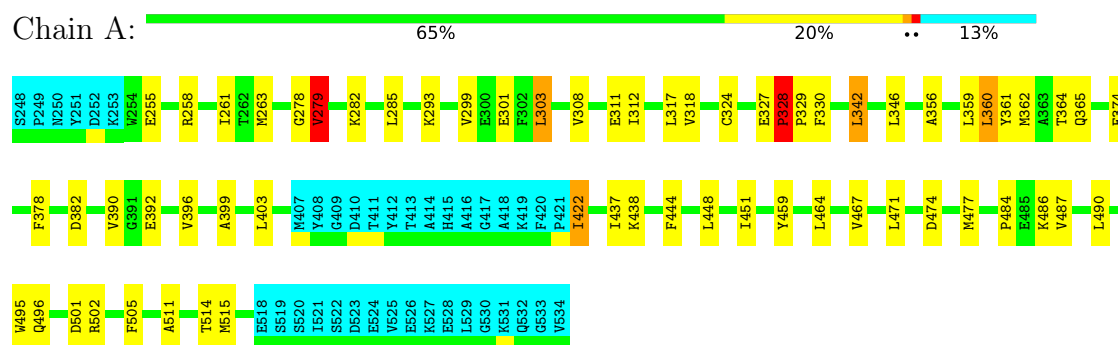
4.2.8 Score per residue for model 8

- Molecule 1: Tyrosine-protein kinase ABL1



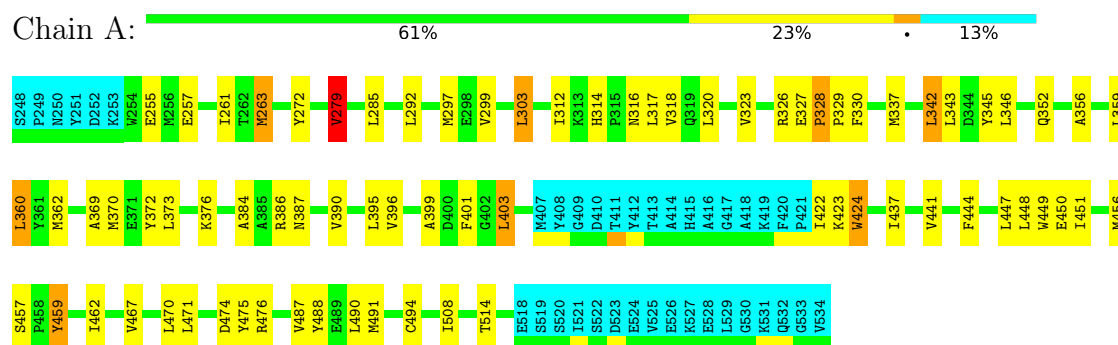
4.2.9 Score per residue for model 9

- Molecule 1: Tyrosine-protein kinase ABL1



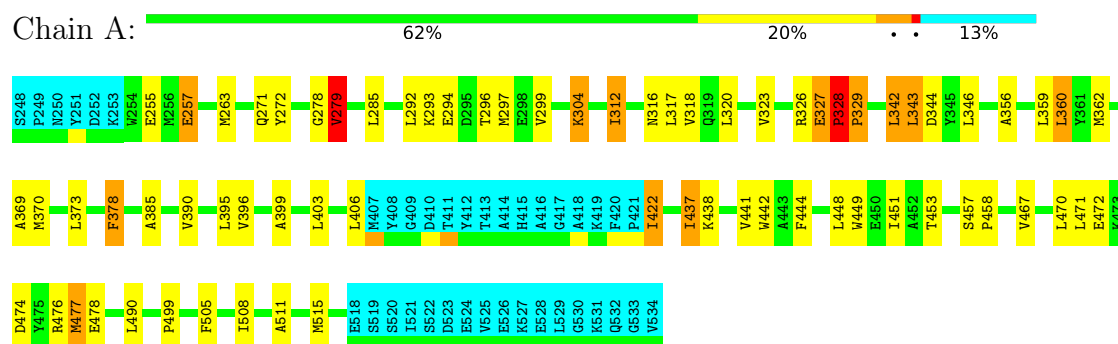
4.2.10 Score per residue for model 10

- Molecule 1: Tyrosine-protein kinase ABL1



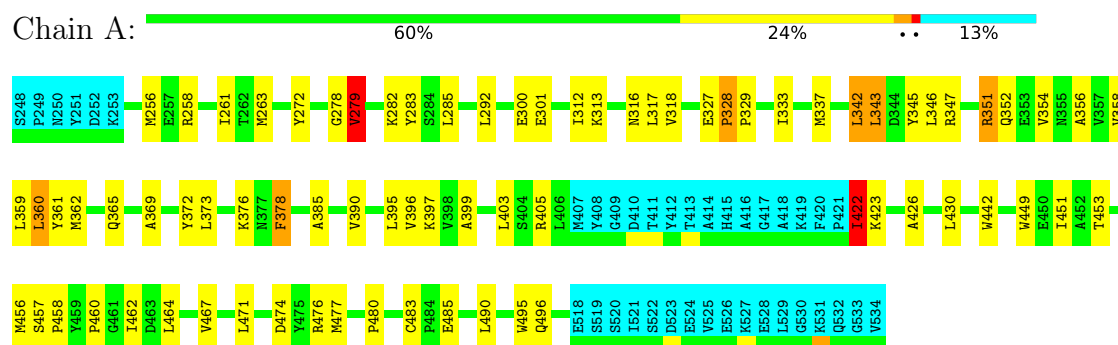
4.2.11 Score per residue for model 11

- Molecule 1: Tyrosine-protein kinase ABL1



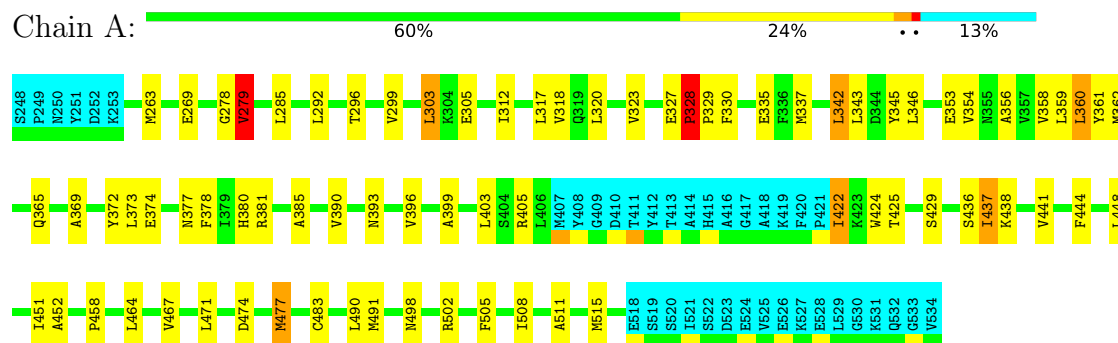
4.2.12 Score per residue for model 12

- Molecule 1: Tyrosine-protein kinase ABL1



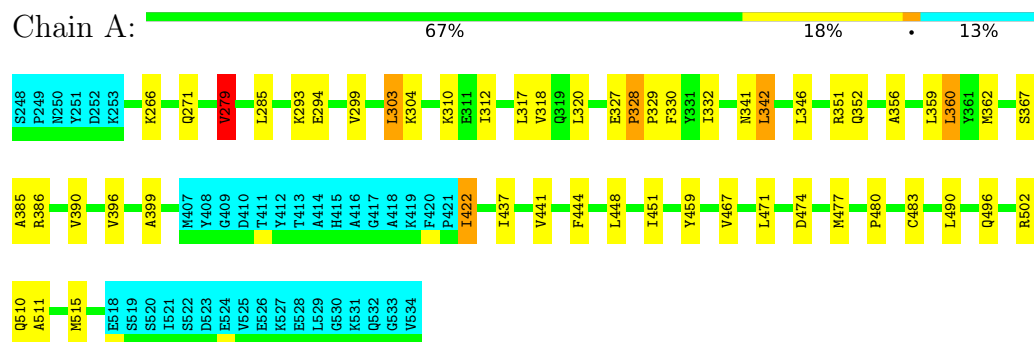
4.2.13 Score per residue for model 13

- Molecule 1: Tyrosine-protein kinase ABL1



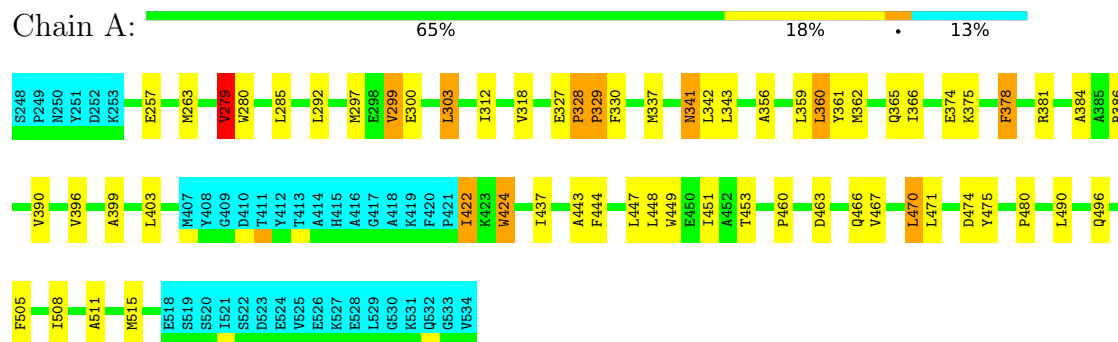
4.2.14 Score per residue for model 14

- Molecule 1: Tyrosine-protein kinase ABL1



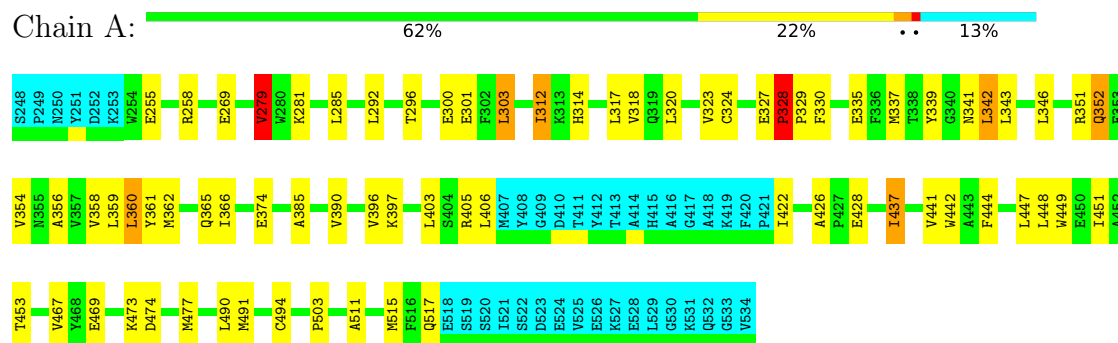
4.2.15 Score per residue for model 15

- Molecule 1: Tyrosine-protein kinase ABL1



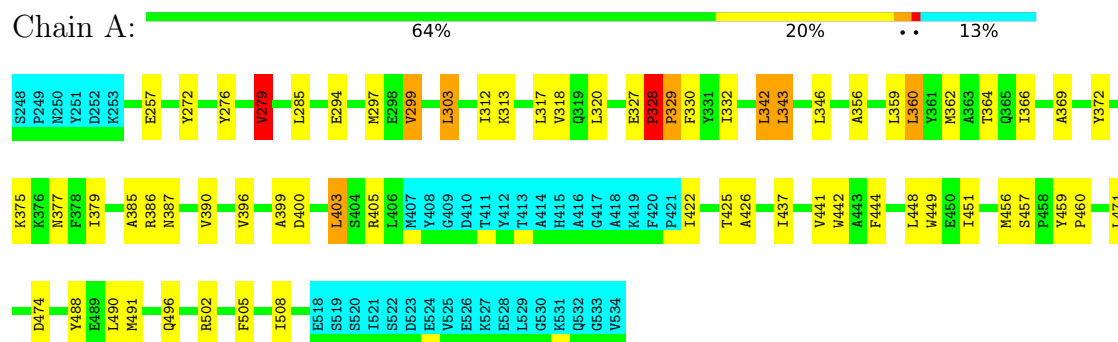
4.2.16 Score per residue for model 16

- Molecule 1: Tyrosine-protein kinase ABL1



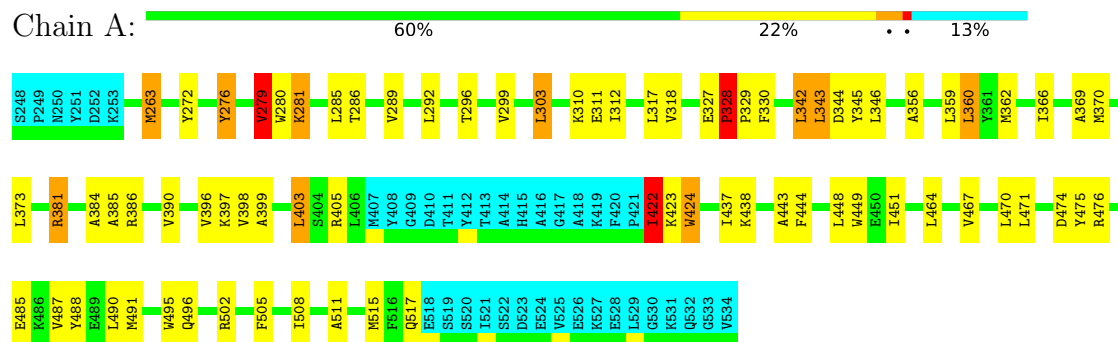
4.2.17 Score per residue for model 17

- Molecule 1: Tyrosine-protein kinase ABL1



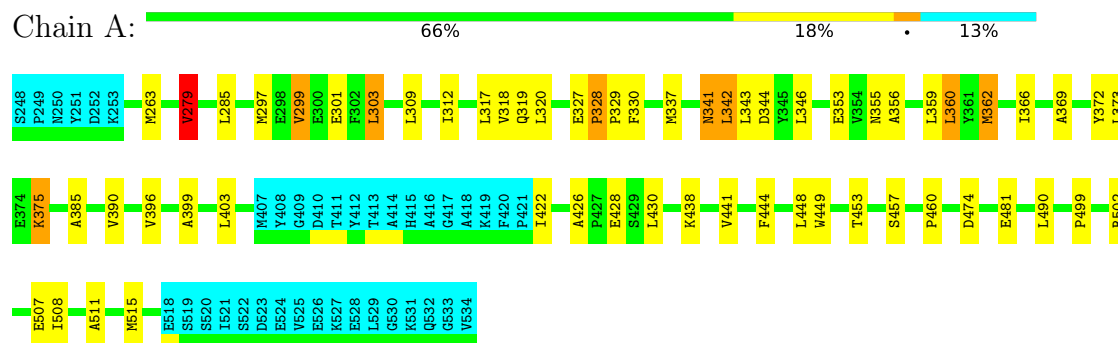
4.2.18 Score per residue for model 18

- Molecule 1: Tyrosine-protein kinase ABL1



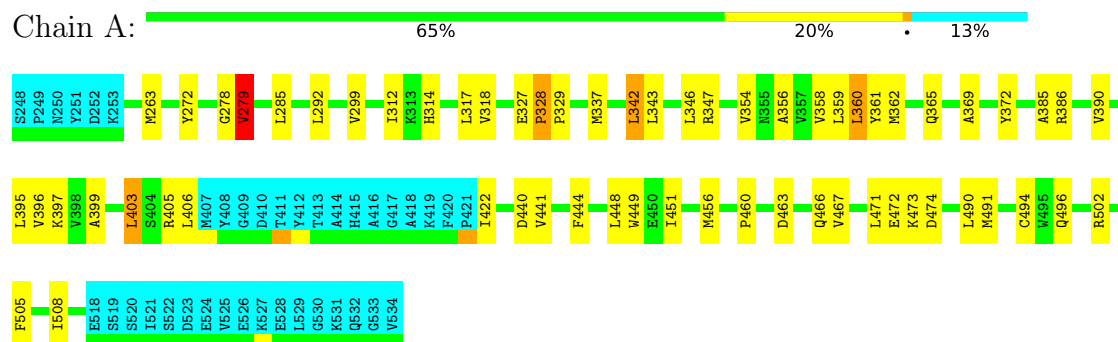
4.2.19 Score per residue for model 19

- Molecule 1: Tyrosine-protein kinase ABL1



4.2.20 Score per residue for model 20

- Molecule 1: Tyrosine-protein kinase ABL1



5 Refinement protocol and experimental data overview

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

Of the 100 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
CNS	refinement	
CYANA	structure calculation	
TALOS	geometry optimization	
PSVS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	553
Number of shifts mapped to atoms	553
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	14%

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.25±0.01	3±1/2101 (0.1± 0.1%)	1.12±0.01	5±1/2846 (0.2± 0.0%)
All	All	1.25	63/42020 (0.1%)	1.12	95/56920 (0.2%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.2±0.4
All	All	0	4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	327	GLU	C-N	6.95	1.41	1.33	13	19
1	A	424	TRP	NE1-CE2	-6.73	1.30	1.37	8	3
1	A	312	ILE	CA-CB	6.30	1.60	1.53	16	5
1	A	279	VAL	CA-CB	6.18	1.62	1.54	19	18
1	A	422	ILE	CA-CB	5.98	1.61	1.54	18	6
1	A	328	PRO	CA-C	5.62	1.57	1.52	3	4
1	A	459	TYR	CA-C	5.46	1.57	1.53	7	3
1	A	467	VAL	CA-CB	5.12	1.60	1.54	5	3
1	A	459	TYR	CA-CB	5.11	1.57	1.52	10	1
1	A	379	ILE	CA-CB	5.01	1.60	1.54	17	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	378	PHE	CA-CB-CG	7.94	121.74	113.80	15	6
1	A	327	GLU	CA-C-N	7.45	128.05	120.38	7	20
1	A	327	GLU	C-N-CA	7.45	128.05	120.38	7	20
1	A	328	PRO	CA-C-N	7.12	128.73	119.84	5	20
1	A	328	PRO	C-N-CA	7.12	128.73	119.84	5	20
1	A	328	PRO	N-CA-C	6.11	118.15	110.70	15	6
1	A	343	LEU	N-CA-CB	5.39	118.05	110.12	12	1
1	A	301	GLU	CA-C-N	5.38	127.74	120.38	5	1
1	A	301	GLU	C-N-CA	5.38	127.74	120.38	5	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	328	PRO	Peptide	3
1	A	402	GLY	Peptide	1

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	2048	2021	2016	32±5
All	All	40960	40420	40320	630

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:317:LEU:HD21	1:A:369:ALA:HB1	0.69	1.63	1	16
1:A:297:MET:HB2	1:A:299:VAL:HG12	0.67	1.65	15	2
1:A:312:ILE:HD11	1:A:317:LEU:HD22	0.67	1.66	12	14
1:A:458:PRO:HA	1:A:477:MET:SD	0.65	2.32	12	1
1:A:303:LEU:HD22	1:A:330:PHE:CZ	0.62	2.29	5	15
1:A:292:LEU:HD12	1:A:296:THR:HG21	0.61	1.73	2	9

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:403:LEU:HD12	1:A:403:LEU:H	0.61	1.55	10	1
1:A:359:LEU:HD22	1:A:451:ILE:HG23	0.61	1.72	18	14
1:A:362:MET:HB2	1:A:396:VAL:HG23	0.61	1.73	9	2
1:A:359:LEU:HA	1:A:362:MET:SD	0.61	2.36	5	15
1:A:256:MET:SD	1:A:333:ILE:HG21	0.61	2.36	12	2
1:A:390:VAL:HG22	1:A:396:VAL:HG22	0.60	1.71	1	19
1:A:385:ALA:HA	1:A:388:CYS:SG	0.60	2.36	7	1
1:A:370:MET:SD	1:A:398:VAL:HG11	0.60	2.37	18	3
1:A:312:ILE:HD12	1:A:373:LEU:HD21	0.59	1.74	13	3
1:A:386:ARG:HH22	1:A:400:ASP:HA	0.59	1.57	4	1
1:A:318:VAL:HG21	1:A:399:ALA:HB2	0.59	1.73	10	19
1:A:362:MET:HG3	1:A:396:VAL:HG21	0.59	1.73	16	1
1:A:449:TRP:CE3	1:A:491:MET:SD	0.58	2.96	10	4
1:A:386:ARG:NH2	1:A:400:ASP:HA	0.58	2.14	4	1
1:A:386:ARG:HG3	1:A:403:LEU:HD13	0.58	1.75	6	4
1:A:403:LEU:HD22	1:A:406:LEU:HD22	0.57	1.75	7	3
1:A:477:MET:SD	1:A:495:TRP:CZ2	0.57	2.97	9	1
1:A:258:ARG:HB3	1:A:324:CYS:SG	0.57	2.40	5	1
1:A:452:ALA:HB1	1:A:483:CYS:SG	0.57	2.39	8	3
1:A:491:MET:HA	1:A:494:CYS:SG	0.57	2.38	16	3
1:A:438:LYS:HD3	1:A:499:PRO:HB3	0.57	1.76	1	1
1:A:297:MET:HG3	1:A:299:VAL:HG12	0.56	1.77	19	1
1:A:384:ALA:HB1	1:A:386:ARG:HH11	0.56	1.61	14	1
1:A:456:MET:SD	1:A:460:PRO:HG3	0.56	2.41	17	1
1:A:423:LYS:HG3	1:A:467:VAL:HG21	0.56	1.76	12	1
1:A:441:VAL:HG13	1:A:508:ILE:HD11	0.56	1.77	17	3
1:A:422:ILE:HG12	1:A:430:LEU:HD22	0.55	1.77	12	2
1:A:341:ASN:ND2	1:A:344:ASP:HB3	0.55	2.16	19	1
1:A:342:LEU:HB3	1:A:385:ALA:HB1	0.55	1.78	6	14
1:A:320:LEU:HD21	1:A:323:VAL:HG23	0.55	1.79	5	5
1:A:258:ARG:HB2	1:A:324:CYS:SG	0.54	2.42	4	4
1:A:441:VAL:HG11	1:A:503:PRO:O	0.54	2.03	6	2
1:A:480:PRO:HB2	1:A:483:CYS:SG	0.54	2.43	14	2
1:A:422:ILE:HG23	1:A:464:LEU:HD21	0.54	1.80	12	1
1:A:356:ALA:O	1:A:360:LEU:HD22	0.53	2.04	18	20
1:A:467:VAL:O	1:A:471:LEU:HG	0.53	2.04	13	15
1:A:261:ILE:HG22	1:A:263:MET:SD	0.53	2.44	6	5
1:A:374:GLU:HB2	1:A:437:ILE:HG13	0.53	1.80	16	1
1:A:441:VAL:HG11	1:A:502:ARG:HE	0.53	1.64	14	1
1:A:370:MET:SD	1:A:373:LEU:HG	0.53	2.44	11	1
1:A:422:ILE:HG12	1:A:425:THR:HB	0.52	1.79	13	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:384:ALA:HA	1:A:424:TRP:CH2	0.52	2.39	10	3
1:A:488:TYR:HA	1:A:491:MET:SD	0.52	2.44	17	3
1:A:386:ARG:NE	1:A:403:LEU:HD13	0.52	2.20	10	1
1:A:437:ILE:HD11	1:A:505:PHE:HE2	0.52	1.63	9	1
1:A:386:ARG:HG2	1:A:403:LEU:HD22	0.52	1.81	10	1
1:A:437:ILE:HG23	1:A:438:LYS:HD2	0.52	1.82	18	1
1:A:441:VAL:HG22	1:A:505:PHE:CE2	0.51	2.39	14	6
1:A:272:TYR:HB3	1:A:292:LEU:HA	0.51	1.80	6	7
1:A:488:TYR:HA	1:A:491:MET:HG2	0.51	1.83	1	1
1:A:463:ASP:HB2	1:A:466:GLN:HG2	0.51	1.82	15	1
1:A:442:TRP:HB2	1:A:502:ARG:HH22	0.51	1.64	2	1
1:A:312:ILE:HD12	1:A:373:LEU:HD11	0.50	1.82	11	1
1:A:337:MET:SD	1:A:397:LYS:HE2	0.50	2.46	16	1
1:A:316:ASN:HA	1:A:395:LEU:HD21	0.50	1.84	12	4
1:A:424:TRP:CZ3	1:A:443:ALA:HB1	0.50	2.40	6	2
1:A:401:PHE:HD2	1:A:403:LEU:HD21	0.50	1.65	6	1
1:A:486:LYS:HB3	1:A:515:MET:HG2	0.50	1.82	9	1
1:A:343:LEU:HD23	1:A:344:ASP:H	0.50	1.65	11	3
1:A:480:PRO:HG2	1:A:483:CYS:SG	0.50	2.47	12	1
1:A:477:MET:HG3	1:A:491:MET:SD	0.50	2.47	13	1
1:A:318:VAL:HG22	1:A:337:MET:HE3	0.49	1.84	16	6
1:A:422:ILE:HG12	1:A:464:LEU:HD11	0.49	1.84	18	1
1:A:496:GLN:HG3	1:A:501:ASP:HB3	0.49	1.82	9	1
1:A:436:SER:HB2	1:A:438:LYS:HG2	0.49	1.84	13	1
1:A:444:PHE:O	1:A:448:LEU:HG	0.49	2.07	8	17
1:A:273:GLY:HA2	1:A:293:LYS:HE3	0.49	1.85	2	1
1:A:425:THR:HA	1:A:442:TRP:CH2	0.49	2.41	17	1
1:A:438:LYS:HD3	1:A:499:PRO:HB2	0.49	1.83	19	1
1:A:359:LEU:HD23	1:A:362:MET:SD	0.49	2.47	12	5
1:A:278:GLY:O	1:A:279:VAL:HG13	0.49	2.08	13	7
1:A:337:MET:SD	1:A:397:LYS:HD2	0.49	2.48	20	2
1:A:320:LEU:HD11	1:A:332:ILE:HB	0.49	1.83	14	2
1:A:342:LEU:O	1:A:346:LEU:HG	0.49	2.08	3	15
1:A:444:PHE:HE2	1:A:508:ILE:HG21	0.49	1.68	11	8
1:A:345:TYR:CD2	1:A:390:VAL:HG21	0.49	2.42	1	7
1:A:449:TRP:O	1:A:453:THR:HG22	0.49	2.08	6	9
1:A:256:MET:SD	1:A:261:ILE:HG21	0.48	2.48	2	1
1:A:466:GLN:HG3	1:A:470:LEU:HD23	0.48	1.83	5	1
1:A:424:TRP:HH2	1:A:447:LEU:HD13	0.48	1.68	10	1
1:A:369:ALA:O	1:A:372:TYR:HB3	0.48	2.08	6	9
1:A:267:LEU:H	1:A:276:TYR:HA	0.48	1.68	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:511:ALA:O	1:A:515:MET:HG3	0.48	2.09	14	13
1:A:314:HIS:HB3	1:A:317:LEU:HD12	0.48	1.83	8	1
1:A:487:VAL:HG22	1:A:515:MET:SD	0.48	2.48	6	1
1:A:341:ASN:HB3	1:A:386:ARG:HA	0.48	1.85	14	1
1:A:463:ASP:HB3	1:A:466:GLN:HE21	0.48	1.68	20	1
1:A:354:VAL:HG13	1:A:358:VAL:HB	0.48	1.86	16	7
1:A:362:MET:HB2	1:A:396:VAL:HG21	0.48	1.85	15	8
1:A:370:MET:HA	1:A:373:LEU:HD13	0.48	1.85	7	3
1:A:444:PHE:CE2	1:A:508:ILE:HG21	0.48	2.44	17	9
1:A:442:TRP:HB2	1:A:502:ARG:NH2	0.48	2.23	2	1
1:A:379:ILE:HD11	1:A:440:ASP:HB2	0.48	1.84	3	1
1:A:306:ALA:HB2	1:A:332:ILE:HG21	0.48	1.86	4	4
1:A:424:TRP:HH2	1:A:447:LEU:HB2	0.48	1.69	6	3
1:A:292:LEU:H	1:A:292:LEU:HD23	0.47	1.69	15	2
1:A:505:PHE:HD1	1:A:508:ILE:HD12	0.47	1.70	7	3
1:A:403:LEU:HD22	1:A:406:LEU:HD13	0.47	1.86	3	1
1:A:275:VAL:HG21	1:A:401:PHE:HB3	0.47	1.85	3	3
1:A:487:VAL:HG12	1:A:491:MET:HE3	0.47	1.86	10	3
1:A:456:MET:SD	1:A:457:SER:O	0.47	2.73	10	3
1:A:401:PHE:HB2	1:A:403:LEU:HG	0.47	1.87	10	2
1:A:426:ALA:O	1:A:430:LEU:HG	0.46	2.10	5	5
1:A:297:MET:SD	1:A:297:MET:N	0.46	2.88	2	3
1:A:343:LEU:HA	1:A:346:LEU:HD12	0.46	1.87	17	2
1:A:367:SER:HA	1:A:505:PHE:HD1	0.46	1.70	3	3
1:A:384:ALA:HB1	1:A:386:ARG:NH1	0.46	2.24	14	1
1:A:303:LEU:HD22	1:A:330:PHE:CE2	0.46	2.45	16	5
1:A:459:TYR:HB3	1:A:462:ILE:HD11	0.46	1.86	10	2
1:A:381:ARG:HH22	1:A:443:ALA:HB2	0.46	1.70	18	1
1:A:470:LEU:HD13	1:A:475:TYR:CD1	0.46	2.45	6	5
1:A:312:ILE:HG13	1:A:317:LEU:HD13	0.46	1.88	12	2
1:A:437:ILE:O	1:A:441:VAL:HG23	0.46	2.11	2	9
1:A:361:TYR:O	1:A:365:GLN:HG2	0.45	2.11	13	6
1:A:342:LEU:HD12	1:A:346:LEU:HD11	0.45	1.87	11	7
1:A:386:ARG:HD2	1:A:403:LEU:HD22	0.45	1.87	6	1
1:A:380:HIS:ND1	1:A:381:ARG:N	0.45	2.65	13	1
1:A:359:LEU:HD22	1:A:451:ILE:CG2	0.45	2.42	3	9
1:A:343:LEU:HD22	1:A:344:ASP:N	0.45	2.26	6	1
1:A:341:ASN:N	1:A:341:ASN:HD22	0.45	2.09	15	1
1:A:362:MET:HB2	1:A:396:VAL:CG2	0.45	2.42	12	7
1:A:343:LEU:HD23	1:A:386:ARG:HH21	0.45	1.72	15	1
1:A:446:VAL:HG13	1:A:477:MET:HE1	0.45	1.88	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:263:MET:HE1	1:A:289:VAL:HG21	0.45	1.88	18	1
1:A:459:TYR:CE1	1:A:471:LEU:HD21	0.45	2.47	17	2
1:A:337:MET:HB3	1:A:390:VAL:C	0.45	2.37	13	2
1:A:477:MET:SD	1:A:477:MET:N	0.45	2.89	16	2
1:A:314:HIS:HB2	1:A:317:LEU:HB2	0.45	1.88	16	1
1:A:264:LYS:HB2	1:A:277:GLU:HG3	0.45	1.88	2	2
1:A:342:LEU:HB2	1:A:385:ALA:O	0.45	2.12	1	2
1:A:444:PHE:HB2	1:A:505:PHE:HE1	0.45	1.72	17	1
1:A:387:ASN:HB3	1:A:403:LEU:HD11	0.44	1.89	10	1
1:A:375:LYS:HE2	1:A:375:LYS:HA	0.44	1.90	4	1
1:A:304:LYS:HA	1:A:304:LYS:HE3	0.44	1.89	11	1
1:A:449:TRP:CE2	1:A:477:MET:HG2	0.44	2.48	7	1
1:A:257:GLU:HG2	1:A:327:GLU:HG3	0.44	1.87	11	1
1:A:480:PRO:HB2	1:A:483:CYS:HB3	0.44	1.88	8	1
1:A:442:TRP:CD1	1:A:495:TRP:HA	0.44	2.48	12	1
1:A:335:GLU:HG2	1:A:337:MET:SD	0.44	2.53	13	2
1:A:469:GLU:O	1:A:473:LYS:HG2	0.44	2.13	16	1
1:A:426:ALA:HB2	1:A:442:TRP:CD2	0.43	2.47	17	1
1:A:466:GLN:O	1:A:470:LEU:HG	0.43	2.13	1	1
1:A:491:MET:SD	1:A:495:TRP:CH2	0.43	3.11	1	1
1:A:362:MET:O	1:A:366:ILE:HG13	0.43	2.14	6	6
1:A:437:ILE:HD11	1:A:505:PHE:CD2	0.43	2.48	1	1
1:A:263:MET:SD	1:A:276:TYR:CE1	0.43	3.12	18	1
1:A:383:LEU:HA	1:A:387:ASN:HD21	0.43	1.74	7	1
1:A:343:LEU:HB2	1:A:386:ARG:NH2	0.43	2.28	1	1
1:A:372:TYR:HD2	1:A:373:LEU:HD12	0.43	1.73	12	1
1:A:303:LEU:N	1:A:303:LEU:HD23	0.43	2.28	14	1
1:A:490:LEU:HD21	1:A:512:PHE:CZ	0.43	2.48	4	1
1:A:424:TRP:CH2	1:A:458:PRO:HG3	0.43	2.49	13	1
1:A:318:VAL:CG2	1:A:399:ALA:HB2	0.43	2.44	15	5
1:A:426:ALA:HB2	1:A:442:TRP:HB3	0.43	1.90	7	1
1:A:422:ILE:HG13	1:A:464:LEU:HD21	0.43	1.91	9	1
1:A:271:GLN:HG3	1:A:402:GLY:HA3	0.42	1.91	1	1
1:A:308:VAL:O	1:A:311:GLU:HG2	0.42	2.14	9	1
1:A:438:LYS:HD2	1:A:499:PRO:HB2	0.42	1.91	6	1
1:A:317:LEU:CD2	1:A:369:ALA:HB1	0.42	2.44	12	2
1:A:351:ARG:HD3	1:A:352:GLN:H	0.42	1.73	12	1
1:A:370:MET:HB3	1:A:505:PHE:CD1	0.42	2.50	14	1
1:A:449:TRP:HE3	1:A:491:MET:HE1	0.42	1.74	2	1
1:A:381:ARG:HG2	1:A:435:PHE:CD1	0.42	2.50	4	1
1:A:385:ALA:N	1:A:447:LEU:HD13	0.42	2.30	5	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:496:GLN:NE2	1:A:502:ARG:HB2	0.42	2.30	14	1
1:A:366:ILE:HD11	1:A:396:VAL:HG11	0.42	1.91	17	3
1:A:476:ARG:HA	1:A:495:TRP:CZ3	0.42	2.49	6	2
1:A:312:ILE:HD13	1:A:317:LEU:HD13	0.42	1.91	16	1
1:A:457:SER:HB2	1:A:460:PRO:HB3	0.42	1.92	19	2
1:A:279:VAL:HG13	1:A:286:THR:HA	0.42	1.92	18	2
1:A:484:PRO:HG2	1:A:487:VAL:HG23	0.42	1.92	9	1
1:A:496:GLN:HG2	1:A:502:ARG:HB2	0.42	1.91	17	1
1:A:422:ILE:HG21	1:A:464:LEU:HD11	0.42	1.92	8	1
1:A:282:LYS:HG2	1:A:283:TYR:H	0.42	1.74	12	1
1:A:343:LEU:HB2	1:A:386:ARG:HH21	0.42	1.75	1	1
1:A:268:GLY:HA3	1:A:406:LEU:HD12	0.42	1.92	4	1
1:A:316:ASN:ND2	1:A:369:ALA:HB2	0.42	2.30	8	1
1:A:449:TRP:CZ2	1:A:456:MET:HE1	0.42	2.50	20	1
1:A:272:TYR:O	1:A:293:LYS:HG3	0.41	2.14	3	1
1:A:449:TRP:CZ2	1:A:477:MET:HG3	0.41	2.50	3	1
1:A:279:VAL:HB	1:A:280:TRP:H	0.41	1.63	15	1
1:A:426:ALA:HB2	1:A:442:TRP:CE3	0.41	2.50	16	1
1:A:473:LYS:O	1:A:474:ASP:HB2	0.41	2.16	4	2
1:A:437:ILE:HD11	1:A:505:PHE:CE2	0.41	2.50	15	1
1:A:449:TRP:HB2	1:A:491:MET:SD	0.41	2.56	8	2
1:A:289:VAL:HG11	1:A:331:TYR:HD2	0.41	1.75	8	1
1:A:442:TRP:HZ2	1:A:471:LEU:HD22	0.41	1.75	11	1
1:A:351:ARG:HD2	1:A:352:GLN:N	0.41	2.30	14	2
1:A:281:LYS:HD3	1:A:281:LYS:H	0.41	1.75	18	1
1:A:428:GLU:HG3	1:A:429:SER:N	0.41	2.31	3	1
1:A:511:ALA:O	1:A:514:THR:HB	0.41	2.16	4	1
1:A:293:LYS:NZ	1:A:295:ASP:HB3	0.41	2.31	5	1
1:A:387:ASN:HB2	1:A:400:ASP:HA	0.41	1.91	17	1
1:A:309:LEU:HB3	1:A:320:LEU:HB2	0.41	1.93	19	1
1:A:496:GLN:O	1:A:502:ARG:HD2	0.41	2.16	20	1
1:A:449:TRP:CH2	1:A:480:PRO:HD3	0.41	2.51	15	1
1:A:384:ALA:HA	1:A:424:TRP:CZ3	0.41	2.51	18	1
1:A:343:LEU:HD23	1:A:386:ARG:HE	0.40	1.75	1	1
1:A:297:MET:HB3	1:A:299:VAL:HG12	0.40	1.93	17	1
1:A:496:GLN:HB3	1:A:502:ARG:HH21	0.40	1.76	18	1
1:A:373:LEU:HB3	1:A:378:PHE:CD1	0.40	2.52	13	1
1:A:375:LYS:NZ	1:A:375:LYS:HB2	0.40	2.30	19	1
1:A:303:LEU:HD23	1:A:303:LEU:N	0.40	2.31	7	1
1:A:384:ALA:HB2	1:A:424:TRP:CZ2	0.40	2.52	5	1
1:A:261:ILE:HG22	1:A:263:MET:HE1	0.40	1.94	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:422:ILE:HD12	1:A:464:LEU:HD11	0.40	1.92	12	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	249/287 (87%)	231±2 (93±1%)	12±2 (5±1%)	6±1 (2±0%)	7	45
All	All	4980/5740 (87%)	4616 (93%)	250 (5%)	114 (2%)	7	45

All 11 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	279	VAL	20
1	A	328	PRO	20
1	A	329	PRO	20
1	A	474	ASP	20
1	A	299	VAL	17
1	A	301	GLU	6
1	A	460	PRO	5
1	A	422	ILE	3
1	A	499	PRO	1
1	A	300	GLU	1
1	A	517	GLN	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	221/252 (88%)	202±3 (91±1%)	19±3 (9±1%)	12	58
All	All	4420/5040 (88%)	4040 (91%)	380 (9%)	12	58

All 87 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	279	VAL	20
1	A	285	LEU	20
1	A	342	LEU	20
1	A	360	LEU	20
1	A	422	ILE	20
1	A	490	LEU	20
1	A	403	LEU	19
1	A	303	LEU	15
1	A	343	LEU	14
1	A	405	ARG	10
1	A	263	MET	10
1	A	314	HIS	8
1	A	257	GLU	6
1	A	502	ARG	6
1	A	374	GLU	5
1	A	477	MET	5
1	A	329	PRO	5
1	A	437	ILE	5
1	A	258	ARG	4
1	A	293	LYS	4
1	A	476	ARG	4
1	A	470	LEU	4
1	A	485	GLU	4
1	A	294	GLU	4
1	A	397	LYS	4
1	A	353	GLU	4
1	A	276	TYR	4
1	A	378	PHE	4
1	A	328	PRO	4
1	A	364	THR	3
1	A	372	TYR	3
1	A	392	GLU	3
1	A	266	LYS	3
1	A	282	LYS	3
1	A	310	LYS	3
1	A	478	GLU	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	264	LYS	3
1	A	300	GLU	3
1	A	326	ARG	3
1	A	424	TRP	3
1	A	428	GLU	3
1	A	496	GLN	3
1	A	381	ARG	3
1	A	341	ASN	3
1	A	375	LYS	3
1	A	433	ASN	2
1	A	311	GLU	2
1	A	319	GLN	2
1	A	371	GLU	2
1	A	473	LYS	2
1	A	498	ASN	2
1	A	438	LYS	2
1	A	514	THR	2
1	A	352	GLN	2
1	A	376	LYS	2
1	A	271	GLN	2
1	A	304	LYS	2
1	A	472	GLU	2
1	A	313	LYS	2
1	A	347	ARG	2
1	A	269	GLU	2
1	A	377	ASN	2
1	A	281	LYS	2
1	A	475	TYR	1
1	A	380	HIS	1
1	A	277	GLU	1
1	A	382	ASP	1
1	A	255	GLU	1
1	A	297	MET	1
1	A	423	LYS	1
1	A	450	GLU	1
1	A	351	ARG	1
1	A	462	ILE	1
1	A	305	GLU	1
1	A	429	SER	1
1	A	510	GLN	1
1	A	339	TYR	1
1	A	406	LEU	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	272	TYR	1
1	A	280	TRP	1
1	A	517	GLN	1
1	A	355	ASN	1
1	A	362	MET	1
1	A	481	GLU	1
1	A	507	GLU	1
1	A	395	LEU	1
1	A	440	ASP	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 14% for the well-defined parts and 14% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: 07112020_inactive2_BMRB.cs.str

7.1.1 Bookkeeping

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

Total number of shifts	553
Number of shifts mapped to atoms	553
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

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 14%, i.e. 505 atoms were assigned a chemical shift out of a possible 3524. 0 out of 44 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/1237 (0%)	0/500 (0%)	0/498 (0%)	0/239 (0%)
Sidechain	452/1937 (23%)	339/1260 (27%)	113/610 (19%)	0/67 (0%)
Aromatic	53/350 (15%)	39/168 (23%)	14/165 (8%)	0/17 (0%)
Overall	505/3524 (14%)	378/1928 (20%)	127/1273 (10%)	0/323 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 14%, i.e. 553 atoms were assigned a chemical shift out of a possible 3993. 0 out of 47 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/1427 (0%)	0/578 (0%)	0/574 (0%)	0/275 (0%)
Sidechain	500/2171 (23%)	375/1410 (27%)	125/688 (18%)	0/73 (0%)
Aromatic	53/395 (13%)	39/189 (21%)	14/187 (7%)	0/19 (0%)
Overall	553/3993 (14%)	414/2177 (19%)	139/1449 (10%)	0/367 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

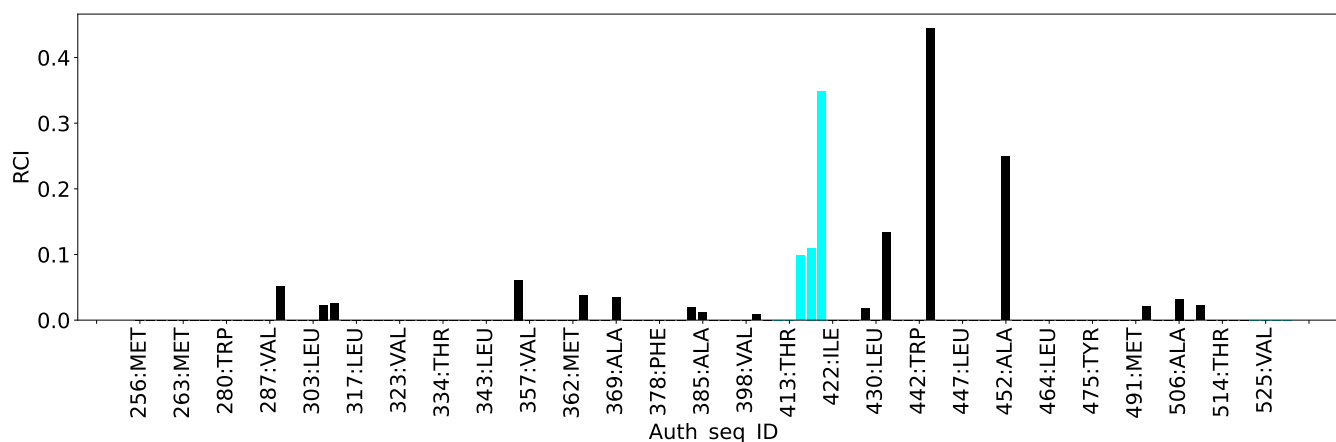
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	453	THR	HG21	-0.20	0.08 – 2.19	-6.4
1	A	453	THR	HG22	-0.20	0.08 – 2.19	-6.4
1	A	453	THR	HG23	-0.20	0.08 – 2.19	-6.4

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	744
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	33
Medium range ($ i-j >1$ and $ i-j <5$)	154
Long range ($ i-j \geq 5$)	527
Inter-chain	0
Hydrogen bond restraints	30
Disulfide bond restraints	0
Total dihedral-angle restraints	496
Number of unmapped restraints	0
Number of restraints per residue	4.3
Number of long range restraints per residue ¹	1.8

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	3.5	0.2
0.2-0.5 (Medium)	0.3	0.47
>0.5 (Large)	0.3	1.57

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	31.6	9.91
10.0-20.0 (Medium)	0.8	17.66
>20.0 (Large)	None	None

9 Distance violation analysis

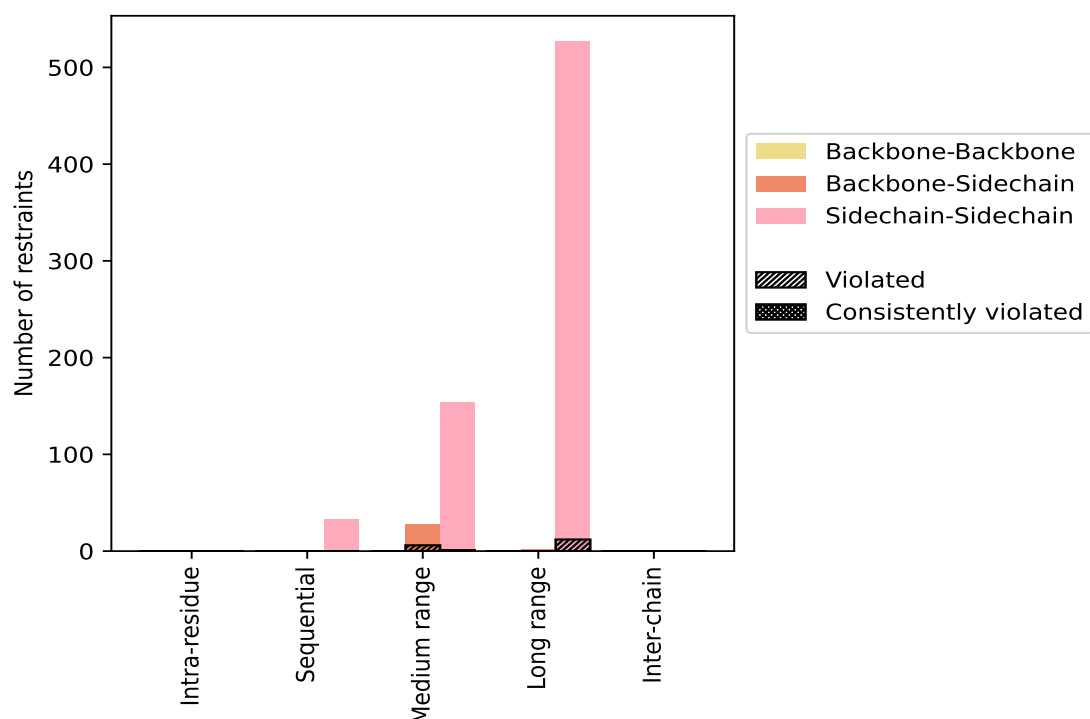
9.1 Summary of distance violations

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	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
Sequential ($i-j =1$)	33	4.4	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	33	4.4	0	0.0	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	154	20.7	1	0.6	0.1	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	154	20.7	1	0.6	0.1	0	0.0	0.0
Long range ($i-j \geq 5$)	527	70.8	12	2.3	1.6	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	527	70.8	12	2.3	1.6	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	30	4.0	6	20.0	0.8	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	744	100.0	19	2.6	2.6	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	30	4.0	6	20.0	0.8	0	0.0	0.0
Sidechain-Sidechain	714	96.0	13	1.8	1.7	0	0.0	0.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	0	1	5	0	6	0.2	0.36	0.08	0.19
2	0	0	3	1	0	4	0.12	0.14	0.02	0.13
3	0	0	2	5	0	7	0.13	0.19	0.03	0.12
4	0	0	1	4	0	5	0.24	0.66	0.21	0.14
5	0	0	1	4	0	5	0.23	0.61	0.19	0.12
6	0	0	2	2	0	4	0.13	0.16	0.02	0.14
7	0	0	2	3	0	5	0.23	0.47	0.13	0.17
8	0	0	1	4	0	5	0.38	1.38	0.5	0.13
9	0	0	3	2	0	5	0.16	0.31	0.08	0.13
10	0	0	1	3	0	4	0.3	0.8	0.29	0.15

Continued on next page...

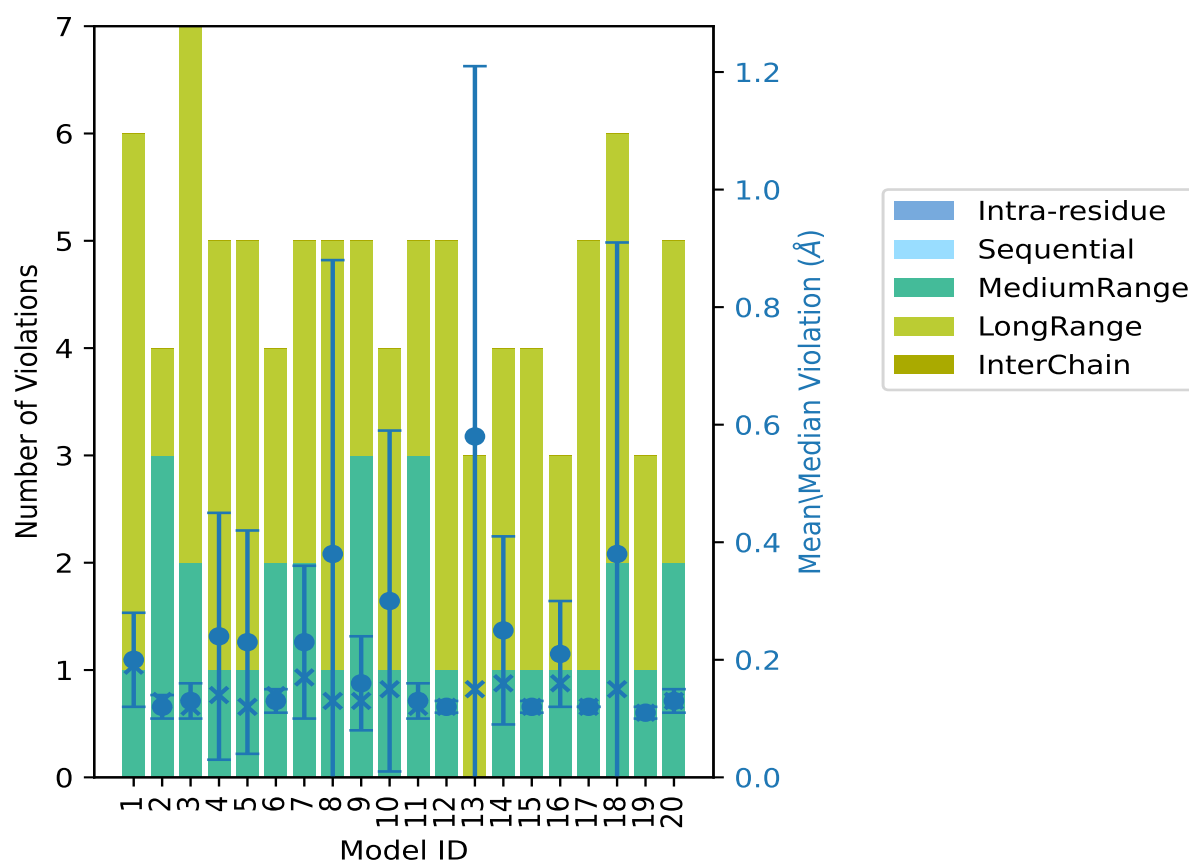
Continued from previous page...

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	0	3	2	0	5	0.13	0.2	0.03	0.12
12	0	0	1	4	0	5	0.12	0.15	0.01	0.12
13	0	0	0	3	0	3	0.58	1.47	0.63	0.15
14	0	0	1	3	0	4	0.25	0.52	0.16	0.16
15	0	0	1	3	0	4	0.12	0.13	0.01	0.12
16	0	0	1	2	0	3	0.21	0.34	0.09	0.16
17	0	0	1	4	0	5	0.12	0.13	0.0	0.12
18	0	0	2	4	0	6	0.38	1.57	0.53	0.15
19	0	0	1	2	0	3	0.11	0.12	0.01	0.11
20	0	0	2	3	0	5	0.13	0.16	0.02	0.13

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

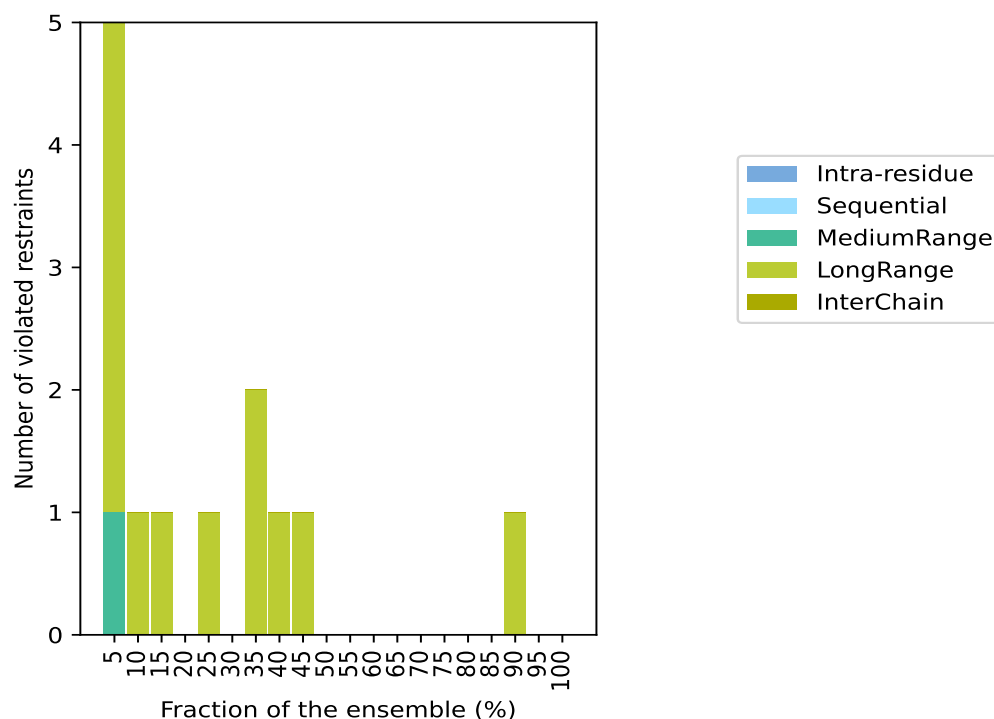
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 701(IR:0, SQ:33, MR:153, LR:515, IC:0) restraints are not 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	%
0	0	1	4	0	5	1	5.0
0	0	0	1	0	1	2	10.0
0	0	0	1	0	1	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	1	0	1	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	2	0	2	7	35.0
0	0	0	1	0	1	8	40.0
0	0	0	1	0	1	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	1	0	1	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

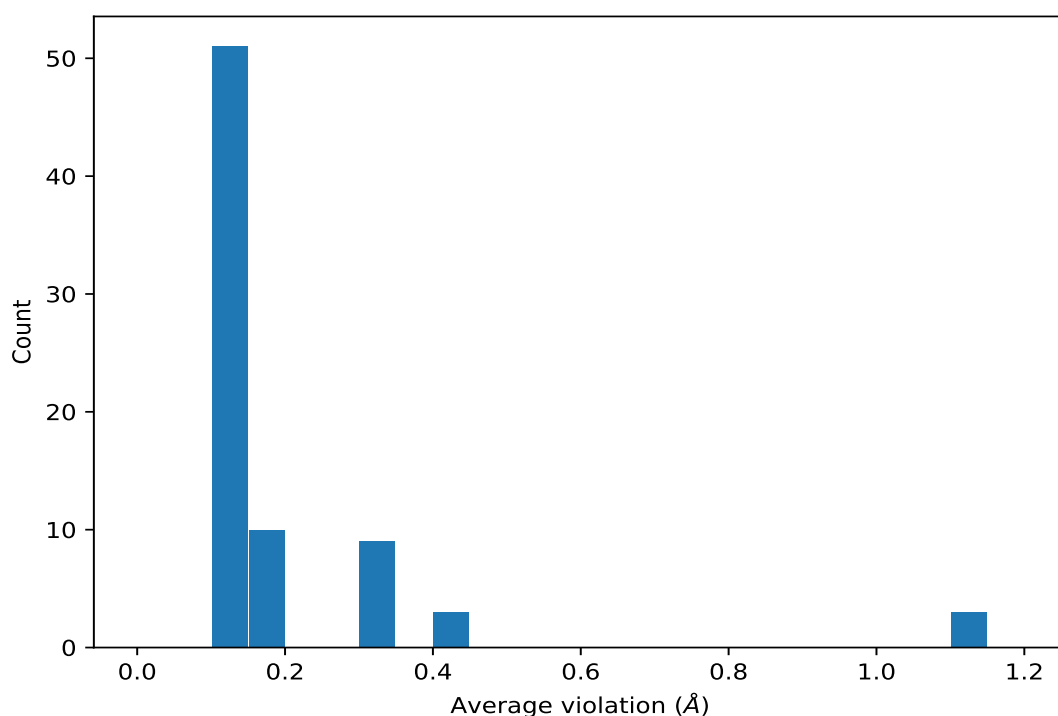
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,30)	1:368:A:SER:O	1:372:A:TYR:H	18	0.15	0.02	0.15
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG21	18	0.14	0.02	0.14
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG22	18	0.14	0.02	0.14
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG23	18	0.14	0.02	0.14
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG21	18	0.14	0.02	0.14
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG22	18	0.14	0.02	0.14
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG23	18	0.14	0.02	0.14
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG21	18	0.14	0.02	0.14
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG22	18	0.14	0.02	0.14
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG23	18	0.14	0.02	0.14
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB1	9	0.15	0.04	0.13
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB2	9	0.15	0.04	0.13
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB3	9	0.15	0.04	0.13
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB1	9	0.15	0.04	0.13
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB2	9	0.15	0.04	0.13
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB3	9	0.15	0.04	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB1	9	0.15	0.04	0.13
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB2	9	0.15	0.04	0.13
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB3	9	0.15	0.04	0.13
(2,695)	1:318:A:VAL:HG11	1:399:A:ALA:HB1	8	0.12	0.01	0.12
(2,695)	1:318:A:VAL:HG11	1:399:A:ALA:HB2	8	0.12	0.01	0.12
(2,695)	1:318:A:VAL:HG11	1:399:A:ALA:HB3	8	0.12	0.01	0.12
(2,695)	1:318:A:VAL:HG12	1:399:A:ALA:HB1	8	0.12	0.01	0.12
(2,695)	1:318:A:VAL:HG12	1:399:A:ALA:HB2	8	0.12	0.01	0.12
(2,695)	1:318:A:VAL:HG12	1:399:A:ALA:HB3	8	0.12	0.01	0.12
(2,695)	1:318:A:VAL:HG13	1:399:A:ALA:HB1	8	0.12	0.01	0.12
(2,695)	1:318:A:VAL:HG13	1:399:A:ALA:HB2	8	0.12	0.01	0.12
(2,695)	1:318:A:VAL:HG13	1:399:A:ALA:HB3	8	0.12	0.01	0.12
(2,695)	1:318:A:VAL:HG21	1:399:A:ALA:HB1	8	0.12	0.01	0.12
(2,695)	1:318:A:VAL:HG21	1:399:A:ALA:HB2	8	0.12	0.01	0.12
(2,695)	1:318:A:VAL:HG21	1:399:A:ALA:HB3	8	0.12	0.01	0.12
(2,695)	1:318:A:VAL:HG22	1:399:A:ALA:HB1	8	0.12	0.01	0.12
(2,695)	1:318:A:VAL:HG22	1:399:A:ALA:HB2	8	0.12	0.01	0.12
(2,695)	1:318:A:VAL:HG22	1:399:A:ALA:HB3	8	0.12	0.01	0.12
(2,695)	1:318:A:VAL:HG23	1:399:A:ALA:HB1	8	0.12	0.01	0.12
(2,695)	1:318:A:VAL:HG23	1:399:A:ALA:HB2	8	0.12	0.01	0.12
(2,695)	1:318:A:VAL:HG23	1:399:A:ALA:HB3	8	0.12	0.01	0.12
(2,420)	1:446:A:VAL:HG11	1:456:A:MET:HE1	7	0.3	0.15	0.31
(2,420)	1:446:A:VAL:HG11	1:456:A:MET:HE2	7	0.3	0.15	0.31
(2,420)	1:446:A:VAL:HG11	1:456:A:MET:HE3	7	0.3	0.15	0.31
(2,420)	1:446:A:VAL:HG12	1:456:A:MET:HE1	7	0.3	0.15	0.31
(2,420)	1:446:A:VAL:HG12	1:456:A:MET:HE2	7	0.3	0.15	0.31
(2,420)	1:446:A:VAL:HG12	1:456:A:MET:HE3	7	0.3	0.15	0.31
(2,420)	1:446:A:VAL:HG13	1:456:A:MET:HE1	7	0.3	0.15	0.31
(2,420)	1:446:A:VAL:HG13	1:456:A:MET:HE2	7	0.3	0.15	0.31
(2,420)	1:446:A:VAL:HG13	1:456:A:MET:HE3	7	0.3	0.15	0.31
(2,693)	1:318:A:VAL:HG11	1:337:A:MET:HE1	7	0.13	0.02	0.12
(2,693)	1:318:A:VAL:HG11	1:337:A:MET:HE2	7	0.13	0.02	0.12
(2,693)	1:318:A:VAL:HG11	1:337:A:MET:HE3	7	0.13	0.02	0.12
(2,693)	1:318:A:VAL:HG12	1:337:A:MET:HE1	7	0.13	0.02	0.12
(2,693)	1:318:A:VAL:HG12	1:337:A:MET:HE2	7	0.13	0.02	0.12
(2,693)	1:318:A:VAL:HG12	1:337:A:MET:HE3	7	0.13	0.02	0.12
(2,693)	1:318:A:VAL:HG13	1:337:A:MET:HE1	7	0.13	0.02	0.12
(2,693)	1:318:A:VAL:HG13	1:337:A:MET:HE2	7	0.13	0.02	0.12
(2,693)	1:318:A:VAL:HG13	1:337:A:MET:HE3	7	0.13	0.02	0.12
(2,693)	1:318:A:VAL:HG21	1:337:A:MET:HE1	7	0.13	0.02	0.12
(2,693)	1:318:A:VAL:HG21	1:337:A:MET:HE2	7	0.13	0.02	0.12
(2,693)	1:318:A:VAL:HG21	1:337:A:MET:HE3	7	0.13	0.02	0.12

Continued on next page...

Continued from previous page...

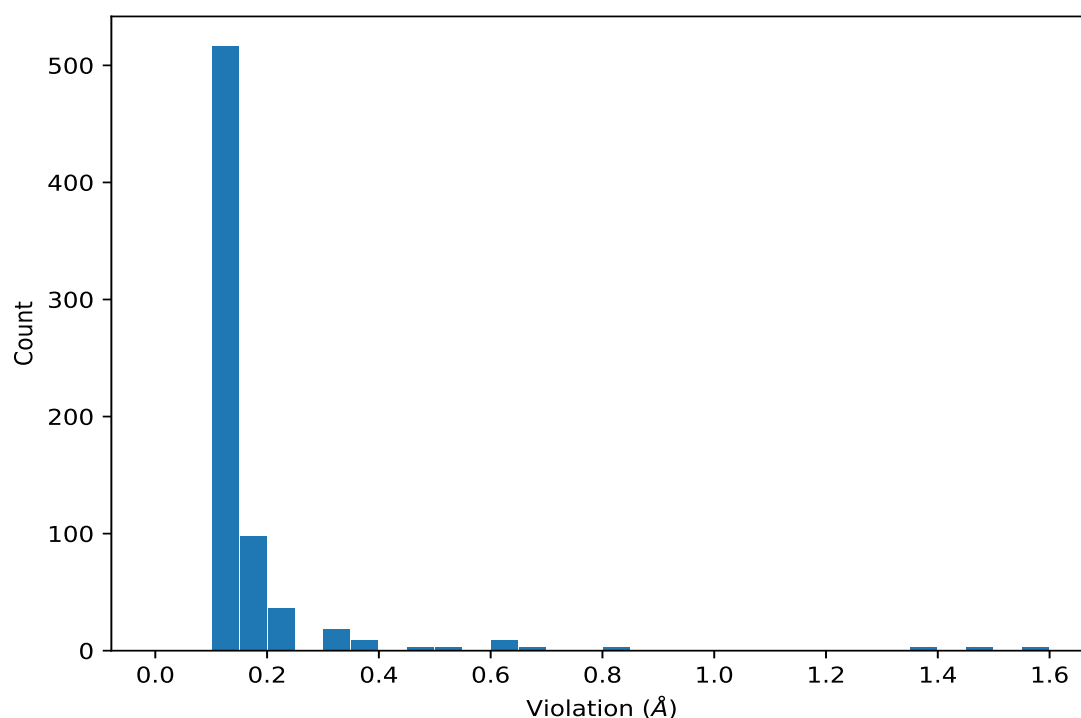
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,693)	1:318:A:VAL:HG22	1:337:A:MET:HE1	7	0.13	0.02	0.12
(2,693)	1:318:A:VAL:HG22	1:337:A:MET:HE2	7	0.13	0.02	0.12
(2,693)	1:318:A:VAL:HG22	1:337:A:MET:HE3	7	0.13	0.02	0.12
(2,693)	1:318:A:VAL:HG23	1:337:A:MET:HE1	7	0.13	0.02	0.12
(2,693)	1:318:A:VAL:HG23	1:337:A:MET:HE2	7	0.13	0.02	0.12
(2,693)	1:318:A:VAL:HG23	1:337:A:MET:HE3	7	0.13	0.02	0.12
(2,678)	1:370:A:MET:HE1	1:505:A:PHE:HE1	5	1.14	0.43	1.38
(2,678)	1:370:A:MET:HE2	1:505:A:PHE:HE1	5	1.14	0.43	1.38
(2,678)	1:370:A:MET:HE3	1:505:A:PHE:HE1	5	1.14	0.43	1.38
(1,4)	1:355:A:ASN:O	1:359:A:LEU:H	4	0.12	0.01	0.12
(2,679)	1:441:A:VAL:HG21	1:505:A:PHE:HE1	3	0.43	0.23	0.52
(2,679)	1:441:A:VAL:HG22	1:505:A:PHE:HE1	3	0.43	0.23	0.52
(2,679)	1:441:A:VAL:HG23	1:505:A:PHE:HE1	3	0.43	0.23	0.52
(1,6)	1:356:A:ALA:O	1:360:A:LEU:H	3	0.11	0.0	0.11
(2,355)	1:342:A:LEU:HD11	1:396:A:VAL:CG2	2	0.11	0.0	0.11
(2,355)	1:342:A:LEU:HD12	1:396:A:VAL:CG2	2	0.11	0.0	0.11
(2,355)	1:342:A:LEU:HD13	1:396:A:VAL:CG2	2	0.11	0.0	0.11
(1,28)	1:367:A:SER:O	1:371:A:GLU: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)
(2,678)	1:370:A:MET:HE1	1:505:A:PHE:HE1	18	1.57
(2,678)	1:370:A:MET:HE2	1:505:A:PHE:HE1	18	1.57
(2,678)	1:370:A:MET:HE3	1:505:A:PHE:HE1	18	1.57
(2,678)	1:370:A:MET:HE1	1:505:A:PHE:HE1	13	1.47
(2,678)	1:370:A:MET:HE2	1:505:A:PHE:HE1	13	1.47
(2,678)	1:370:A:MET:HE3	1:505:A:PHE:HE1	13	1.47
(2,678)	1:370:A:MET:HE1	1:505:A:PHE:HE1	8	1.38
(2,678)	1:370:A:MET:HE2	1:505:A:PHE:HE1	8	1.38
(2,678)	1:370:A:MET:HE3	1:505:A:PHE:HE1	8	1.38
(2,678)	1:370:A:MET:HE1	1:505:A:PHE:HE1	10	0.8
(2,678)	1:370:A:MET:HE2	1:505:A:PHE:HE1	10	0.8
(2,678)	1:370:A:MET:HE3	1:505:A:PHE:HE1	10	0.8
(2,679)	1:441:A:VAL:HG21	1:505:A:PHE:HE1	4	0.66
(2,679)	1:441:A:VAL:HG22	1:505:A:PHE:HE1	4	0.66
(2,679)	1:441:A:VAL:HG23	1:505:A:PHE:HE1	4	0.66
(2,420)	1:446:A:VAL:HG11	1:456:A:MET:HE1	5	0.61

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,420)	1:446:A:VAL:HG11	1:456:A:MET:HE2	5	0.61
(2,420)	1:446:A:VAL:HG11	1:456:A:MET:HE3	5	0.61
(2,420)	1:446:A:VAL:HG12	1:456:A:MET:HE1	5	0.61
(2,420)	1:446:A:VAL:HG12	1:456:A:MET:HE2	5	0.61
(2,420)	1:446:A:VAL:HG12	1:456:A:MET:HE3	5	0.61
(2,420)	1:446:A:VAL:HG13	1:456:A:MET:HE1	5	0.61
(2,420)	1:446:A:VAL:HG13	1:456:A:MET:HE2	5	0.61
(2,420)	1:446:A:VAL:HG13	1:456:A:MET:HE3	5	0.61
(2,679)	1:441:A:VAL:HG21	1:505:A:PHE:HE1	14	0.52
(2,679)	1:441:A:VAL:HG22	1:505:A:PHE:HE1	14	0.52
(2,679)	1:441:A:VAL:HG23	1:505:A:PHE:HE1	14	0.52
(2,678)	1:370:A:MET:HE1	1:505:A:PHE:HE1	7	0.47
(2,678)	1:370:A:MET:HE2	1:505:A:PHE:HE1	7	0.47
(2,678)	1:370:A:MET:HE3	1:505:A:PHE:HE1	7	0.47
(2,420)	1:446:A:VAL:HG11	1:456:A:MET:HE1	1	0.36
(2,420)	1:446:A:VAL:HG11	1:456:A:MET:HE2	1	0.36
(2,420)	1:446:A:VAL:HG11	1:456:A:MET:HE3	1	0.36
(2,420)	1:446:A:VAL:HG12	1:456:A:MET:HE1	1	0.36
(2,420)	1:446:A:VAL:HG12	1:456:A:MET:HE2	1	0.36
(2,420)	1:446:A:VAL:HG12	1:456:A:MET:HE3	1	0.36
(2,420)	1:446:A:VAL:HG13	1:456:A:MET:HE1	1	0.36
(2,420)	1:446:A:VAL:HG13	1:456:A:MET:HE2	1	0.36
(2,420)	1:446:A:VAL:HG13	1:456:A:MET:HE3	1	0.36
(2,420)	1:446:A:VAL:HG11	1:456:A:MET:HE1	16	0.34
(2,420)	1:446:A:VAL:HG11	1:456:A:MET:HE2	16	0.34
(2,420)	1:446:A:VAL:HG11	1:456:A:MET:HE3	16	0.34
(2,420)	1:446:A:VAL:HG12	1:456:A:MET:HE1	16	0.34
(2,420)	1:446:A:VAL:HG12	1:456:A:MET:HE2	16	0.34
(2,420)	1:446:A:VAL:HG12	1:456:A:MET:HE3	16	0.34
(2,420)	1:446:A:VAL:HG13	1:456:A:MET:HE1	16	0.34
(2,420)	1:446:A:VAL:HG13	1:456:A:MET:HE2	16	0.34
(2,420)	1:446:A:VAL:HG13	1:456:A:MET:HE3	16	0.34
(2,420)	1:446:A:VAL:HG11	1:456:A:MET:HE1	9	0.31
(2,420)	1:446:A:VAL:HG11	1:456:A:MET:HE2	9	0.31
(2,420)	1:446:A:VAL:HG11	1:456:A:MET:HE3	9	0.31
(2,420)	1:446:A:VAL:HG12	1:456:A:MET:HE1	9	0.31
(2,420)	1:446:A:VAL:HG12	1:456:A:MET:HE2	9	0.31
(2,420)	1:446:A:VAL:HG12	1:456:A:MET:HE3	9	0.31
(2,420)	1:446:A:VAL:HG13	1:456:A:MET:HE1	9	0.31
(2,420)	1:446:A:VAL:HG13	1:456:A:MET:HE2	9	0.31
(2,420)	1:446:A:VAL:HG13	1:456:A:MET:HE3	9	0.31
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB1	1	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB2	1	0.23
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB3	1	0.23
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB1	1	0.23
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB2	1	0.23
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB3	1	0.23
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB1	1	0.23
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB2	1	0.23
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB3	1	0.23
(2,420)	1:446:A:VAL:HG11	1:456:A:MET:HE1	7	0.23
(2,420)	1:446:A:VAL:HG11	1:456:A:MET:HE2	7	0.23
(2,420)	1:446:A:VAL:HG11	1:456:A:MET:HE3	7	0.23
(2,420)	1:446:A:VAL:HG12	1:456:A:MET:HE1	7	0.23
(2,420)	1:446:A:VAL:HG12	1:456:A:MET:HE2	7	0.23
(2,420)	1:446:A:VAL:HG12	1:456:A:MET:HE3	7	0.23
(2,420)	1:446:A:VAL:HG13	1:456:A:MET:HE1	7	0.23
(2,420)	1:446:A:VAL:HG13	1:456:A:MET:HE2	7	0.23
(2,420)	1:446:A:VAL:HG13	1:456:A:MET:HE3	7	0.23
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG21	1	0.2
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG22	1	0.2
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG23	1	0.2
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG21	1	0.2
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG22	1	0.2
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG23	1	0.2
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG21	1	0.2
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG22	1	0.2
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG23	1	0.2
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB1	11	0.2
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB2	11	0.2
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB3	11	0.2
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB1	11	0.2
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB2	11	0.2
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB3	11	0.2
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB1	11	0.2
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB2	11	0.2
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB3	11	0.2
(1,30)	1:368:A:SER:O	1:372:A:TYR:H	3	0.19
(1,30)	1:368:A:SER:O	1:372:A:TYR:H	5	0.19
(2,710)	1:525:A:VAL:HG11	1:529:A:LEU:HD11	1	0.18
(2,710)	1:525:A:VAL:HG11	1:529:A:LEU:HD12	1	0.18
(2,710)	1:525:A:VAL:HG11	1:529:A:LEU:HD13	1	0.18
(2,710)	1:525:A:VAL:HG11	1:529:A:LEU:HD21	1	0.18
(2,710)	1:525:A:VAL:HG11	1:529:A:LEU:HD22	1	0.18

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,710)	1:525:A:VAL:HG11	1:529:A:LEU:HD23	1	0.18
(2,710)	1:525:A:VAL:HG12	1:529:A:LEU:HD11	1	0.18
(2,710)	1:525:A:VAL:HG12	1:529:A:LEU:HD12	1	0.18
(2,710)	1:525:A:VAL:HG12	1:529:A:LEU:HD13	1	0.18
(2,710)	1:525:A:VAL:HG12	1:529:A:LEU:HD21	1	0.18
(2,710)	1:525:A:VAL:HG12	1:529:A:LEU:HD22	1	0.18
(2,710)	1:525:A:VAL:HG12	1:529:A:LEU:HD23	1	0.18
(2,710)	1:525:A:VAL:HG13	1:529:A:LEU:HD11	1	0.18
(2,710)	1:525:A:VAL:HG13	1:529:A:LEU:HD12	1	0.18
(2,710)	1:525:A:VAL:HG13	1:529:A:LEU:HD13	1	0.18
(2,710)	1:525:A:VAL:HG13	1:529:A:LEU:HD21	1	0.18
(2,710)	1:525:A:VAL:HG13	1:529:A:LEU:HD22	1	0.18
(2,710)	1:525:A:VAL:HG13	1:529:A:LEU:HD23	1	0.18
(2,710)	1:525:A:VAL:HG21	1:529:A:LEU:HD11	1	0.18
(2,710)	1:525:A:VAL:HG21	1:529:A:LEU:HD12	1	0.18
(2,710)	1:525:A:VAL:HG21	1:529:A:LEU:HD13	1	0.18
(2,710)	1:525:A:VAL:HG21	1:529:A:LEU:HD21	1	0.18
(2,710)	1:525:A:VAL:HG21	1:529:A:LEU:HD22	1	0.18
(2,710)	1:525:A:VAL:HG21	1:529:A:LEU:HD23	1	0.18
(2,710)	1:525:A:VAL:HG22	1:529:A:LEU:HD11	1	0.18
(2,710)	1:525:A:VAL:HG22	1:529:A:LEU:HD12	1	0.18
(2,710)	1:525:A:VAL:HG22	1:529:A:LEU:HD13	1	0.18
(2,710)	1:525:A:VAL:HG22	1:529:A:LEU:HD21	1	0.18
(2,710)	1:525:A:VAL:HG22	1:529:A:LEU:HD22	1	0.18
(2,710)	1:525:A:VAL:HG22	1:529:A:LEU:HD23	1	0.18
(2,710)	1:525:A:VAL:HG23	1:529:A:LEU:HD11	1	0.18
(2,710)	1:525:A:VAL:HG23	1:529:A:LEU:HD12	1	0.18
(2,710)	1:525:A:VAL:HG23	1:529:A:LEU:HD13	1	0.18
(2,710)	1:525:A:VAL:HG23	1:529:A:LEU:HD21	1	0.18
(2,710)	1:525:A:VAL:HG23	1:529:A:LEU:HD22	1	0.18
(2,710)	1:525:A:VAL:HG23	1:529:A:LEU:HD23	1	0.18
(1,30)	1:368:A:SER:O	1:372:A:TYR:H	7	0.17
(1,30)	1:368:A:SER:O	1:372:A:TYR:H	8	0.17
(1,30)	1:368:A:SER:O	1:372:A:TYR:H	14	0.17
(2,693)	1:318:A:VAL:HG11	1:337:A:MET:HE1	16	0.16
(2,693)	1:318:A:VAL:HG11	1:337:A:MET:HE2	16	0.16
(2,693)	1:318:A:VAL:HG11	1:337:A:MET:HE3	16	0.16
(2,693)	1:318:A:VAL:HG12	1:337:A:MET:HE1	16	0.16
(2,693)	1:318:A:VAL:HG12	1:337:A:MET:HE2	16	0.16
(2,693)	1:318:A:VAL:HG12	1:337:A:MET:HE3	16	0.16
(2,693)	1:318:A:VAL:HG13	1:337:A:MET:HE1	16	0.16
(2,693)	1:318:A:VAL:HG13	1:337:A:MET:HE2	16	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,693)	1:318:A:VAL:HG13	1:337:A:MET:HE3	16	0.16
(2,693)	1:318:A:VAL:HG21	1:337:A:MET:HE1	16	0.16
(2,693)	1:318:A:VAL:HG21	1:337:A:MET:HE2	16	0.16
(2,693)	1:318:A:VAL:HG21	1:337:A:MET:HE3	16	0.16
(2,693)	1:318:A:VAL:HG22	1:337:A:MET:HE1	16	0.16
(2,693)	1:318:A:VAL:HG22	1:337:A:MET:HE2	16	0.16
(2,693)	1:318:A:VAL:HG22	1:337:A:MET:HE3	16	0.16
(2,693)	1:318:A:VAL:HG23	1:337:A:MET:HE1	16	0.16
(2,693)	1:318:A:VAL:HG23	1:337:A:MET:HE2	16	0.16
(2,693)	1:318:A:VAL:HG23	1:337:A:MET:HE3	16	0.16
(2,661)	1:416:A:ALA:HB1	1:430:A:LEU:HD21	7	0.16
(2,661)	1:416:A:ALA:HB1	1:430:A:LEU:HD22	7	0.16
(2,661)	1:416:A:ALA:HB1	1:430:A:LEU:HD23	7	0.16
(2,661)	1:416:A:ALA:HB2	1:430:A:LEU:HD21	7	0.16
(2,661)	1:416:A:ALA:HB2	1:430:A:LEU:HD22	7	0.16
(2,661)	1:416:A:ALA:HB2	1:430:A:LEU:HD23	7	0.16
(2,661)	1:416:A:ALA:HB3	1:430:A:LEU:HD21	7	0.16
(2,661)	1:416:A:ALA:HB3	1:430:A:LEU:HD22	7	0.16
(2,661)	1:416:A:ALA:HB3	1:430:A:LEU:HD23	7	0.16
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG21	14	0.16
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG22	14	0.16
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG23	14	0.16
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG21	14	0.16
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG22	14	0.16
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG23	14	0.16
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG21	14	0.16
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG22	14	0.16
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG23	14	0.16
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG21	18	0.16
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG22	18	0.16
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG23	18	0.16
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG21	18	0.16
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG22	18	0.16
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG23	18	0.16
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG21	18	0.16
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG22	18	0.16
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG23	18	0.16
(2,418)	1:456:A:MET:HE1	1:477:A:MET:HE1	20	0.16
(2,418)	1:456:A:MET:HE1	1:477:A:MET:HE2	20	0.16
(2,418)	1:456:A:MET:HE1	1:477:A:MET:HE3	20	0.16
(2,418)	1:456:A:MET:HE2	1:477:A:MET:HE1	20	0.16
(2,418)	1:456:A:MET:HE2	1:477:A:MET:HE2	20	0.16

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,418)	1:456:A:MET:HE2	1:477:A:MET:HE3	20	0.16
(2,418)	1:456:A:MET:HE3	1:477:A:MET:HE1	20	0.16
(2,418)	1:456:A:MET:HE3	1:477:A:MET:HE2	20	0.16
(2,418)	1:456:A:MET:HE3	1:477:A:MET:HE3	20	0.16
(1,30)	1:368:A:SER:O	1:372:A:TYR:H	4	0.16
(1,30)	1:368:A:SER:O	1:372:A:TYR:H	6	0.16
(1,30)	1:368:A:SER:O	1:372:A:TYR:H	10	0.16
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG21	12	0.15
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG22	12	0.15
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG23	12	0.15
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG21	12	0.15
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG22	12	0.15
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG23	12	0.15
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG21	12	0.15
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG22	12	0.15
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG23	12	0.15
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG21	13	0.15
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG22	13	0.15
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG23	13	0.15
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG21	13	0.15
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG22	13	0.15
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG23	13	0.15
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG21	13	0.15
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG22	13	0.15
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG23	13	0.15
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG21	20	0.15
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG22	20	0.15
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG23	20	0.15
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG21	20	0.15
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG22	20	0.15
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG23	20	0.15
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG21	20	0.15
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG22	20	0.15
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG23	20	0.15
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB1	18	0.15
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB2	18	0.15
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB3	18	0.15
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB1	18	0.15
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB2	18	0.15
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB3	18	0.15
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB1	18	0.15
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB2	18	0.15

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB3	18	0.15
(2,420)	1:446:A:VAL:HG11	1:456:A:MET:HE1	3	0.15
(2,420)	1:446:A:VAL:HG11	1:456:A:MET:HE2	3	0.15
(2,420)	1:446:A:VAL:HG11	1:456:A:MET:HE3	3	0.15
(2,420)	1:446:A:VAL:HG12	1:456:A:MET:HE1	3	0.15
(2,420)	1:446:A:VAL:HG12	1:456:A:MET:HE2	3	0.15
(2,420)	1:446:A:VAL:HG12	1:456:A:MET:HE3	3	0.15
(2,420)	1:446:A:VAL:HG13	1:456:A:MET:HE1	3	0.15
(2,420)	1:446:A:VAL:HG13	1:456:A:MET:HE2	3	0.15
(2,420)	1:446:A:VAL:HG13	1:456:A:MET:HE3	3	0.15
(1,30)	1:368:A:SER:O	1:372:A:TYR:H	18	0.15
(2,695)	1:318:A:VAL:HG11	1:399:A:ALA:HB1	18	0.14
(2,695)	1:318:A:VAL:HG11	1:399:A:ALA:HB2	18	0.14
(2,695)	1:318:A:VAL:HG11	1:399:A:ALA:HB3	18	0.14
(2,695)	1:318:A:VAL:HG12	1:399:A:ALA:HB1	18	0.14
(2,695)	1:318:A:VAL:HG12	1:399:A:ALA:HB2	18	0.14
(2,695)	1:318:A:VAL:HG12	1:399:A:ALA:HB3	18	0.14
(2,695)	1:318:A:VAL:HG13	1:399:A:ALA:HB1	18	0.14
(2,695)	1:318:A:VAL:HG13	1:399:A:ALA:HB2	18	0.14
(2,695)	1:318:A:VAL:HG13	1:399:A:ALA:HB3	18	0.14
(2,695)	1:318:A:VAL:HG21	1:399:A:ALA:HB1	18	0.14
(2,695)	1:318:A:VAL:HG21	1:399:A:ALA:HB2	18	0.14
(2,695)	1:318:A:VAL:HG21	1:399:A:ALA:HB3	18	0.14
(2,695)	1:318:A:VAL:HG22	1:399:A:ALA:HB1	18	0.14
(2,695)	1:318:A:VAL:HG22	1:399:A:ALA:HB2	18	0.14
(2,695)	1:318:A:VAL:HG22	1:399:A:ALA:HB3	18	0.14
(2,695)	1:318:A:VAL:HG23	1:399:A:ALA:HB1	18	0.14
(2,695)	1:318:A:VAL:HG23	1:399:A:ALA:HB2	18	0.14
(2,695)	1:318:A:VAL:HG23	1:399:A:ALA:HB3	18	0.14
(2,693)	1:318:A:VAL:HG11	1:337:A:MET:HE1	4	0.14
(2,693)	1:318:A:VAL:HG11	1:337:A:MET:HE2	4	0.14
(2,693)	1:318:A:VAL:HG11	1:337:A:MET:HE3	4	0.14
(2,693)	1:318:A:VAL:HG12	1:337:A:MET:HE1	4	0.14
(2,693)	1:318:A:VAL:HG12	1:337:A:MET:HE2	4	0.14
(2,693)	1:318:A:VAL:HG12	1:337:A:MET:HE3	4	0.14
(2,693)	1:318:A:VAL:HG13	1:337:A:MET:HE1	4	0.14
(2,693)	1:318:A:VAL:HG13	1:337:A:MET:HE2	4	0.14
(2,693)	1:318:A:VAL:HG13	1:337:A:MET:HE3	4	0.14
(2,693)	1:318:A:VAL:HG21	1:337:A:MET:HE1	4	0.14
(2,693)	1:318:A:VAL:HG21	1:337:A:MET:HE2	4	0.14
(2,693)	1:318:A:VAL:HG21	1:337:A:MET:HE3	4	0.14
(2,693)	1:318:A:VAL:HG22	1:337:A:MET:HE1	4	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,693)	1:318:A:VAL:HG22	1:337:A:MET:HE2	4	0.14
(2,693)	1:318:A:VAL:HG22	1:337:A:MET:HE3	4	0.14
(2,693)	1:318:A:VAL:HG23	1:337:A:MET:HE1	4	0.14
(2,693)	1:318:A:VAL:HG23	1:337:A:MET:HE2	4	0.14
(2,693)	1:318:A:VAL:HG23	1:337:A:MET:HE3	4	0.14
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG21	2	0.14
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG22	2	0.14
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG23	2	0.14
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG21	2	0.14
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG22	2	0.14
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG23	2	0.14
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG21	2	0.14
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG22	2	0.14
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG23	2	0.14
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG21	3	0.14
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG22	3	0.14
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG23	3	0.14
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG21	3	0.14
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG22	3	0.14
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG23	3	0.14
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG21	3	0.14
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG22	3	0.14
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG23	3	0.14
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG21	6	0.14
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG22	6	0.14
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG23	6	0.14
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG21	6	0.14
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG22	6	0.14
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG23	6	0.14
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG21	6	0.14
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG22	6	0.14
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG23	6	0.14
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB1	14	0.14
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB2	14	0.14
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB3	14	0.14
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB1	14	0.14
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB2	14	0.14
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB3	14	0.14
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB1	14	0.14
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB2	14	0.14
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB3	14	0.14
(1,30)	1:368:A:SER:O	1:372:A:TYR:H	2	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,4)	1:355:A:ASN:O	1:359:A:LEU:H	9	0.14
(2,695)	1:318:A:VAL:HG11	1:399:A:ALA:HB1	6	0.13
(2,695)	1:318:A:VAL:HG11	1:399:A:ALA:HB2	6	0.13
(2,695)	1:318:A:VAL:HG11	1:399:A:ALA:HB3	6	0.13
(2,695)	1:318:A:VAL:HG12	1:399:A:ALA:HB1	6	0.13
(2,695)	1:318:A:VAL:HG12	1:399:A:ALA:HB2	6	0.13
(2,695)	1:318:A:VAL:HG12	1:399:A:ALA:HB3	6	0.13
(2,695)	1:318:A:VAL:HG13	1:399:A:ALA:HB1	6	0.13
(2,695)	1:318:A:VAL:HG13	1:399:A:ALA:HB2	6	0.13
(2,695)	1:318:A:VAL:HG13	1:399:A:ALA:HB3	6	0.13
(2,695)	1:318:A:VAL:HG21	1:399:A:ALA:HB1	6	0.13
(2,695)	1:318:A:VAL:HG21	1:399:A:ALA:HB2	6	0.13
(2,695)	1:318:A:VAL:HG21	1:399:A:ALA:HB3	6	0.13
(2,695)	1:318:A:VAL:HG22	1:399:A:ALA:HB1	6	0.13
(2,695)	1:318:A:VAL:HG22	1:399:A:ALA:HB2	6	0.13
(2,695)	1:318:A:VAL:HG22	1:399:A:ALA:HB3	6	0.13
(2,695)	1:318:A:VAL:HG23	1:399:A:ALA:HB1	6	0.13
(2,695)	1:318:A:VAL:HG23	1:399:A:ALA:HB2	6	0.13
(2,695)	1:318:A:VAL:HG23	1:399:A:ALA:HB3	6	0.13
(2,695)	1:318:A:VAL:HG11	1:399:A:ALA:HB1	10	0.13
(2,695)	1:318:A:VAL:HG11	1:399:A:ALA:HB2	10	0.13
(2,695)	1:318:A:VAL:HG11	1:399:A:ALA:HB3	10	0.13
(2,695)	1:318:A:VAL:HG12	1:399:A:ALA:HB1	10	0.13
(2,695)	1:318:A:VAL:HG12	1:399:A:ALA:HB2	10	0.13
(2,695)	1:318:A:VAL:HG12	1:399:A:ALA:HB3	10	0.13
(2,695)	1:318:A:VAL:HG13	1:399:A:ALA:HB1	10	0.13
(2,695)	1:318:A:VAL:HG13	1:399:A:ALA:HB2	10	0.13
(2,695)	1:318:A:VAL:HG13	1:399:A:ALA:HB3	10	0.13
(2,695)	1:318:A:VAL:HG21	1:399:A:ALA:HB1	10	0.13
(2,695)	1:318:A:VAL:HG21	1:399:A:ALA:HB2	10	0.13
(2,695)	1:318:A:VAL:HG21	1:399:A:ALA:HB3	10	0.13
(2,695)	1:318:A:VAL:HG22	1:399:A:ALA:HB1	10	0.13
(2,695)	1:318:A:VAL:HG22	1:399:A:ALA:HB2	10	0.13
(2,695)	1:318:A:VAL:HG22	1:399:A:ALA:HB3	10	0.13
(2,695)	1:318:A:VAL:HG23	1:399:A:ALA:HB1	10	0.13
(2,695)	1:318:A:VAL:HG23	1:399:A:ALA:HB2	10	0.13
(2,695)	1:318:A:VAL:HG23	1:399:A:ALA:HB3	10	0.13
(2,693)	1:318:A:VAL:HG11	1:337:A:MET:HE1	15	0.13
(2,693)	1:318:A:VAL:HG11	1:337:A:MET:HE2	15	0.13
(2,693)	1:318:A:VAL:HG11	1:337:A:MET:HE3	15	0.13
(2,693)	1:318:A:VAL:HG12	1:337:A:MET:HE1	15	0.13
(2,693)	1:318:A:VAL:HG12	1:337:A:MET:HE2	15	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,693)	1:318:A:VAL:HG12	1:337:A:MET:HE3	15	0.13
(2,693)	1:318:A:VAL:HG13	1:337:A:MET:HE1	15	0.13
(2,693)	1:318:A:VAL:HG13	1:337:A:MET:HE2	15	0.13
(2,693)	1:318:A:VAL:HG13	1:337:A:MET:HE3	15	0.13
(2,693)	1:318:A:VAL:HG21	1:337:A:MET:HE1	15	0.13
(2,693)	1:318:A:VAL:HG21	1:337:A:MET:HE2	15	0.13
(2,693)	1:318:A:VAL:HG21	1:337:A:MET:HE3	15	0.13
(2,693)	1:318:A:VAL:HG22	1:337:A:MET:HE1	15	0.13
(2,693)	1:318:A:VAL:HG22	1:337:A:MET:HE2	15	0.13
(2,693)	1:318:A:VAL:HG22	1:337:A:MET:HE3	15	0.13
(2,693)	1:318:A:VAL:HG23	1:337:A:MET:HE1	15	0.13
(2,693)	1:318:A:VAL:HG23	1:337:A:MET:HE2	15	0.13
(2,693)	1:318:A:VAL:HG23	1:337:A:MET:HE3	15	0.13
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG21	4	0.13
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG22	4	0.13
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG23	4	0.13
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG21	4	0.13
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG22	4	0.13
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG23	4	0.13
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG21	4	0.13
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG22	4	0.13
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG23	4	0.13
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG21	8	0.13
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG22	8	0.13
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG23	8	0.13
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG21	8	0.13
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG22	8	0.13
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG23	8	0.13
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG21	8	0.13
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG22	8	0.13
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG23	8	0.13
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG21	9	0.13
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG22	9	0.13
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG23	9	0.13
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG21	9	0.13
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG22	9	0.13
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG23	9	0.13
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG21	9	0.13
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG22	9	0.13
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG23	9	0.13
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG21	17	0.13
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG22	17	0.13

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG23	17	0.13
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG21	17	0.13
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG22	17	0.13
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG23	17	0.13
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG21	17	0.13
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG22	17	0.13
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG23	17	0.13
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB1	12	0.13
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB2	12	0.13
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB3	12	0.13
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB1	12	0.13
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB2	12	0.13
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB3	12	0.13
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB1	12	0.13
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB2	12	0.13
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB3	12	0.13
(2,420)	1:446:A:VAL:HG11	1:456:A:MET:HE1	17	0.13
(2,420)	1:446:A:VAL:HG11	1:456:A:MET:HE2	17	0.13
(2,420)	1:446:A:VAL:HG11	1:456:A:MET:HE3	17	0.13
(2,420)	1:446:A:VAL:HG12	1:456:A:MET:HE1	17	0.13
(2,420)	1:446:A:VAL:HG12	1:456:A:MET:HE2	17	0.13
(2,420)	1:446:A:VAL:HG12	1:456:A:MET:HE3	17	0.13
(2,420)	1:446:A:VAL:HG13	1:456:A:MET:HE1	17	0.13
(2,420)	1:446:A:VAL:HG13	1:456:A:MET:HE2	17	0.13
(2,420)	1:446:A:VAL:HG13	1:456:A:MET:HE3	17	0.13
(1,30)	1:368:A:SER:O	1:372:A:TYR:H	9	0.13
(1,30)	1:368:A:SER:O	1:372:A:TYR:H	11	0.13
(1,30)	1:368:A:SER:O	1:372:A:TYR:H	15	0.13
(1,30)	1:368:A:SER:O	1:372:A:TYR:H	16	0.13
(1,30)	1:368:A:SER:O	1:372:A:TYR:H	20	0.13
(2,695)	1:318:A:VAL:HG11	1:399:A:ALA:HB1	12	0.12
(2,695)	1:318:A:VAL:HG11	1:399:A:ALA:HB2	12	0.12
(2,695)	1:318:A:VAL:HG11	1:399:A:ALA:HB3	12	0.12
(2,695)	1:318:A:VAL:HG12	1:399:A:ALA:HB1	12	0.12
(2,695)	1:318:A:VAL:HG12	1:399:A:ALA:HB2	12	0.12
(2,695)	1:318:A:VAL:HG12	1:399:A:ALA:HB3	12	0.12
(2,695)	1:318:A:VAL:HG13	1:399:A:ALA:HB1	12	0.12
(2,695)	1:318:A:VAL:HG13	1:399:A:ALA:HB2	12	0.12
(2,695)	1:318:A:VAL:HG13	1:399:A:ALA:HB3	12	0.12
(2,695)	1:318:A:VAL:HG21	1:399:A:ALA:HB1	12	0.12
(2,695)	1:318:A:VAL:HG21	1:399:A:ALA:HB2	12	0.12
(2,695)	1:318:A:VAL:HG21	1:399:A:ALA:HB3	12	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,695)	1:318:A:VAL:HG22	1:399:A:ALA:HB1	12	0.12
(2,695)	1:318:A:VAL:HG22	1:399:A:ALA:HB2	12	0.12
(2,695)	1:318:A:VAL:HG22	1:399:A:ALA:HB3	12	0.12
(2,695)	1:318:A:VAL:HG23	1:399:A:ALA:HB1	12	0.12
(2,695)	1:318:A:VAL:HG23	1:399:A:ALA:HB2	12	0.12
(2,695)	1:318:A:VAL:HG23	1:399:A:ALA:HB3	12	0.12
(2,695)	1:318:A:VAL:HG11	1:399:A:ALA:HB1	15	0.12
(2,695)	1:318:A:VAL:HG11	1:399:A:ALA:HB2	15	0.12
(2,695)	1:318:A:VAL:HG11	1:399:A:ALA:HB3	15	0.12
(2,695)	1:318:A:VAL:HG12	1:399:A:ALA:HB1	15	0.12
(2,695)	1:318:A:VAL:HG12	1:399:A:ALA:HB2	15	0.12
(2,695)	1:318:A:VAL:HG12	1:399:A:ALA:HB3	15	0.12
(2,695)	1:318:A:VAL:HG13	1:399:A:ALA:HB1	15	0.12
(2,695)	1:318:A:VAL:HG13	1:399:A:ALA:HB2	15	0.12
(2,695)	1:318:A:VAL:HG13	1:399:A:ALA:HB3	15	0.12
(2,695)	1:318:A:VAL:HG21	1:399:A:ALA:HB1	15	0.12
(2,695)	1:318:A:VAL:HG21	1:399:A:ALA:HB2	15	0.12
(2,695)	1:318:A:VAL:HG21	1:399:A:ALA:HB3	15	0.12
(2,695)	1:318:A:VAL:HG22	1:399:A:ALA:HB1	15	0.12
(2,695)	1:318:A:VAL:HG22	1:399:A:ALA:HB2	15	0.12
(2,695)	1:318:A:VAL:HG22	1:399:A:ALA:HB3	15	0.12
(2,695)	1:318:A:VAL:HG23	1:399:A:ALA:HB1	15	0.12
(2,695)	1:318:A:VAL:HG23	1:399:A:ALA:HB2	15	0.12
(2,695)	1:318:A:VAL:HG23	1:399:A:ALA:HB3	15	0.12
(2,695)	1:318:A:VAL:HG11	1:399:A:ALA:HB1	17	0.12
(2,695)	1:318:A:VAL:HG11	1:399:A:ALA:HB2	17	0.12
(2,695)	1:318:A:VAL:HG11	1:399:A:ALA:HB3	17	0.12
(2,695)	1:318:A:VAL:HG12	1:399:A:ALA:HB1	17	0.12
(2,695)	1:318:A:VAL:HG12	1:399:A:ALA:HB2	17	0.12
(2,695)	1:318:A:VAL:HG12	1:399:A:ALA:HB3	17	0.12
(2,695)	1:318:A:VAL:HG13	1:399:A:ALA:HB1	17	0.12
(2,695)	1:318:A:VAL:HG13	1:399:A:ALA:HB2	17	0.12
(2,695)	1:318:A:VAL:HG13	1:399:A:ALA:HB3	17	0.12
(2,695)	1:318:A:VAL:HG21	1:399:A:ALA:HB1	17	0.12
(2,695)	1:318:A:VAL:HG21	1:399:A:ALA:HB2	17	0.12
(2,695)	1:318:A:VAL:HG21	1:399:A:ALA:HB3	17	0.12
(2,695)	1:318:A:VAL:HG22	1:399:A:ALA:HB1	17	0.12
(2,695)	1:318:A:VAL:HG22	1:399:A:ALA:HB2	17	0.12
(2,695)	1:318:A:VAL:HG22	1:399:A:ALA:HB3	17	0.12
(2,695)	1:318:A:VAL:HG23	1:399:A:ALA:HB1	17	0.12
(2,695)	1:318:A:VAL:HG23	1:399:A:ALA:HB2	17	0.12
(2,695)	1:318:A:VAL:HG23	1:399:A:ALA:HB3	17	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,693)	1:318:A:VAL:HG11	1:337:A:MET:HE1	20	0.12
(2,693)	1:318:A:VAL:HG11	1:337:A:MET:HE2	20	0.12
(2,693)	1:318:A:VAL:HG11	1:337:A:MET:HE3	20	0.12
(2,693)	1:318:A:VAL:HG12	1:337:A:MET:HE1	20	0.12
(2,693)	1:318:A:VAL:HG12	1:337:A:MET:HE2	20	0.12
(2,693)	1:318:A:VAL:HG12	1:337:A:MET:HE3	20	0.12
(2,693)	1:318:A:VAL:HG13	1:337:A:MET:HE1	20	0.12
(2,693)	1:318:A:VAL:HG13	1:337:A:MET:HE2	20	0.12
(2,693)	1:318:A:VAL:HG13	1:337:A:MET:HE3	20	0.12
(2,693)	1:318:A:VAL:HG21	1:337:A:MET:HE1	20	0.12
(2,693)	1:318:A:VAL:HG21	1:337:A:MET:HE2	20	0.12
(2,693)	1:318:A:VAL:HG21	1:337:A:MET:HE3	20	0.12
(2,693)	1:318:A:VAL:HG22	1:337:A:MET:HE1	20	0.12
(2,693)	1:318:A:VAL:HG22	1:337:A:MET:HE2	20	0.12
(2,693)	1:318:A:VAL:HG22	1:337:A:MET:HE3	20	0.12
(2,693)	1:318:A:VAL:HG23	1:337:A:MET:HE1	20	0.12
(2,693)	1:318:A:VAL:HG23	1:337:A:MET:HE2	20	0.12
(2,693)	1:318:A:VAL:HG23	1:337:A:MET:HE3	20	0.12
(2,679)	1:441:A:VAL:HG21	1:505:A:PHE:HE1	3	0.12
(2,679)	1:441:A:VAL:HG22	1:505:A:PHE:HE1	3	0.12
(2,679)	1:441:A:VAL:HG23	1:505:A:PHE:HE1	3	0.12
(2,629)	1:441:A:VAL:HG11	1:508:A:ILE:HD11	17	0.12
(2,629)	1:441:A:VAL:HG11	1:508:A:ILE:HD12	17	0.12
(2,629)	1:441:A:VAL:HG11	1:508:A:ILE:HD13	17	0.12
(2,629)	1:441:A:VAL:HG12	1:508:A:ILE:HD11	17	0.12
(2,629)	1:441:A:VAL:HG12	1:508:A:ILE:HD12	17	0.12
(2,629)	1:441:A:VAL:HG12	1:508:A:ILE:HD13	17	0.12
(2,629)	1:441:A:VAL:HG13	1:508:A:ILE:HD11	17	0.12
(2,629)	1:441:A:VAL:HG13	1:508:A:ILE:HD12	17	0.12
(2,629)	1:441:A:VAL:HG13	1:508:A:ILE:HD13	17	0.12
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG21	5	0.12
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG22	5	0.12
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG23	5	0.12
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG21	5	0.12
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG22	5	0.12
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG23	5	0.12
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG21	5	0.12
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG22	5	0.12
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG23	5	0.12
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG21	11	0.12
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG22	11	0.12
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG23	11	0.12

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG21	11	0.12
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG22	11	0.12
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG23	11	0.12
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG21	11	0.12
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG22	11	0.12
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG23	11	0.12
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB1	3	0.12
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB2	3	0.12
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB3	3	0.12
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB1	3	0.12
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB2	3	0.12
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB3	3	0.12
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB1	3	0.12
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB2	3	0.12
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB3	3	0.12
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB1	13	0.12
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB2	13	0.12
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB3	13	0.12
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB1	13	0.12
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB2	13	0.12
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB3	13	0.12
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB1	13	0.12
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB2	13	0.12
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB3	13	0.12
(1,30)	1:368:A:SER:O	1:372:A:TYR:H	17	0.12
(1,30)	1:368:A:SER:O	1:372:A:TYR:H	19	0.12
(1,4)	1:355:A:ASN:O	1:359:A:LEU:H	2	0.12
(2,695)	1:318:A:VAL:HG11	1:399:A:ALA:HB1	1	0.11
(2,695)	1:318:A:VAL:HG11	1:399:A:ALA:HB2	1	0.11
(2,695)	1:318:A:VAL:HG11	1:399:A:ALA:HB3	1	0.11
(2,695)	1:318:A:VAL:HG12	1:399:A:ALA:HB1	1	0.11
(2,695)	1:318:A:VAL:HG12	1:399:A:ALA:HB2	1	0.11
(2,695)	1:318:A:VAL:HG12	1:399:A:ALA:HB3	1	0.11
(2,695)	1:318:A:VAL:HG13	1:399:A:ALA:HB1	1	0.11
(2,695)	1:318:A:VAL:HG13	1:399:A:ALA:HB2	1	0.11
(2,695)	1:318:A:VAL:HG13	1:399:A:ALA:HB3	1	0.11
(2,695)	1:318:A:VAL:HG21	1:399:A:ALA:HB1	1	0.11
(2,695)	1:318:A:VAL:HG21	1:399:A:ALA:HB2	1	0.11
(2,695)	1:318:A:VAL:HG21	1:399:A:ALA:HB3	1	0.11
(2,695)	1:318:A:VAL:HG22	1:399:A:ALA:HB1	1	0.11
(2,695)	1:318:A:VAL:HG22	1:399:A:ALA:HB2	1	0.11
(2,695)	1:318:A:VAL:HG22	1:399:A:ALA:HB3	1	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,695)	1:318:A:VAL:HG23	1:399:A:ALA:HB1	1	0.11
(2,695)	1:318:A:VAL:HG23	1:399:A:ALA:HB2	1	0.11
(2,695)	1:318:A:VAL:HG23	1:399:A:ALA:HB3	1	0.11
(2,693)	1:318:A:VAL:HG11	1:337:A:MET:HE1	1	0.11
(2,693)	1:318:A:VAL:HG11	1:337:A:MET:HE2	1	0.11
(2,693)	1:318:A:VAL:HG11	1:337:A:MET:HE3	1	0.11
(2,693)	1:318:A:VAL:HG12	1:337:A:MET:HE1	1	0.11
(2,693)	1:318:A:VAL:HG12	1:337:A:MET:HE2	1	0.11
(2,693)	1:318:A:VAL:HG12	1:337:A:MET:HE3	1	0.11
(2,693)	1:318:A:VAL:HG13	1:337:A:MET:HE1	1	0.11
(2,693)	1:318:A:VAL:HG13	1:337:A:MET:HE2	1	0.11
(2,693)	1:318:A:VAL:HG13	1:337:A:MET:HE3	1	0.11
(2,693)	1:318:A:VAL:HG21	1:337:A:MET:HE1	1	0.11
(2,693)	1:318:A:VAL:HG21	1:337:A:MET:HE2	1	0.11
(2,693)	1:318:A:VAL:HG21	1:337:A:MET:HE3	1	0.11
(2,693)	1:318:A:VAL:HG22	1:337:A:MET:HE1	1	0.11
(2,693)	1:318:A:VAL:HG22	1:337:A:MET:HE2	1	0.11
(2,693)	1:318:A:VAL:HG22	1:337:A:MET:HE3	1	0.11
(2,693)	1:318:A:VAL:HG23	1:337:A:MET:HE1	1	0.11
(2,693)	1:318:A:VAL:HG23	1:337:A:MET:HE2	1	0.11
(2,693)	1:318:A:VAL:HG23	1:337:A:MET:HE3	1	0.11
(2,693)	1:318:A:VAL:HG11	1:337:A:MET:HE1	12	0.11
(2,693)	1:318:A:VAL:HG11	1:337:A:MET:HE2	12	0.11
(2,693)	1:318:A:VAL:HG11	1:337:A:MET:HE3	12	0.11
(2,693)	1:318:A:VAL:HG12	1:337:A:MET:HE1	12	0.11
(2,693)	1:318:A:VAL:HG12	1:337:A:MET:HE2	12	0.11
(2,693)	1:318:A:VAL:HG12	1:337:A:MET:HE3	12	0.11
(2,693)	1:318:A:VAL:HG13	1:337:A:MET:HE1	12	0.11
(2,693)	1:318:A:VAL:HG13	1:337:A:MET:HE2	12	0.11
(2,693)	1:318:A:VAL:HG13	1:337:A:MET:HE3	12	0.11
(2,693)	1:318:A:VAL:HG21	1:337:A:MET:HE1	12	0.11
(2,693)	1:318:A:VAL:HG21	1:337:A:MET:HE2	12	0.11
(2,693)	1:318:A:VAL:HG21	1:337:A:MET:HE3	12	0.11
(2,693)	1:318:A:VAL:HG22	1:337:A:MET:HE1	12	0.11
(2,693)	1:318:A:VAL:HG22	1:337:A:MET:HE2	12	0.11
(2,693)	1:318:A:VAL:HG22	1:337:A:MET:HE3	12	0.11
(2,693)	1:318:A:VAL:HG23	1:337:A:MET:HE1	12	0.11
(2,693)	1:318:A:VAL:HG23	1:337:A:MET:HE2	12	0.11
(2,693)	1:318:A:VAL:HG23	1:337:A:MET:HE3	12	0.11
(2,693)	1:318:A:VAL:HG11	1:337:A:MET:HE1	19	0.11
(2,693)	1:318:A:VAL:HG11	1:337:A:MET:HE2	19	0.11
(2,693)	1:318:A:VAL:HG11	1:337:A:MET:HE3	19	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,693)	1:318:A:VAL:HG12	1:337:A:MET:HE1	19	0.11
(2,693)	1:318:A:VAL:HG12	1:337:A:MET:HE2	19	0.11
(2,693)	1:318:A:VAL:HG12	1:337:A:MET:HE3	19	0.11
(2,693)	1:318:A:VAL:HG13	1:337:A:MET:HE1	19	0.11
(2,693)	1:318:A:VAL:HG13	1:337:A:MET:HE2	19	0.11
(2,693)	1:318:A:VAL:HG13	1:337:A:MET:HE3	19	0.11
(2,693)	1:318:A:VAL:HG21	1:337:A:MET:HE1	19	0.11
(2,693)	1:318:A:VAL:HG21	1:337:A:MET:HE2	19	0.11
(2,693)	1:318:A:VAL:HG21	1:337:A:MET:HE3	19	0.11
(2,693)	1:318:A:VAL:HG22	1:337:A:MET:HE1	19	0.11
(2,693)	1:318:A:VAL:HG22	1:337:A:MET:HE2	19	0.11
(2,693)	1:318:A:VAL:HG22	1:337:A:MET:HE3	19	0.11
(2,693)	1:318:A:VAL:HG23	1:337:A:MET:HE1	19	0.11
(2,693)	1:318:A:VAL:HG23	1:337:A:MET:HE2	19	0.11
(2,693)	1:318:A:VAL:HG23	1:337:A:MET:HE3	19	0.11
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB1	5	0.11
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB2	5	0.11
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB3	5	0.11
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB1	5	0.11
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB2	5	0.11
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB3	5	0.11
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB1	5	0.11
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB2	5	0.11
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB3	5	0.11
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB1	8	0.11
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB2	8	0.11
(2,446)	1:317:A:LEU:HD21	1:369:A:ALA:HB3	8	0.11
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB1	8	0.11
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB2	8	0.11
(2,446)	1:317:A:LEU:HD22	1:369:A:ALA:HB3	8	0.11
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB1	8	0.11
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB2	8	0.11
(2,446)	1:317:A:LEU:HD23	1:369:A:ALA:HB3	8	0.11
(2,355)	1:342:A:LEU:HD11	1:396:A:VAL:CG2	3	0.11
(2,355)	1:342:A:LEU:HD12	1:396:A:VAL:CG2	3	0.11
(2,355)	1:342:A:LEU:HD13	1:396:A:VAL:CG2	3	0.11
(2,355)	1:342:A:LEU:HD11	1:396:A:VAL:CG2	4	0.11
(2,355)	1:342:A:LEU:HD12	1:396:A:VAL:CG2	4	0.11
(2,355)	1:342:A:LEU:HD13	1:396:A:VAL:CG2	4	0.11
(1,30)	1:368:A:SER:O	1:372:A:TYR:H	12	0.11
(1,28)	1:367:A:SER:O	1:371:A:GLU:H	20	0.11
(1,6)	1:356:A:ALA:O	1:360:A:LEU:H	7	0.11

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:356:A:ALA:O	1:360:A:LEU:H	11	0.11
(1,4)	1:355:A:ASN:O	1:359:A:LEU:H	11	0.11
(2,695)	1:318:A:VAL:HG11	1:399:A:ALA:HB1	8	0.1
(2,695)	1:318:A:VAL:HG11	1:399:A:ALA:HB2	8	0.1
(2,695)	1:318:A:VAL:HG11	1:399:A:ALA:HB3	8	0.1
(2,695)	1:318:A:VAL:HG12	1:399:A:ALA:HB1	8	0.1
(2,695)	1:318:A:VAL:HG12	1:399:A:ALA:HB2	8	0.1
(2,695)	1:318:A:VAL:HG12	1:399:A:ALA:HB3	8	0.1
(2,695)	1:318:A:VAL:HG13	1:399:A:ALA:HB1	8	0.1
(2,695)	1:318:A:VAL:HG13	1:399:A:ALA:HB2	8	0.1
(2,695)	1:318:A:VAL:HG13	1:399:A:ALA:HB3	8	0.1
(2,695)	1:318:A:VAL:HG21	1:399:A:ALA:HB1	8	0.1
(2,695)	1:318:A:VAL:HG21	1:399:A:ALA:HB2	8	0.1
(2,695)	1:318:A:VAL:HG21	1:399:A:ALA:HB3	8	0.1
(2,695)	1:318:A:VAL:HG22	1:399:A:ALA:HB1	8	0.1
(2,695)	1:318:A:VAL:HG22	1:399:A:ALA:HB2	8	0.1
(2,695)	1:318:A:VAL:HG22	1:399:A:ALA:HB3	8	0.1
(2,695)	1:318:A:VAL:HG23	1:399:A:ALA:HB1	8	0.1
(2,695)	1:318:A:VAL:HG23	1:399:A:ALA:HB2	8	0.1
(2,695)	1:318:A:VAL:HG23	1:399:A:ALA:HB3	8	0.1
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG21	10	0.1
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG22	10	0.1
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG23	10	0.1
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG21	10	0.1
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG22	10	0.1
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG23	10	0.1
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG21	10	0.1
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG22	10	0.1
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG23	10	0.1
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG21	15	0.1
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG22	15	0.1
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG23	15	0.1
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG21	15	0.1
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG22	15	0.1
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG23	15	0.1
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG21	15	0.1
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG22	15	0.1
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG23	15	0.1
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG21	19	0.1
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG22	19	0.1
(2,609)	1:390:A:VAL:HG21	1:396:A:VAL:HG23	19	0.1
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG21	19	0.1

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG22	19	0.1
(2,609)	1:390:A:VAL:HG22	1:396:A:VAL:HG23	19	0.1
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG21	19	0.1
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG22	19	0.1
(2,609)	1:390:A:VAL:HG23	1:396:A:VAL:HG23	19	0.1
(2,422)	1:446:A:VAL:HG11	1:477:A:MET:HE1	5	0.1
(2,422)	1:446:A:VAL:HG11	1:477:A:MET:HE2	5	0.1
(2,422)	1:446:A:VAL:HG11	1:477:A:MET:HE3	5	0.1
(2,422)	1:446:A:VAL:HG12	1:477:A:MET:HE1	5	0.1
(2,422)	1:446:A:VAL:HG12	1:477:A:MET:HE2	5	0.1
(2,422)	1:446:A:VAL:HG12	1:477:A:MET:HE3	5	0.1
(2,422)	1:446:A:VAL:HG13	1:477:A:MET:HE1	5	0.1
(2,422)	1:446:A:VAL:HG13	1:477:A:MET:HE2	5	0.1
(2,422)	1:446:A:VAL:HG13	1:477:A:MET:HE3	5	0.1
(1,29)	1:368:A:SER:O	1:372:A:TYR:N	3	0.1
(1,28)	1:367:A:SER:O	1:371:A:GLU:H	2	0.1
(1,16)	1:361:A:TYR:O	1:365:A:GLN:H	18	0.1
(1,6)	1:356:A:ALA:O	1:360:A:LEU:H	9	0.1
(1,4)	1:355:A:ASN:O	1:359:A:LEU:H	6	0.1

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

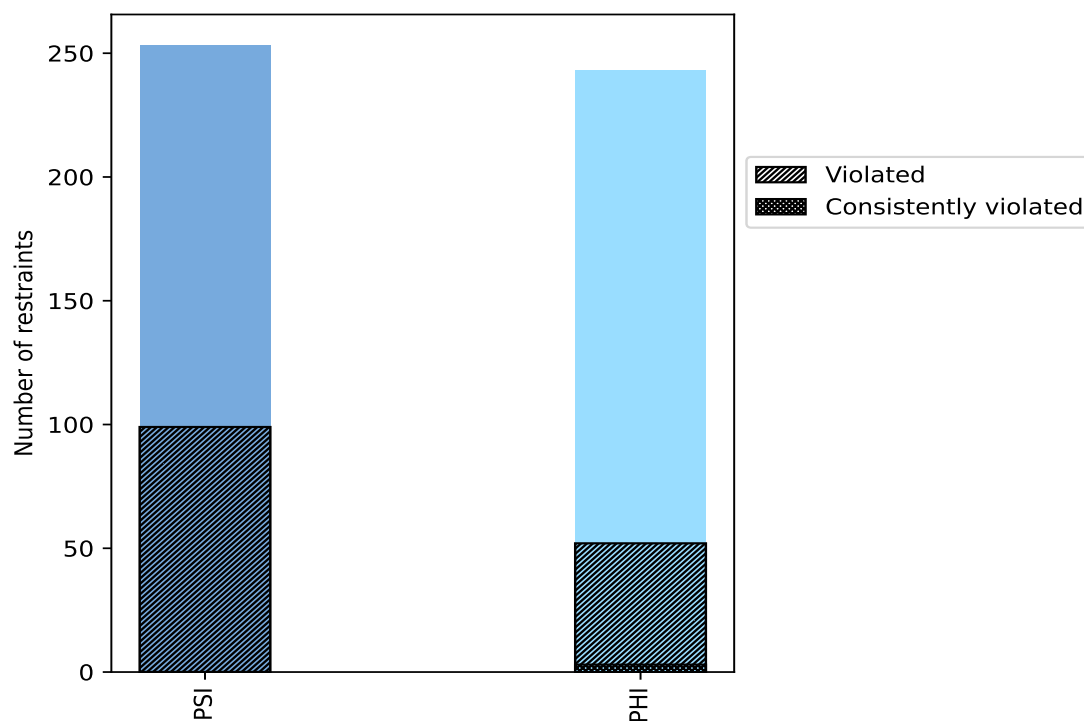
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	253	51.0	99	39.1	20.0	0	0.0	0.0
PHI	243	49.0	52	21.4	10.5	3	1.2	0.6
Total	496	100.0	151	30.4	30.4	3	0.6	0.6

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

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



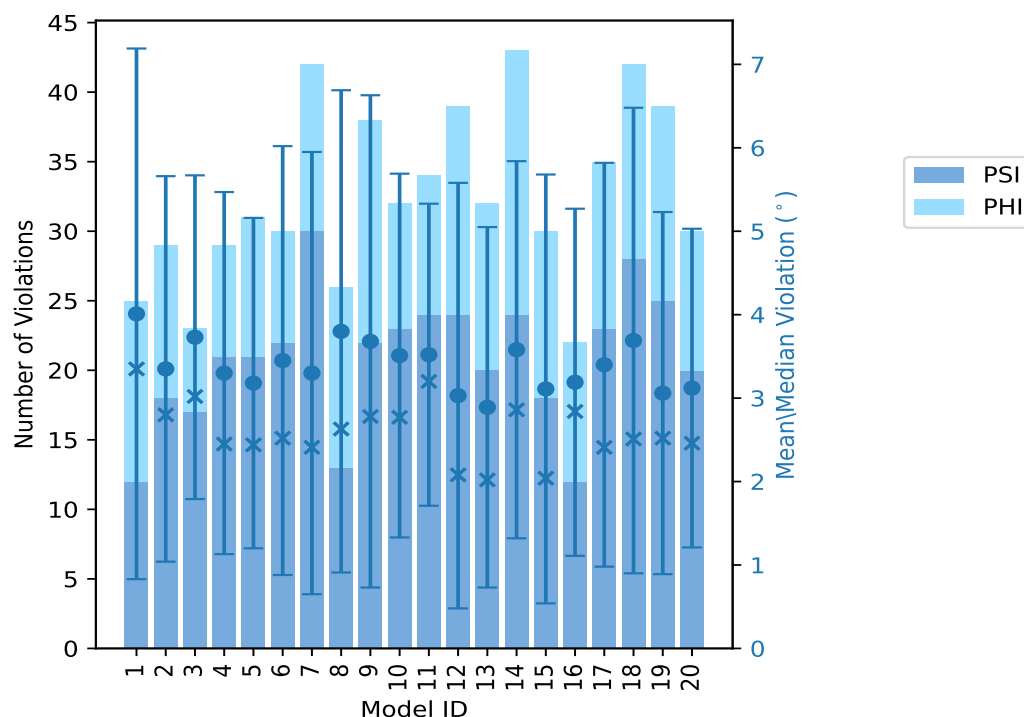
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	12	13	25	4.01	17.3	3.18	3.35
2	18	11	29	3.35	9.77	2.31	2.8
3	17	6	23	3.73	7.86	1.94	3.02
4	21	8	29	3.3	10.86	2.17	2.45
5	21	10	31	3.18	8.44	1.98	2.44
6	22	8	30	3.45	9.91	2.57	2.52
7	30	12	42	3.3	14.37	2.65	2.41
8	13	13	26	3.8	10.9	2.89	2.63
9	22	16	38	3.68	17.66	2.95	2.78
10	23	9	32	3.51	8.92	2.18	2.77
11	24	10	34	3.52	10.07	1.81	3.2
12	24	15	39	3.03	15.08	2.55	2.08
13	20	12	32	2.89	9.3	2.16	2.02
14	24	19	43	3.58	11.29	2.26	2.86
15	18	12	30	3.11	12.42	2.57	2.04
16	12	10	22	3.19	10.71	2.08	2.84
17	23	12	35	3.4	10.51	2.42	2.41
18	28	14	42	3.69	11.38	2.79	2.51
19	25	14	39	3.06	12.86	2.17	2.52
20	20	10	30	3.12	9.17	1.91	2.46

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
29	21	50	1	5.0
15	8	23	2	10.0
11	4	15	3	15.0
9	6	15	4	20.0
12	1	13	5	25.0
4	1	5	6	30.0
4	2	6	7	35.0
3	2	5	8	40.0
2	1	3	9	45.0
3	0	3	10	50.0
1	0	1	11	55.0

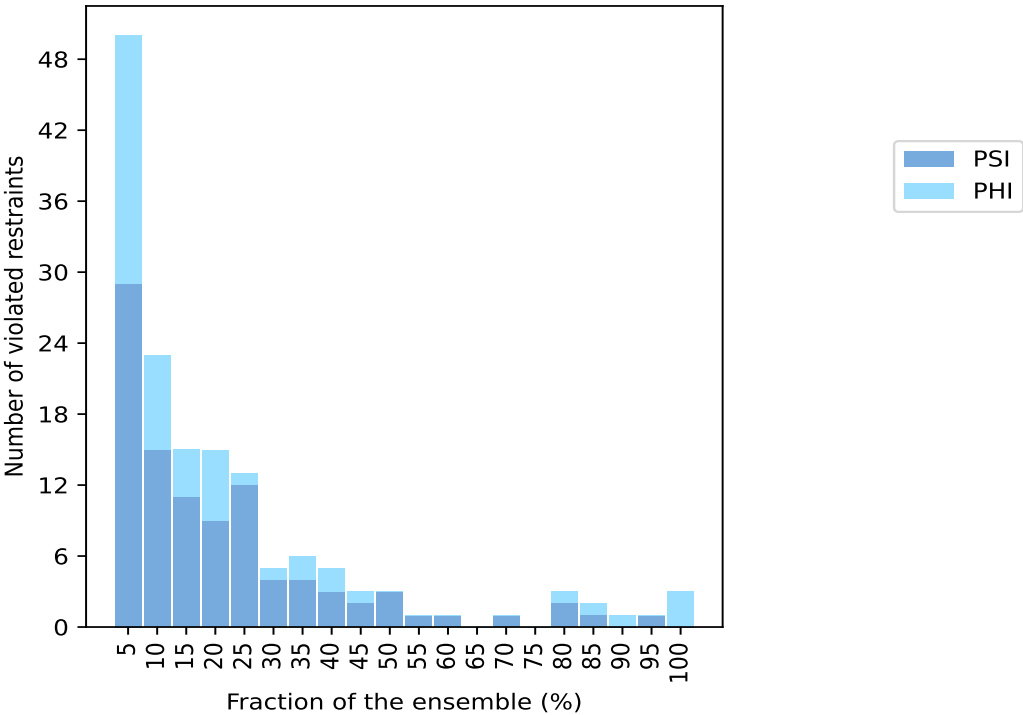
Continued on next page...

Continued from previous page...

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

¹ Number of models with violations

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

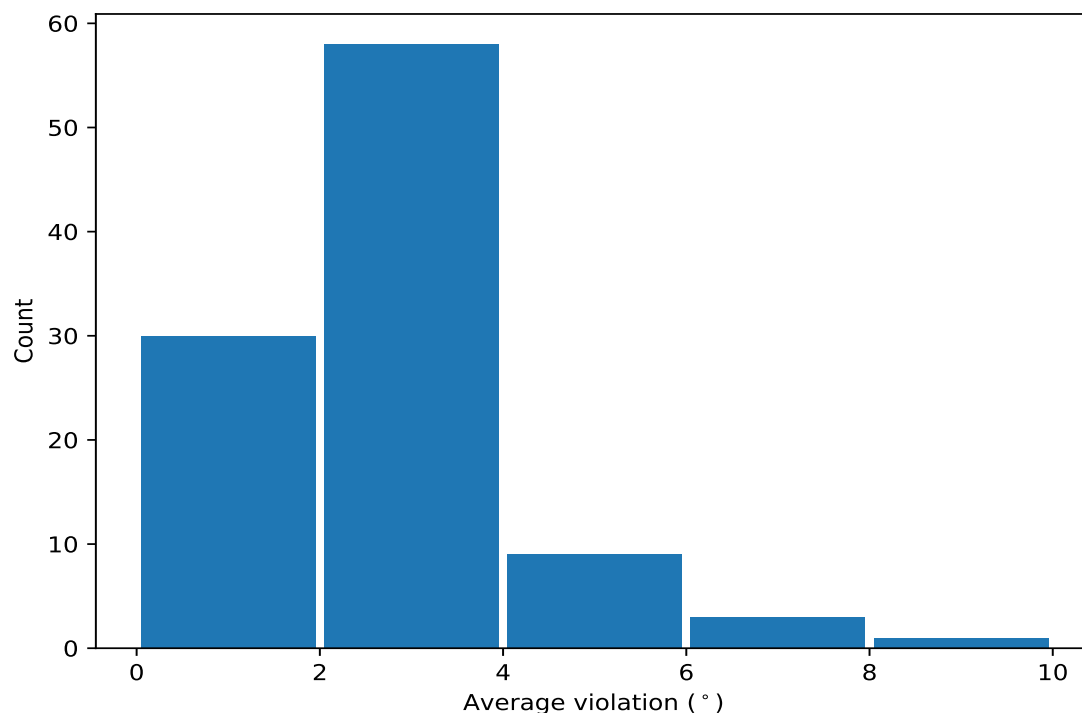


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,147)	1:398:A:VAL:C	1:399:A:ALA:N	1:399:A:ALA:CA	1:399:A:ALA:C	20	8.7	1.84	8.64
(1,148)	1:400:A:ASP:C	1:401:A:PHE:N	1:401:A:PHE:CA	1:401:A:PHE:C	20	6.08	2.36	5.58
(1,30)	1:278:A:GLY:C	1:279:A:VAL:N	1:279:A:VAL:CA	1:279:A:VAL:C	20	5.49	1.85	5.22
(1,394)	1:400:A:ASP:N	1:400:A:ASP:CA	1:400:A:ASP:C	1:401:A:PHE:N	19	4.49	1.82	4.38
(1,151)	1:404:A:SER:C	1:405:A:ARG:N	1:405:A:ARG:CA	1:405:A:ARG:C	18	7.54	3.11	8.15
(1,155)	1:410:A:ASP:C	1:411:A:THR:N	1:411:A:THR:CA	1:411:A:THR:C	17	6.95	5.33	4.98
(1,365)	1:369:A:ALA:N	1:369:A:ALA:CA	1:369:A:ALA:C	1:370:A:MET:N	17	2.68	1.08	2.46
(1,338)	1:342:A:LEU:N	1:342:A:LEU:CA	1:342:A:LEU:C	1:343:A:LEU:N	16	4.51	1.37	4.23
(1,296)	1:300:A:GLU:N	1:300:A:GLU:CA	1:300:A:GLU:C	1:301:A:GLU:N	16	3.26	1.15	3.07
(1,38)	1:286:A:THR:C	1:287:A:VAL:N	1:287:A:VAL:CA	1:287:A:VAL:C	16	2.22	0.53	2.08
(1,294)	1:298:A:GLU:N	1:298:A:GLU:CA	1:298:A:GLU:C	1:299:A:VAL:N	14	4.5	1.87	4.25
(1,295)	1:299:A:VAL:N	1:299:A:VAL:CA	1:299:A:VAL:C	1:300:A:GLU:N	12	2.23	1.15	1.92
(1,339)	1:343:A:LEU:N	1:343:A:LEU:CA	1:343:A:LEU:C	1:344:A:ASP:N	11	2.6	1.1	2.34
(1,314)	1:318:A:VAL:N	1:318:A:VAL:CA	1:318:A:VAL:C	1:319:A:GLN:N	10	3.15	1.74	3.12
(1,398)	1:404:A:SER:N	1:404:A:SER:CA	1:404:A:SER:C	1:405:A:ARG:N	10	2.79	1.15	2.66
(1,283)	1:287:A:VAL:N	1:287:A:VAL:CA	1:287:A:VAL:C	1:288:A:ALA:N	10	1.55	0.35	1.52
(1,149)	1:402:A:GLY:C	1:403:A:LEU:N	1:403:A:LEU:CA	1:403:A:LEU:C	9	3.51	1.4	3.0
(1,293)	1:297:A:MET:N	1:297:A:MET:CA	1:297:A:MET:C	1:298:A:GLU:N	9	2.46	1.42	2.15
(1,323)	1:327:A:GLU:N	1:327:A:GLU:CA	1:327:A:GLU:C	1:328:A:PRO:N	9	2.17	1.35	1.68
(1,484)	1:504:A:SER:N	1:504:A:SER:CA	1:504:A:SER:C	1:505:A:PHE:N	8	3.99	0.83	3.72

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,12)	1:260:A:ASP:C	1:261:A:ILE:N	1:261:A:ILE:CA	1:261:A:ILE:C	8	3.24	0.76	3.14
(1,456)	1:476:A:ARG:N	1:476:A:ARG:CA	1:476:A:ARG:C	1:477:A:MET:N	8	2.92	1.46	2.25
(1,31)	1:279:A:VAL:C	1:280:A:TRP:N	1:280:A:TRP:CA	1:280:A:TRP:C	8	2.29	0.98	2.08
(1,292)	1:296:A:THR:N	1:296:A:THR:CA	1:296:A:THR:C	1:297:A:MET:N	8	2.1	0.91	1.86
(1,6)	1:254:A:TRP:C	1:255:A:GLU:N	1:255:A:GLU:CA	1:255:A:GLU:C	7	5.84	0.93	5.95
(1,376)	1:380:A:HIS:N	1:380:A:HIS:CA	1:380:A:HIS:C	1:381:A:ARG:N	7	4.71	3.73	3.17
(1,478)	1:498:A:ASN:N	1:498:A:ASN:CA	1:498:A:ASN:C	1:499:A:PRO:N	7	3.21	1.35	2.97
(1,401)	1:409:A:GLY:N	1:409:A:GLY:CA	1:409:A:GLY:C	1:410:A:ASP:N	7	3.13	1.17	3.48
(1,189)	1:456:A:MET:C	1:457:A:SER:N	1:457:A:SER:CA	1:457:A:SER:C	7	2.65	1.12	2.35
(1,494)	1:514:A:THR:N	1:514:A:THR:CA	1:514:A:THR:C	1:515:A:MET:N	7	2.06	1.16	1.64
(1,379)	1:383:A:LEU:N	1:383:A:LEU:CA	1:383:A:LEU:C	1:384:A:ALA:N	6	3.83	0.69	3.84
(1,482)	1:502:A:ARG:N	1:502:A:ARG:CA	1:502:A:ARG:C	1:503:A:PRO:N	6	3.54	2.0	2.69
(1,325)	1:329:A:PRO:N	1:329:A:PRO:CA	1:329:A:PRO:C	1:330:A:PHE:N	6	2.22	0.6	2.32
(1,50)	1:298:A:GLU:C	1:299:A:VAL:N	1:299:A:VAL:CA	1:299:A:VAL:C	6	1.88	0.44	1.99
(1,464)	1:484:A:PRO:N	1:484:A:PRO:CA	1:484:A:PRO:C	1:485:A:GLU:N	6	1.85	0.42	1.94
(1,397)	1:403:A:LEU:N	1:403:A:LEU:CA	1:403:A:LEU:C	1:404:A:SER:N	5	4.55	1.78	5.03
(1,457)	1:477:A:MET:N	1:477:A:MET:CA	1:477:A:MET:C	1:478:A:GLU:N	5	3.26	1.62	2.81
(1,251)	1:255:A:GLU:N	1:255:A:GLU:CA	1:255:A:GLU:C	1:256:A:MET:N	5	3.25	0.32	3.28
(1,488)	1:508:A:ILE:N	1:508:A:ILE:CA	1:508:A:ILE:C	1:509:A:HIS:N	5	3.24	1.77	2.34
(1,414)	1:434:A:LYS:N	1:434:A:LYS:CA	1:434:A:LYS:C	1:435:A:PHE:N	5	3.17	1.67	2.1
(1,437)	1:457:A:SER:N	1:457:A:SER:CA	1:457:A:SER:C	1:458:A:PRO:N	5	2.86	1.22	2.82
(1,402)	1:412:A:TYR:N	1:412:A:TYR:CA	1:412:A:TYR:C	1:413:A:THR:N	5	2.8	1.25	2.7
(1,485)	1:505:A:PHE:N	1:505:A:PHE:CA	1:505:A:PHE:C	1:506:A:ALA:N	5	2.76	0.68	2.67
(1,326)	1:330:A:PHE:N	1:330:A:PHE:CA	1:330:A:PHE:C	1:331:A:TYR:N	5	2.25	0.71	2.62
(1,374)	1:378:A:PHE:N	1:378:A:PHE:CA	1:378:A:PHE:C	1:379:A:ILE:N	5	2.25	0.87	2.18
(1,150)	1:403:A:LEU:C	1:404:A:SER:N	1:404:A:SER:CA	1:404:A:SER:C	5	2.16	0.65	2.55
(1,357)	1:361:A:TYR:N	1:361:A:TYR:CA	1:361:A:TYR:C	1:362:A:MET:N	5	2.12	1.41	1.44
(1,403)	1:423:A:LYS:N	1:423:A:LYS:CA	1:423:A:LYS:C	1:424:A:TRP:N	5	1.86	0.77	1.49
(1,475)	1:495:A:TRP:N	1:495:A:TRP:CA	1:495:A:TRP:C	1:496:A:GLN:N	4	5.28	3.16	3.73
(1,404)	1:424:A:TRP:N	1:424:A:TRP:CA	1:424:A:TRP:C	1:425:A:THR:N	4	4.53	2.12	3.72
(1,154)	1:409:A:GLY:C	1:410:A:ASP:N	1:410:A:ASP:CA	1:410:A:ASP:C	4	3.86	1.7	4.33
(1,307)	1:311:A:GLU:N	1:311:A:GLU:CA	1:311:A:GLU:C	1:312:A:ILE:N	4	2.76	1.29	2.72
(1,269)	1:273:A:GLY:N	1:273:A:GLY:CA	1:273:A:GLY:C	1:274:A:GLU:N	4	2.59	1.71	1.78
(1,287)	1:291:A:THR:N	1:291:A:THR:CA	1:291:A:THR:C	1:292:A:LEU:N	4	2.56	1.09	2.53
(1,271)	1:275:A:VAL:N	1:275:A:VAL:CA	1:275:A:VAL:C	1:276:A:TYR:N	4	2.36	0.83	2.13
(1,7)	1:255:A:GLU:C	1:256:A:MET:N	1:256:A:MET:CA	1:256:A:MET:C	4	2.34	0.77	2.16
(1,64)	1:312:A:ILE:C	1:313:A:LYS:N	1:313:A:LYS:CA	1:313:A:LYS:C	4	1.98	0.67	1.92
(1,483)	1:503:A:PRO:N	1:503:A:PRO:CA	1:503:A:PRO:C	1:504:A:SER:N	4	1.78	0.64	1.48
(1,434)	1:454:A:TYR:N	1:454:A:TYR:CA	1:454:A:TYR:C	1:455:A:GLY:N	4	1.74	0.62	1.7
(1,242)	1:515:A:MET:C	1:516:A:PHE:N	1:516:A:PHE:CA	1:516:A:PHE:C	4	1.74	0.53	1.81
(1,204)	1:473:A:LYS:C	1:474:A:ASP:N	1:474:A:ASP:CA	1:474:A:ASP:C	4	1.74	0.66	1.47
(1,409)	1:429:A:SER:N	1:429:A:SER:CA	1:429:A:SER:C	1:430:A:LEU:N	4	1.72	0.28	1.76
(1,197)	1:466:A:GLN:C	1:467:A:VAL:N	1:467:A:VAL:CA	1:467:A:VAL:C	4	1.39	0.17	1.46
(1,377)	1:381:A:ARG:N	1:381:A:ARG:CA	1:381:A:ARG:C	1:382:A:ASP:N	3	3.8	2.38	3.4
(1,130)	1:381:A:ARG:C	1:382:A:ASP:N	1:382:A:ASP:CA	1:382:A:ASP:C	3	3.28	1.61	2.36
(1,124)	1:375:A:LYS:C	1:376:A:LYS:N	1:376:A:LYS:CA	1:376:A:LYS:C	3	2.9	0.84	2.66
(1,274)	1:278:A:GLY:N	1:278:A:GLY:CA	1:278:A:GLY:C	1:279:A:VAL:N	3	2.89	0.98	2.62
(1,205)	1:474:A:ASP:C	1:475:A:TYR:N	1:475:A:TYR:CA	1:475:A:TYR:C	3	2.82	0.89	2.45
(1,453)	1:473:A:LYS:N	1:473:A:LYS:CA	1:473:A:LYS:C	1:474:A:ASP:N	3	2.53	1.02	2.75
(1,495)	1:515:A:MET:N	1:515:A:MET:CA	1:515:A:MET:C	1:516:A:PHE:N	3	2.32	1.0	1.91
(1,459)	1:479:A:ARG:N	1:479:A:ARG:CA	1:479:A:ARG:C	1:480:A:PRO:N	3	2.31	1.32	1.56

Continued on next page...

Continued from previous page...

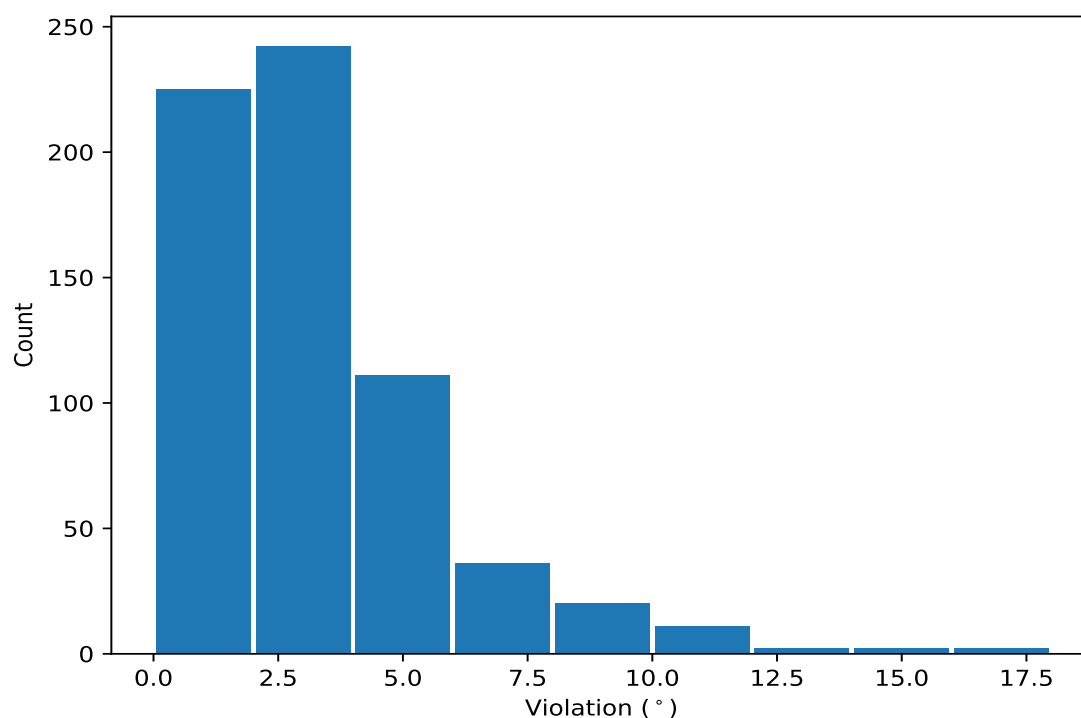
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,395)	1:401:A:PHE:N	1:401:A:PHE:CA	1:401:A:PHE:C	1:402:A:GLY:N	3	2.29	0.36	2.06
(1,393)	1:397:A:LYS:N	1:397:A:LYS:CA	1:397:A:LYS:C	1:398:A:VAL:N	3	2.27	0.72	2.49
(1,43)	1:291:A:THR:C	1:292:A:LEU:N	1:292:A:LEU:CA	1:292:A:LEU:C	3	2.24	1.03	1.69
(1,252)	1:256:A:MET:N	1:256:A:MET:CA	1:256:A:MET:C	1:257:A:GLU:N	3	1.94	0.43	2.23
(1,378)	1:382:A:ASP:N	1:382:A:ASP:CA	1:382:A:ASP:C	1:383:A:LEU:N	3	1.76	0.31	1.56
(1,412)	1:432:A:TYR:N	1:432:A:TYR:CA	1:432:A:TYR:C	1:433:A:ASN:N	3	1.6	0.27	1.72
(1,331)	1:335:A:GLU:N	1:335:A:GLU:CA	1:335:A:GLU:C	1:336:A:PHE:N	3	1.5	0.56	1.11
(1,157)	1:423:A:LYS:C	1:424:A:TRP:N	1:424:A:TRP:CA	1:424:A:TRP:C	2	3.14	1.5	3.14
(1,248)	1:252:A:ASP:N	1:252:A:ASP:CA	1:252:A:ASP:C	1:253:A:LYS:N	2	2.96	0.39	2.96
(1,396)	1:402:A:GLY:N	1:402:A:GLY:CA	1:402:A:GLY:C	1:403:A:LEU:N	2	2.67	1.1	2.67
(1,132)	1:383:A:LEU:C	1:384:A:ALA:N	1:384:A:ALA:CA	1:384:A:ALA:C	2	2.25	0.13	2.25
(1,305)	1:309:A:LEU:N	1:309:A:LEU:CA	1:309:A:LEU:C	1:310:A:LYS:N	2	2.22	1.2	2.22
(1,420)	1:440:A:ASP:N	1:440:A:ASP:CA	1:440:A:ASP:C	1:441:A:VAL:N	2	2.05	0.48	2.05
(1,246)	1:250:A:ASN:N	1:250:A:ASN:CA	1:250:A:ASN:C	1:251:A:TYR:N	2	2.04	0.77	2.04
(1,458)	1:478:A:GLU:N	1:478:A:GLU:CA	1:478:A:GLU:C	1:479:A:ARG:N	2	2.0	0.44	2.0
(1,309)	1:313:A:LYS:N	1:313:A:LYS:CA	1:313:A:LYS:C	1:314:A:HIS:N	2	1.92	0.35	1.92
(1,84)	1:335:A:GLU:C	1:336:A:PHE:N	1:336:A:PHE:CA	1:336:A:PHE:C	2	1.81	0.2	1.81
(1,53)	1:301:A:GLU:C	1:302:A:PHE:N	1:302:A:PHE:CA	1:302:A:PHE:C	2	1.8	0.08	1.8
(1,471)	1:491:A:MET:N	1:491:A:MET:CA	1:491:A:MET:C	1:492:A:ARG:N	2	1.79	0.37	1.79
(1,371)	1:375:A:LYS:N	1:375:A:LYS:CA	1:375:A:LYS:C	1:376:A:LYS:N	2	1.68	0.44	1.68
(1,382)	1:386:A:ARG:N	1:386:A:ARG:CA	1:386:A:ARG:C	1:387:A:ASN:N	2	1.64	0.26	1.64
(1,2)	1:250:A:ASN:C	1:251:A:TYR:N	1:251:A:TYR:CA	1:251:A:TYR:C	2	1.56	0.48	1.56
(1,8)	1:256:A:MET:C	1:257:A:GLU:N	1:257:A:GLU:CA	1:257:A:GLU:C	2	1.52	0.01	1.52
(1,336)	1:340:A:GLY:N	1:340:A:GLY:CA	1:340:A:GLY:C	1:341:A:ASN:N	2	1.52	0.28	1.52
(1,267)	1:271:A:GLN:N	1:271:A:GLN:CA	1:271:A:GLN:C	1:272:A:TYR:N	2	1.5	0.1	1.5
(1,95)	1:346:A:LEU:C	1:347:A:ARG:N	1:347:A:ARG:CA	1:347:A:ARG:C	2	1.42	0.16	1.42
(1,366)	1:370:A:MET:N	1:370:A:MET:CA	1:370:A:MET:C	1:371:A:GLU:N	2	1.42	0.09	1.42
(1,312)	1:316:A:ASN:N	1:316:A:ASN:CA	1:316:A:ASN:C	1:317:A:LEU:N	2	1.08	0.07	1.08
(1,473)	1:493:A:ALA:N	1:493:A:ALA:CA	1:493:A:ALA:C	1:494:A:CYS:N	2	1.08	0.04	1.08
(1,16)	1:264:A:LYS:C	1:265:A:HIS:N	1:265:A:HIS:CA	1:265:A:HIS:C	2	1.08	0.05	1.08

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

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,155)	1:410:A:ASP:C	1:411:A:THR:N	1:411:A:THR:CA	1:411:A:THR:C	9	17.66
(1,155)	1:410:A:ASP:C	1:411:A:THR:N	1:411:A:THR:CA	1:411:A:THR:C	1	17.3
(1,155)	1:410:A:ASP:C	1:411:A:THR:N	1:411:A:THR:CA	1:411:A:THR:C	12	15.08
(1,155)	1:410:A:ASP:C	1:411:A:THR:N	1:411:A:THR:CA	1:411:A:THR:C	7	14.37
(1,151)	1:404:A:SER:C	1:405:A:ARG:N	1:405:A:ARG:CA	1:405:A:ARG:C	19	12.86
(1,147)	1:398:A:VAL:C	1:399:A:ALA:N	1:399:A:ALA:CA	1:399:A:ALA:C	15	12.42
(1,147)	1:398:A:VAL:C	1:399:A:ALA:N	1:399:A:ALA:CA	1:399:A:ALA:C	18	11.38
(1,147)	1:398:A:VAL:C	1:399:A:ALA:N	1:399:A:ALA:CA	1:399:A:ALA:C	7	11.34
(1,376)	1:380:A:HIS:N	1:380:A:HIS:CA	1:380:A:HIS:C	1:381:A:ARG:N	14	11.29
(1,148)	1:400:A:ASP:C	1:401:A:PHE:N	1:401:A:PHE:CA	1:401:A:PHE:C	18	11.15
(1,148)	1:400:A:ASP:C	1:401:A:PHE:N	1:401:A:PHE:CA	1:401:A:PHE:C	8	10.9
(1,151)	1:404:A:SER:C	1:405:A:ARG:N	1:405:A:ARG:CA	1:405:A:ARG:C	4	10.86
(1,151)	1:404:A:SER:C	1:405:A:ARG:N	1:405:A:ARG:CA	1:405:A:ARG:C	16	10.71
(1,475)	1:495:A:TRP:N	1:495:A:TRP:CA	1:495:A:TRP:C	1:496:A:GLN:N	18	10.67
(1,147)	1:398:A:VAL:C	1:399:A:ALA:N	1:399:A:ALA:CA	1:399:A:ALA:C	17	10.51
(1,151)	1:404:A:SER:C	1:405:A:ARG:N	1:405:A:ARG:CA	1:405:A:ARG:C	11	10.07
(1,147)	1:398:A:VAL:C	1:399:A:ALA:N	1:399:A:ALA:CA	1:399:A:ALA:C	8	10.03
(1,30)	1:278:A:GLY:C	1:279:A:VAL:N	1:279:A:VAL:CA	1:279:A:VAL:C	6	9.91
(1,151)	1:404:A:SER:C	1:405:A:ARG:N	1:405:A:ARG:CA	1:405:A:ARG:C	15	9.88
(1,151)	1:404:A:SER:C	1:405:A:ARG:N	1:405:A:ARG:CA	1:405:A:ARG:C	2	9.77
(1,147)	1:398:A:VAL:C	1:399:A:ALA:N	1:399:A:ALA:CA	1:399:A:ALA:C	6	9.67

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,151)	1:404:A:SER:C	1:405:A:ARG:N	1:405:A:ARG:CA	1:405:A:ARG:C	17	9.65
(1,151)	1:404:A:SER:C	1:405:A:ARG:N	1:405:A:ARG:CA	1:405:A:ARG:C	8	9.35
(1,147)	1:398:A:VAL:C	1:399:A:ALA:N	1:399:A:ALA:CA	1:399:A:ALA:C	2	9.31
(1,156)	1:422:A:ILE:C	1:423:A:LYS:N	1:423:A:LYS:CA	1:423:A:LYS:C	13	9.3
(1,147)	1:398:A:VAL:C	1:399:A:ALA:N	1:399:A:ALA:CA	1:399:A:ALA:C	20	9.17
(1,151)	1:404:A:SER:C	1:405:A:ARG:N	1:405:A:ARG:CA	1:405:A:ARG:C	6	9.11
(1,147)	1:398:A:VAL:C	1:399:A:ALA:N	1:399:A:ALA:CA	1:399:A:ALA:C	10	8.92
(1,148)	1:400:A:ASP:C	1:401:A:PHE:N	1:401:A:PHE:CA	1:401:A:PHE:C	6	8.85
(1,147)	1:398:A:VAL:C	1:399:A:ALA:N	1:399:A:ALA:CA	1:399:A:ALA:C	9	8.85
(1,147)	1:398:A:VAL:C	1:399:A:ALA:N	1:399:A:ALA:CA	1:399:A:ALA:C	4	8.44
(1,30)	1:278:A:GLY:C	1:279:A:VAL:N	1:279:A:VAL:CA	1:279:A:VAL:C	5	8.44
(1,147)	1:398:A:VAL:C	1:399:A:ALA:N	1:399:A:ALA:CA	1:399:A:ALA:C	5	8.3
(1,148)	1:400:A:ASP:C	1:401:A:PHE:N	1:401:A:PHE:CA	1:401:A:PHE:C	14	8.14
(1,294)	1:298:A:GLU:N	1:298:A:GLU:CA	1:298:A:GLU:C	1:299:A:VAL:N	14	8.1
(1,404)	1:424:A:TRP:N	1:424:A:TRP:CA	1:424:A:TRP:C	1:425:A:THR:N	20	8.08
(1,394)	1:400:A:ASP:N	1:400:A:ASP:CA	1:400:A:ASP:C	1:401:A:PHE:N	18	8.05
(1,147)	1:398:A:VAL:C	1:399:A:ALA:N	1:399:A:ALA:CA	1:399:A:ALA:C	12	7.99
(1,376)	1:380:A:HIS:N	1:380:A:HIS:CA	1:380:A:HIS:C	1:381:A:ARG:N	18	7.97
(1,148)	1:400:A:ASP:C	1:401:A:PHE:N	1:401:A:PHE:CA	1:401:A:PHE:C	17	7.96
(1,30)	1:278:A:GLY:C	1:279:A:VAL:N	1:279:A:VAL:CA	1:279:A:VAL:C	2	7.95
(1,148)	1:400:A:ASP:C	1:401:A:PHE:N	1:401:A:PHE:CA	1:401:A:PHE:C	10	7.94
(1,147)	1:398:A:VAL:C	1:399:A:ALA:N	1:399:A:ALA:CA	1:399:A:ALA:C	1	7.9
(1,147)	1:398:A:VAL:C	1:399:A:ALA:N	1:399:A:ALA:CA	1:399:A:ALA:C	3	7.86
(1,147)	1:398:A:VAL:C	1:399:A:ALA:N	1:399:A:ALA:CA	1:399:A:ALA:C	14	7.81
(1,294)	1:298:A:GLU:N	1:298:A:GLU:CA	1:298:A:GLU:C	1:299:A:VAL:N	8	7.74
(1,338)	1:342:A:LEU:N	1:342:A:LEU:CA	1:342:A:LEU:C	1:343:A:LEU:N	10	7.68
(1,394)	1:400:A:ASP:N	1:400:A:ASP:CA	1:400:A:ASP:C	1:401:A:PHE:N	9	7.31
(1,6)	1:254:A:TRP:C	1:255:A:GLU:N	1:255:A:GLU:CA	1:255:A:GLU:C	19	7.26
(1,151)	1:404:A:SER:C	1:405:A:ARG:N	1:405:A:ARG:CA	1:405:A:ARG:C	13	7.2
(1,151)	1:404:A:SER:C	1:405:A:ARG:N	1:405:A:ARG:CA	1:405:A:ARG:C	12	7.15
(1,155)	1:410:A:ASP:C	1:411:A:THR:N	1:411:A:THR:CA	1:411:A:THR:C	18	7.06
(1,147)	1:398:A:VAL:C	1:399:A:ALA:N	1:399:A:ALA:CA	1:399:A:ALA:C	13	6.96
(1,30)	1:278:A:GLY:C	1:279:A:VAL:N	1:279:A:VAL:CA	1:279:A:VAL:C	17	6.92
(1,338)	1:342:A:LEU:N	1:342:A:LEU:CA	1:342:A:LEU:C	1:343:A:LEU:N	7	6.91
(1,397)	1:403:A:LEU:N	1:403:A:LEU:CA	1:403:A:LEU:C	1:404:A:SER:N	10	6.9
(1,377)	1:381:A:ARG:N	1:381:A:ARG:CA	1:381:A:ARG:C	1:382:A:ASP:N	14	6.89
(1,155)	1:410:A:ASP:C	1:411:A:THR:N	1:411:A:THR:CA	1:411:A:THR:C	10	6.86
(1,6)	1:254:A:TRP:C	1:255:A:GLU:N	1:255:A:GLU:CA	1:255:A:GLU:C	18	6.86
(1,376)	1:380:A:HIS:N	1:380:A:HIS:CA	1:380:A:HIS:C	1:381:A:ARG:N	15	6.85
(1,30)	1:278:A:GLY:C	1:279:A:VAL:N	1:279:A:VAL:CA	1:279:A:VAL:C	3	6.8
(1,30)	1:278:A:GLY:C	1:279:A:VAL:N	1:279:A:VAL:CA	1:279:A:VAL:C	8	6.55
(1,482)	1:502:A:ARG:N	1:502:A:ARG:CA	1:502:A:ARG:C	1:503:A:PRO:N	3	6.54
(1,147)	1:398:A:VAL:C	1:399:A:ALA:N	1:399:A:ALA:CA	1:399:A:ALA:C	19	6.48
(1,148)	1:400:A:ASP:C	1:401:A:PHE:N	1:401:A:PHE:CA	1:401:A:PHE:C	13	6.43
(1,314)	1:318:A:VAL:N	1:318:A:VAL:CA	1:318:A:VAL:C	1:319:A:GLN:N	4	6.39
(1,148)	1:400:A:ASP:C	1:401:A:PHE:N	1:401:A:PHE:CA	1:401:A:PHE:C	15	6.39
(1,294)	1:298:A:GLU:N	1:298:A:GLU:CA	1:298:A:GLU:C	1:299:A:VAL:N	7	6.29
(1,151)	1:404:A:SER:C	1:405:A:ARG:N	1:405:A:ARG:CA	1:405:A:ARG:C	18	6.18
(1,394)	1:400:A:ASP:N	1:400:A:ASP:CA	1:400:A:ASP:C	1:401:A:PHE:N	1	6.09
(1,6)	1:254:A:TRP:C	1:255:A:GLU:N	1:255:A:GLU:CA	1:255:A:GLU:C	9	6.02
(1,394)	1:400:A:ASP:N	1:400:A:ASP:CA	1:400:A:ASP:C	1:401:A:PHE:N	7	6.01

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,293)	1:297:A:MET:N	1:297:A:MET:CA	1:297:A:MET:C	1:298:A:GLU:N	18	6.0
(1,394)	1:400:A:ASP:N	1:400:A:ASP:CA	1:400:A:ASP:C	1:401:A:PHE:N	10	5.99
(1,482)	1:502:A:ARG:N	1:502:A:ARG:CA	1:502:A:ARG:C	1:503:A:PRO:N	11	5.95
(1,148)	1:400:A:ASP:C	1:401:A:PHE:N	1:401:A:PHE:CA	1:401:A:PHE:C	7	5.95
(1,6)	1:254:A:TRP:C	1:255:A:GLU:N	1:255:A:GLU:CA	1:255:A:GLU:C	17	5.95
(1,148)	1:400:A:ASP:C	1:401:A:PHE:N	1:401:A:PHE:CA	1:401:A:PHE:C	9	5.93
(1,155)	1:410:A:ASP:C	1:411:A:THR:N	1:411:A:THR:CA	1:411:A:THR:C	2	5.89
(1,414)	1:434:A:LYS:N	1:434:A:LYS:CA	1:434:A:LYS:C	1:435:A:PHE:N	9	5.88
(1,30)	1:278:A:GLY:C	1:279:A:VAL:N	1:279:A:VAL:CA	1:279:A:VAL:C	11	5.88
(1,457)	1:477:A:MET:N	1:477:A:MET:CA	1:477:A:MET:C	1:478:A:GLU:N	11	5.83
(1,151)	1:404:A:SER:C	1:405:A:ARG:N	1:405:A:ARG:CA	1:405:A:ARG:C	3	5.78
(1,394)	1:400:A:ASP:N	1:400:A:ASP:CA	1:400:A:ASP:C	1:401:A:PHE:N	8	5.76
(1,338)	1:342:A:LEU:N	1:342:A:LEU:CA	1:342:A:LEU:C	1:343:A:LEU:N	17	5.7
(1,478)	1:498:A:ASN:N	1:498:A:ASN:CA	1:498:A:ASN:C	1:499:A:PRO:N	19	5.69
(1,394)	1:400:A:ASP:N	1:400:A:ASP:CA	1:400:A:ASP:C	1:401:A:PHE:N	5	5.68
(1,323)	1:327:A:GLU:N	1:327:A:GLU:CA	1:327:A:GLU:C	1:328:A:PRO:N	14	5.68
(1,154)	1:409:A:GLY:C	1:410:A:ASP:N	1:410:A:ASP:CA	1:410:A:ASP:C	1	5.64
(1,488)	1:508:A:ILE:N	1:508:A:ILE:CA	1:508:A:ILE:C	1:509:A:HIS:N	12	5.58
(1,155)	1:410:A:ASP:C	1:411:A:THR:N	1:411:A:THR:CA	1:411:A:THR:C	6	5.58
(1,397)	1:403:A:LEU:N	1:403:A:LEU:CA	1:403:A:LEU:C	1:404:A:SER:N	20	5.56
(1,130)	1:381:A:ARG:C	1:382:A:ASP:N	1:382:A:ASP:CA	1:382:A:ASP:C	14	5.54
(1,269)	1:273:A:GLY:N	1:273:A:GLY:CA	1:273:A:GLY:C	1:274:A:GLU:N	9	5.53
(1,147)	1:398:A:VAL:C	1:399:A:ALA:N	1:399:A:ALA:CA	1:399:A:ALA:C	11	5.5
(1,484)	1:504:A:SER:N	1:504:A:SER:CA	1:504:A:SER:C	1:505:A:PHE:N	5	5.48
(1,30)	1:278:A:GLY:C	1:279:A:VAL:N	1:279:A:VAL:CA	1:279:A:VAL:C	7	5.48
(1,30)	1:278:A:GLY:C	1:279:A:VAL:N	1:279:A:VAL:CA	1:279:A:VAL:C	10	5.47
(1,394)	1:400:A:ASP:N	1:400:A:ASP:CA	1:400:A:ASP:C	1:401:A:PHE:N	20	5.46
(1,294)	1:298:A:GLU:N	1:298:A:GLU:CA	1:298:A:GLU:C	1:299:A:VAL:N	3	5.45
(1,314)	1:318:A:VAL:N	1:318:A:VAL:CA	1:318:A:VAL:C	1:319:A:GLN:N	11	5.44
(1,149)	1:402:A:GLY:C	1:403:A:LEU:N	1:403:A:LEU:CA	1:403:A:LEU:C	5	5.41
(1,338)	1:342:A:LEU:N	1:342:A:LEU:CA	1:342:A:LEU:C	1:343:A:LEU:N	13	5.4
(1,456)	1:476:A:ARG:N	1:476:A:ARG:CA	1:476:A:ARG:C	1:477:A:MET:N	1	5.39
(1,365)	1:369:A:ALA:N	1:369:A:ALA:CA	1:369:A:ALA:C	1:370:A:MET:N	18	5.36
(1,189)	1:456:A:MET:C	1:457:A:SER:N	1:457:A:SER:CA	1:457:A:SER:C	16	5.31
(1,338)	1:342:A:LEU:N	1:342:A:LEU:CA	1:342:A:LEU:C	1:343:A:LEU:N	3	5.29
(1,149)	1:402:A:GLY:C	1:403:A:LEU:N	1:403:A:LEU:CA	1:403:A:LEU:C	14	5.27
(1,149)	1:402:A:GLY:C	1:403:A:LEU:N	1:403:A:LEU:CA	1:403:A:LEU:C	17	5.27
(1,30)	1:278:A:GLY:C	1:279:A:VAL:N	1:279:A:VAL:CA	1:279:A:VAL:C	13	5.26
(1,147)	1:398:A:VAL:C	1:399:A:ALA:N	1:399:A:ALA:CA	1:399:A:ALA:C	16	5.25
(1,148)	1:400:A:ASP:C	1:401:A:PHE:N	1:401:A:PHE:CA	1:401:A:PHE:C	3	5.23
(1,6)	1:254:A:TRP:C	1:255:A:GLU:N	1:255:A:GLU:CA	1:255:A:GLU:C	8	5.23
(1,401)	1:409:A:GLY:N	1:409:A:GLY:CA	1:409:A:GLY:C	1:410:A:ASP:N	5	5.21
(1,6)	1:254:A:TRP:C	1:255:A:GLU:N	1:255:A:GLU:CA	1:255:A:GLU:C	14	5.21
(1,30)	1:278:A:GLY:C	1:279:A:VAL:N	1:279:A:VAL:CA	1:279:A:VAL:C	4	5.18
(1,488)	1:508:A:ILE:N	1:508:A:ILE:CA	1:508:A:ILE:C	1:509:A:HIS:N	7	5.16
(1,30)	1:278:A:GLY:C	1:279:A:VAL:N	1:279:A:VAL:CA	1:279:A:VAL:C	14	5.11
(1,484)	1:504:A:SER:N	1:504:A:SER:CA	1:504:A:SER:C	1:505:A:PHE:N	3	5.1
(1,294)	1:298:A:GLU:N	1:298:A:GLU:CA	1:298:A:GLU:C	1:299:A:VAL:N	13	5.1
(1,148)	1:400:A:ASP:C	1:401:A:PHE:N	1:401:A:PHE:CA	1:401:A:PHE:C	12	5.07
(1,402)	1:412:A:TYR:N	1:412:A:TYR:CA	1:412:A:TYR:C	1:413:A:THR:N	17	5.06
(1,148)	1:400:A:ASP:C	1:401:A:PHE:N	1:401:A:PHE:CA	1:401:A:PHE:C	4	5.06

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,30)	1:278:A:GLY:C	1:279:A:VAL:N	1:279:A:VAL:CA	1:279:A:VAL:C	16	5.05
(1,296)	1:300:A:GLU:N	1:300:A:GLU:CA	1:300:A:GLU:C	1:301:A:GLU:N	5	5.04
(1,456)	1:476:A:ARG:N	1:476:A:ARG:CA	1:476:A:ARG:C	1:477:A:MET:N	2	5.03
(1,397)	1:403:A:LEU:N	1:403:A:LEU:CA	1:403:A:LEU:C	1:404:A:SER:N	14	5.03
(1,394)	1:400:A:ASP:N	1:400:A:ASP:CA	1:400:A:ASP:C	1:401:A:PHE:N	17	5.0
(1,338)	1:342:A:LEU:N	1:342:A:LEU:CA	1:342:A:LEU:C	1:343:A:LEU:N	5	4.99
(1,155)	1:410:A:ASP:C	1:411:A:THR:N	1:411:A:THR:CA	1:411:A:THR:C	19	4.98
(1,151)	1:404:A:SER:C	1:405:A:ARG:N	1:405:A:ARG:CA	1:405:A:ARG:C	1	4.96
(1,357)	1:361:A:TYR:N	1:361:A:TYR:CA	1:361:A:TYR:C	1:362:A:MET:N	9	4.94
(1,296)	1:300:A:GLU:N	1:300:A:GLU:CA	1:300:A:GLU:C	1:301:A:GLU:N	9	4.94
(1,151)	1:404:A:SER:C	1:405:A:ARG:N	1:405:A:ARG:CA	1:405:A:ARG:C	14	4.93
(1,437)	1:457:A:SER:N	1:457:A:SER:CA	1:457:A:SER:C	1:458:A:PRO:N	3	4.91
(1,294)	1:298:A:GLU:N	1:298:A:GLU:CA	1:298:A:GLU:C	1:299:A:VAL:N	11	4.91
(1,296)	1:300:A:GLU:N	1:300:A:GLU:CA	1:300:A:GLU:C	1:301:A:GLU:N	4	4.84
(1,154)	1:409:A:GLY:C	1:410:A:ASP:N	1:410:A:ASP:CA	1:410:A:ASP:C	7	4.82
(1,379)	1:383:A:LEU:N	1:383:A:LEU:CA	1:383:A:LEU:C	1:384:A:ALA:N	9	4.8
(1,148)	1:400:A:ASP:C	1:401:A:PHE:N	1:401:A:PHE:CA	1:401:A:PHE:C	11	4.79
(1,494)	1:514:A:THR:N	1:514:A:THR:CA	1:514:A:THR:C	1:515:A:MET:N	14	4.78
(1,295)	1:299:A:VAL:N	1:299:A:VAL:CA	1:299:A:VAL:C	1:300:A:GLU:N	2	4.75
(1,294)	1:298:A:GLU:N	1:298:A:GLU:CA	1:298:A:GLU:C	1:299:A:VAL:N	18	4.75
(1,12)	1:260:A:ASP:C	1:261:A:ILE:N	1:261:A:ILE:CA	1:261:A:ILE:C	9	4.74
(1,339)	1:343:A:LEU:N	1:343:A:LEU:CA	1:343:A:LEU:C	1:344:A:ASP:N	10	4.73
(1,338)	1:342:A:LEU:N	1:342:A:LEU:CA	1:342:A:LEU:C	1:343:A:LEU:N	18	4.71
(1,399)	1:405:A:ARG:N	1:405:A:ARG:CA	1:405:A:ARG:C	1:406:A:LEU:N	4	4.64
(1,157)	1:423:A:LYS:C	1:424:A:TRP:N	1:424:A:TRP:CA	1:424:A:TRP:C	8	4.64
(1,478)	1:498:A:ASN:N	1:498:A:ASN:CA	1:498:A:ASN:C	1:499:A:PRO:N	11	4.62
(1,398)	1:404:A:SER:N	1:404:A:SER:CA	1:404:A:SER:C	1:405:A:ARG:N	19	4.6
(1,307)	1:311:A:GLU:N	1:311:A:GLU:CA	1:311:A:GLU:C	1:312:A:ILE:N	12	4.58
(1,295)	1:299:A:VAL:N	1:299:A:VAL:CA	1:299:A:VAL:C	1:300:A:GLU:N	16	4.57
(1,30)	1:278:A:GLY:C	1:279:A:VAL:N	1:279:A:VAL:CA	1:279:A:VAL:C	20	4.54
(1,30)	1:278:A:GLY:C	1:279:A:VAL:N	1:279:A:VAL:CA	1:279:A:VAL:C	15	4.51
(1,296)	1:300:A:GLU:N	1:300:A:GLU:CA	1:300:A:GLU:C	1:301:A:GLU:N	1	4.48
(1,338)	1:342:A:LEU:N	1:342:A:LEU:CA	1:342:A:LEU:C	1:343:A:LEU:N	20	4.47
(1,148)	1:400:A:ASP:C	1:401:A:PHE:N	1:401:A:PHE:CA	1:401:A:PHE:C	1	4.47
(1,30)	1:278:A:GLY:C	1:279:A:VAL:N	1:279:A:VAL:CA	1:279:A:VAL:C	1	4.44
(1,365)	1:369:A:ALA:N	1:369:A:ALA:CA	1:369:A:ALA:C	1:370:A:MET:N	10	4.43
(1,475)	1:495:A:TRP:N	1:495:A:TRP:CA	1:495:A:TRP:C	1:496:A:GLN:N	17	4.4
(1,379)	1:383:A:LEU:N	1:383:A:LEU:CA	1:383:A:LEU:C	1:384:A:ALA:N	1	4.4
(1,394)	1:400:A:ASP:N	1:400:A:ASP:CA	1:400:A:ASP:C	1:401:A:PHE:N	6	4.38
(1,6)	1:254:A:TRP:C	1:255:A:GLU:N	1:255:A:GLU:CA	1:255:A:GLU:C	15	4.38
(1,414)	1:434:A:LYS:N	1:434:A:LYS:CA	1:434:A:LYS:C	1:435:A:PHE:N	13	4.37
(1,314)	1:318:A:VAL:N	1:318:A:VAL:CA	1:318:A:VAL:C	1:319:A:GLN:N	5	4.37
(1,339)	1:343:A:LEU:N	1:343:A:LEU:CA	1:343:A:LEU:C	1:344:A:ASP:N	12	4.31
(1,148)	1:400:A:ASP:C	1:401:A:PHE:N	1:401:A:PHE:CA	1:401:A:PHE:C	20	4.3
(1,457)	1:477:A:MET:N	1:477:A:MET:CA	1:477:A:MET:C	1:478:A:GLU:N	6	4.27
(1,394)	1:400:A:ASP:N	1:400:A:ASP:CA	1:400:A:ASP:C	1:401:A:PHE:N	2	4.24
(1,274)	1:278:A:GLY:N	1:278:A:GLY:CA	1:278:A:GLY:C	1:279:A:VAL:N	6	4.21
(1,484)	1:504:A:SER:N	1:504:A:SER:CA	1:504:A:SER:C	1:505:A:PHE:N	17	4.17
(1,459)	1:479:A:ARG:N	1:479:A:ARG:CA	1:479:A:ARG:C	1:480:A:PRO:N	9	4.16
(1,404)	1:424:A:TRP:N	1:424:A:TRP:CA	1:424:A:TRP:C	1:425:A:THR:N	3	4.14
(1,379)	1:383:A:LEU:N	1:383:A:LEU:CA	1:383:A:LEU:C	1:384:A:ALA:N	19	4.09

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,296)	1:300:A:GLU:N	1:300:A:GLU:CA	1:300:A:GLU:C	1:301:A:GLU:N	12	4.07
(1,148)	1:400:A:ASP:C	1:401:A:PHE:N	1:401:A:PHE:CA	1:401:A:PHE:C	19	4.07
(1,110)	1:361:A:TYR:C	1:362:A:MET:N	1:362:A:MET:CA	1:362:A:MET:C	9	4.07
(1,30)	1:278:A:GLY:C	1:279:A:VAL:N	1:279:A:VAL:CA	1:279:A:VAL:C	18	4.06
(1,436)	1:456:A:MET:N	1:456:A:MET:CA	1:456:A:MET:C	1:457:A:SER:N	2	4.05
(1,205)	1:474:A:ASP:C	1:475:A:TYR:N	1:475:A:TYR:CA	1:475:A:TYR:C	11	4.05
(1,124)	1:375:A:LYS:C	1:376:A:LYS:N	1:376:A:LYS:CA	1:376:A:LYS:C	10	4.02
(1,365)	1:369:A:ALA:N	1:369:A:ALA:CA	1:369:A:ALA:C	1:370:A:MET:N	8	4.0
(1,338)	1:342:A:LEU:N	1:342:A:LEU:CA	1:342:A:LEU:C	1:343:A:LEU:N	8	4.0
(1,287)	1:291:A:THR:N	1:291:A:THR:CA	1:291:A:THR:C	1:292:A:LEU:N	14	4.0
(1,398)	1:404:A:SER:N	1:404:A:SER:CA	1:404:A:SER:C	1:405:A:ARG:N	12	3.95
(1,31)	1:279:A:VAL:C	1:280:A:TRP:N	1:280:A:TRP:CA	1:280:A:TRP:C	11	3.95
(1,401)	1:409:A:GLY:N	1:409:A:GLY:CA	1:409:A:GLY:C	1:410:A:ASP:N	1	3.91
(1,338)	1:342:A:LEU:N	1:342:A:LEU:CA	1:342:A:LEU:C	1:343:A:LEU:N	19	3.88
(1,454)	1:474:A:ASP:N	1:474:A:ASP:CA	1:474:A:ASP:C	1:475:A:TYR:N	11	3.87
(1,398)	1:404:A:SER:N	1:404:A:SER:CA	1:404:A:SER:C	1:405:A:ARG:N	17	3.86
(1,398)	1:404:A:SER:N	1:404:A:SER:CA	1:404:A:SER:C	1:405:A:ARG:N	16	3.85
(1,154)	1:409:A:GLY:C	1:410:A:ASP:N	1:410:A:ASP:CA	1:410:A:ASP:C	9	3.84
(1,374)	1:378:A:PHE:N	1:378:A:PHE:CA	1:378:A:PHE:C	1:379:A:ILE:N	18	3.83
(1,484)	1:504:A:SER:N	1:504:A:SER:CA	1:504:A:SER:C	1:505:A:PHE:N	19	3.82
(1,31)	1:279:A:VAL:C	1:280:A:TRP:N	1:280:A:TRP:CA	1:280:A:TRP:C	14	3.81
(1,485)	1:505:A:PHE:N	1:505:A:PHE:CA	1:505:A:PHE:C	1:506:A:ALA:N	11	3.78
(1,396)	1:402:A:GLY:N	1:402:A:GLY:CA	1:402:A:GLY:C	1:403:A:LEU:N	14	3.77
(1,296)	1:300:A:GLU:N	1:300:A:GLU:CA	1:300:A:GLU:C	1:301:A:GLU:N	20	3.76
(1,294)	1:298:A:GLU:N	1:298:A:GLU:CA	1:298:A:GLU:C	1:299:A:VAL:N	10	3.75
(1,296)	1:300:A:GLU:N	1:300:A:GLU:CA	1:300:A:GLU:C	1:301:A:GLU:N	10	3.72
(1,251)	1:255:A:GLU:N	1:255:A:GLU:CA	1:255:A:GLU:C	1:256:A:MET:N	12	3.72
(1,12)	1:260:A:ASP:C	1:261:A:ILE:N	1:261:A:ILE:CA	1:261:A:ILE:C	7	3.72
(1,495)	1:515:A:MET:N	1:515:A:MET:CA	1:515:A:MET:C	1:516:A:PHE:N	2	3.7
(1,257)	1:261:A:ILE:N	1:261:A:ILE:CA	1:261:A:ILE:C	1:262:A:THR:N	8	3.69
(1,271)	1:275:A:VAL:N	1:275:A:VAL:CA	1:275:A:VAL:C	1:276:A:TYR:N	12	3.68
(1,43)	1:291:A:THR:C	1:292:A:LEU:N	1:292:A:LEU:CA	1:292:A:LEU:C	14	3.68
(1,394)	1:400:A:ASP:N	1:400:A:ASP:CA	1:400:A:ASP:C	1:401:A:PHE:N	3	3.67
(1,148)	1:400:A:ASP:C	1:401:A:PHE:N	1:401:A:PHE:CA	1:401:A:PHE:C	2	3.67
(1,453)	1:473:A:LYS:N	1:473:A:LYS:CA	1:473:A:LYS:C	1:474:A:ASP:N	4	3.65
(1,155)	1:410:A:ASP:C	1:411:A:THR:N	1:411:A:THR:CA	1:411:A:THR:C	15	3.65
(1,484)	1:504:A:SER:N	1:504:A:SER:CA	1:504:A:SER:C	1:505:A:PHE:N	12	3.63
(1,294)	1:298:A:GLU:N	1:298:A:GLU:CA	1:298:A:GLU:C	1:299:A:VAL:N	20	3.63
(1,484)	1:504:A:SER:N	1:504:A:SER:CA	1:504:A:SER:C	1:505:A:PHE:N	10	3.62
(1,365)	1:369:A:ALA:N	1:369:A:ALA:CA	1:369:A:ALA:C	1:370:A:MET:N	7	3.61
(1,379)	1:383:A:LEU:N	1:383:A:LEU:CA	1:383:A:LEU:C	1:384:A:ALA:N	11	3.6
(1,292)	1:296:A:THR:N	1:296:A:THR:CA	1:296:A:THR:C	1:297:A:MET:N	19	3.6
(1,30)	1:278:A:GLY:C	1:279:A:VAL:N	1:279:A:VAL:CA	1:279:A:VAL:C	19	3.6
(1,456)	1:476:A:ARG:N	1:476:A:ARG:CA	1:476:A:ARG:C	1:477:A:MET:N	5	3.58
(1,294)	1:298:A:GLU:N	1:298:A:GLU:CA	1:298:A:GLU:C	1:299:A:VAL:N	17	3.58
(1,155)	1:410:A:ASP:C	1:411:A:THR:N	1:411:A:THR:CA	1:411:A:THR:C	20	3.58
(1,12)	1:260:A:ASP:C	1:261:A:ILE:N	1:261:A:ILE:CA	1:261:A:ILE:C	12	3.58
(1,338)	1:342:A:LEU:N	1:342:A:LEU:CA	1:342:A:LEU:C	1:343:A:LEU:N	6	3.57
(1,7)	1:255:A:GLU:C	1:256:A:MET:N	1:256:A:MET:CA	1:256:A:MET:C	1	3.55
(1,314)	1:318:A:VAL:N	1:318:A:VAL:CA	1:318:A:VAL:C	1:319:A:GLN:N	16	3.53
(1,397)	1:403:A:LEU:N	1:403:A:LEU:CA	1:403:A:LEU:C	1:404:A:SER:N	6	3.52

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,401)	1:409:A:GLY:N	1:409:A:GLY:CA	1:409:A:GLY:C	1:410:A:ASP:N	7	3.5
(1,394)	1:400:A:ASP:N	1:400:A:ASP:CA	1:400:A:ASP:C	1:401:A:PHE:N	4	3.5
(1,401)	1:409:A:GLY:N	1:409:A:GLY:CA	1:409:A:GLY:C	1:410:A:ASP:N	9	3.48
(1,155)	1:410:A:ASP:C	1:411:A:THR:N	1:411:A:THR:CA	1:411:A:THR:C	13	3.48
(1,338)	1:342:A:LEU:N	1:342:A:LEU:CA	1:342:A:LEU:C	1:343:A:LEU:N	14	3.47
(1,149)	1:402:A:GLY:C	1:403:A:LEU:N	1:403:A:LEU:CA	1:403:A:LEU:C	10	3.45
(1,155)	1:410:A:ASP:C	1:411:A:THR:N	1:411:A:THR:CA	1:411:A:THR:C	11	3.44
(1,305)	1:309:A:LEU:N	1:309:A:LEU:CA	1:309:A:LEU:C	1:310:A:LYS:N	9	3.41
(1,379)	1:383:A:LEU:N	1:383:A:LEU:CA	1:383:A:LEU:C	1:384:A:ALA:N	5	3.4
(1,377)	1:381:A:ARG:N	1:381:A:ARG:CA	1:381:A:ARG:C	1:382:A:ASP:N	18	3.4
(1,403)	1:423:A:LYS:N	1:423:A:LYS:CA	1:423:A:LYS:C	1:424:A:TRP:N	8	3.36
(1,314)	1:318:A:VAL:N	1:318:A:VAL:CA	1:318:A:VAL:C	1:319:A:GLN:N	2	3.36
(1,293)	1:297:A:MET:N	1:297:A:MET:CA	1:297:A:MET:C	1:298:A:GLU:N	6	3.36
(1,251)	1:255:A:GLU:N	1:255:A:GLU:CA	1:255:A:GLU:C	1:256:A:MET:N	1	3.35
(1,248)	1:252:A:ASP:N	1:252:A:ASP:CA	1:252:A:ASP:C	1:253:A:LYS:N	19	3.35
(1,292)	1:296:A:THR:N	1:296:A:THR:CA	1:296:A:THR:C	1:297:A:MET:N	6	3.34
(1,151)	1:404:A:SER:C	1:405:A:ARG:N	1:405:A:ARG:CA	1:405:A:ARG:C	9	3.34
(1,38)	1:286:A:THR:C	1:287:A:VAL:N	1:287:A:VAL:CA	1:287:A:VAL:C	11	3.31
(1,404)	1:424:A:TRP:N	1:424:A:TRP:CA	1:424:A:TRP:C	1:425:A:THR:N	2	3.29
(1,251)	1:255:A:GLU:N	1:255:A:GLU:CA	1:255:A:GLU:C	1:256:A:MET:N	7	3.28
(1,485)	1:505:A:PHE:N	1:505:A:PHE:CA	1:505:A:PHE:C	1:506:A:ALA:N	7	3.26
(1,394)	1:400:A:ASP:N	1:400:A:ASP:CA	1:400:A:ASP:C	1:401:A:PHE:N	19	3.26
(1,339)	1:343:A:LEU:N	1:343:A:LEU:CA	1:343:A:LEU:C	1:344:A:ASP:N	20	3.26
(1,48)	1:296:A:THR:C	1:297:A:MET:N	1:297:A:MET:CA	1:297:A:MET:C	20	3.24
(1,12)	1:260:A:ASP:C	1:261:A:ILE:N	1:261:A:ILE:CA	1:261:A:ILE:C	11	3.24
(1,338)	1:342:A:LEU:N	1:342:A:LEU:CA	1:342:A:LEU:C	1:343:A:LEU:N	2	3.21
(1,294)	1:298:A:GLU:N	1:298:A:GLU:CA	1:298:A:GLU:C	1:299:A:VAL:N	5	3.21
(1,482)	1:502:A:ARG:N	1:502:A:ARG:CA	1:502:A:ARG:C	1:503:A:PRO:N	19	3.17
(1,376)	1:380:A:HIS:N	1:380:A:HIS:CA	1:380:A:HIS:C	1:381:A:ARG:N	9	3.17
(1,296)	1:300:A:GLU:N	1:300:A:GLU:CA	1:300:A:GLU:C	1:301:A:GLU:N	7	3.17
(1,365)	1:369:A:ALA:N	1:369:A:ALA:CA	1:369:A:ALA:C	1:370:A:MET:N	11	3.16
(1,287)	1:291:A:THR:N	1:291:A:THR:CA	1:291:A:THR:C	1:292:A:LEU:N	17	3.16
(1,251)	1:255:A:GLU:N	1:255:A:GLU:CA	1:255:A:GLU:C	1:256:A:MET:N	11	3.15
(1,478)	1:498:A:ASN:N	1:498:A:ASN:CA	1:498:A:ASN:C	1:499:A:PRO:N	15	3.1
(1,325)	1:329:A:PRO:N	1:329:A:PRO:CA	1:329:A:PRO:C	1:330:A:PHE:N	15	3.1
(1,437)	1:457:A:SER:N	1:457:A:SER:CA	1:457:A:SER:C	1:458:A:PRO:N	11	3.07
(1,484)	1:504:A:SER:N	1:504:A:SER:CA	1:504:A:SER:C	1:505:A:PHE:N	18	3.06
(1,475)	1:495:A:TRP:N	1:495:A:TRP:CA	1:495:A:TRP:C	1:496:A:GLN:N	7	3.06
(1,12)	1:260:A:ASP:C	1:261:A:ILE:N	1:261:A:ILE:CA	1:261:A:ILE:C	14	3.05
(1,484)	1:504:A:SER:N	1:504:A:SER:CA	1:504:A:SER:C	1:505:A:PHE:N	11	3.04
(1,338)	1:342:A:LEU:N	1:342:A:LEU:CA	1:342:A:LEU:C	1:343:A:LEU:N	4	3.04
(1,307)	1:311:A:GLU:N	1:311:A:GLU:CA	1:311:A:GLU:C	1:312:A:ILE:N	14	3.04
(1,339)	1:343:A:LEU:N	1:343:A:LEU:CA	1:343:A:LEU:C	1:344:A:ASP:N	13	3.02
(1,326)	1:330:A:PHE:N	1:330:A:PHE:CA	1:330:A:PHE:C	1:331:A:TYR:N	3	3.02
(1,322)	1:326:A:ARG:N	1:326:A:ARG:CA	1:326:A:ARG:C	1:327:A:GLU:N	12	3.02
(1,38)	1:286:A:THR:C	1:287:A:VAL:N	1:287:A:VAL:CA	1:287:A:VAL:C	4	3.02
(1,393)	1:397:A:LYS:N	1:397:A:LYS:CA	1:397:A:LYS:C	1:398:A:VAL:N	17	3.01
(1,338)	1:342:A:LEU:N	1:342:A:LEU:CA	1:342:A:LEU:C	1:343:A:LEU:N	11	3.01
(1,149)	1:402:A:GLY:C	1:403:A:LEU:N	1:403:A:LEU:CA	1:403:A:LEU:C	15	3.0
(1,475)	1:495:A:TRP:N	1:495:A:TRP:CA	1:495:A:TRP:C	1:496:A:GLN:N	14	2.98
(1,155)	1:410:A:ASP:C	1:411:A:THR:N	1:411:A:THR:CA	1:411:A:THR:C	16	2.98

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,64)	1:312:A:ILE:C	1:313:A:LYS:N	1:313:A:LYS:CA	1:313:A:LYS:C	4	2.98
(1,12)	1:260:A:ASP:C	1:261:A:ILE:N	1:261:A:ILE:CA	1:261:A:ILE:C	17	2.98
(1,478)	1:498:A:ASN:N	1:498:A:ASN:CA	1:498:A:ASN:C	1:499:A:PRO:N	10	2.97
(1,358)	1:362:A:MET:N	1:362:A:MET:CA	1:362:A:MET:C	1:363:A:ALA:N	16	2.97
(1,296)	1:300:A:GLU:N	1:300:A:GLU:CA	1:300:A:GLU:C	1:301:A:GLU:N	3	2.97
(1,229)	1:501:A:ASP:C	1:502:A:ARG:N	1:502:A:ARG:CA	1:502:A:ARG:C	9	2.93
(1,402)	1:412:A:TYR:N	1:412:A:TYR:CA	1:412:A:TYR:C	1:413:A:THR:N	20	2.92
(1,338)	1:342:A:LEU:N	1:342:A:LEU:CA	1:342:A:LEU:C	1:343:A:LEU:N	16	2.9
(1,314)	1:318:A:VAL:N	1:318:A:VAL:CA	1:318:A:VAL:C	1:319:A:GLN:N	18	2.89
(1,483)	1:503:A:PRO:N	1:503:A:PRO:CA	1:503:A:PRO:C	1:504:A:SER:N	7	2.88
(1,150)	1:403:A:LEU:C	1:404:A:SER:N	1:404:A:SER:CA	1:404:A:SER:C	7	2.88
(1,149)	1:402:A:GLY:C	1:403:A:LEU:N	1:403:A:LEU:CA	1:403:A:LEU:C	2	2.88
(1,148)	1:400:A:ASP:C	1:401:A:PHE:N	1:401:A:PHE:CA	1:401:A:PHE:C	16	2.87
(1,204)	1:473:A:LYS:C	1:474:A:ASP:N	1:474:A:ASP:CA	1:474:A:ASP:C	14	2.86
(1,437)	1:457:A:SER:N	1:457:A:SER:CA	1:457:A:SER:C	1:458:A:PRO:N	10	2.82
(1,398)	1:404:A:SER:N	1:404:A:SER:CA	1:404:A:SER:C	1:405:A:ARG:N	1	2.82
(1,457)	1:477:A:MET:N	1:477:A:MET:CA	1:477:A:MET:C	1:478:A:GLU:N	4	2.81
(1,339)	1:343:A:LEU:N	1:343:A:LEU:CA	1:343:A:LEU:C	1:344:A:ASP:N	5	2.81
(1,246)	1:250:A:ASN:N	1:250:A:ASN:CA	1:250:A:ASN:C	1:251:A:TYR:N	16	2.81
(1,395)	1:401:A:PHE:N	1:401:A:PHE:CA	1:401:A:PHE:C	1:402:A:GLY:N	18	2.8
(1,38)	1:286:A:THR:C	1:287:A:VAL:N	1:287:A:VAL:CA	1:287:A:VAL:C	2	2.8
(1,296)	1:300:A:GLU:N	1:300:A:GLU:CA	1:300:A:GLU:C	1:301:A:GLU:N	16	2.77
(1,296)	1:300:A:GLU:N	1:300:A:GLU:CA	1:300:A:GLU:C	1:301:A:GLU:N	8	2.76
(1,453)	1:473:A:LYS:N	1:473:A:LYS:CA	1:473:A:LYS:C	1:474:A:ASP:N	11	2.75
(1,251)	1:255:A:GLU:N	1:255:A:GLU:CA	1:255:A:GLU:C	1:256:A:MET:N	13	2.73
(1,326)	1:330:A:PHE:N	1:330:A:PHE:CA	1:330:A:PHE:C	1:331:A:TYR:N	4	2.72
(1,38)	1:286:A:THR:C	1:287:A:VAL:N	1:287:A:VAL:CA	1:287:A:VAL:C	10	2.72
(1,155)	1:410:A:ASP:C	1:411:A:THR:N	1:411:A:THR:CA	1:411:A:THR:C	14	2.71
(1,402)	1:412:A:TYR:N	1:412:A:TYR:CA	1:412:A:TYR:C	1:413:A:THR:N	6	2.7
(1,379)	1:383:A:LEU:N	1:383:A:LEU:CA	1:383:A:LEU:C	1:384:A:ALA:N	12	2.7
(1,323)	1:327:A:GLU:N	1:327:A:GLU:CA	1:327:A:GLU:C	1:328:A:PRO:N	19	2.68
(1,149)	1:402:A:GLY:C	1:403:A:LEU:N	1:403:A:LEU:CA	1:403:A:LEU:C	19	2.68
(1,485)	1:505:A:PHE:N	1:505:A:PHE:CA	1:505:A:PHE:C	1:506:A:ALA:N	10	2.67
(1,394)	1:400:A:ASP:N	1:400:A:ASP:CA	1:400:A:ASP:C	1:401:A:PHE:N	14	2.67
(1,293)	1:297:A:MET:N	1:297:A:MET:CA	1:297:A:MET:C	1:298:A:GLU:N	20	2.67
(1,124)	1:375:A:LYS:C	1:376:A:LYS:N	1:376:A:LYS:CA	1:376:A:LYS:C	18	2.66
(1,365)	1:369:A:ALA:N	1:369:A:ALA:CA	1:369:A:ALA:C	1:370:A:MET:N	3	2.64
(1,294)	1:298:A:GLU:N	1:298:A:GLU:CA	1:298:A:GLU:C	1:299:A:VAL:N	19	2.64
(1,30)	1:278:A:GLY:C	1:279:A:VAL:N	1:279:A:VAL:CA	1:279:A:VAL:C	9	2.64
(1,326)	1:330:A:PHE:N	1:330:A:PHE:CA	1:330:A:PHE:C	1:331:A:TYR:N	7	2.62
(1,274)	1:278:A:GLY:N	1:278:A:GLY:CA	1:278:A:GLY:C	1:279:A:VAL:N	17	2.62
(1,404)	1:424:A:TRP:N	1:424:A:TRP:CA	1:424:A:TRP:C	1:425:A:THR:N	6	2.61
(1,347)	1:351:A:ARG:N	1:351:A:ARG:CA	1:351:A:ARG:C	1:352:A:GLN:N	19	2.6
(1,150)	1:403:A:LEU:C	1:404:A:SER:N	1:404:A:SER:CA	1:404:A:SER:C	6	2.59
(1,248)	1:252:A:ASP:N	1:252:A:ASP:CA	1:252:A:ASP:C	1:253:A:LYS:N	18	2.57
(1,150)	1:403:A:LEU:C	1:404:A:SER:N	1:404:A:SER:CA	1:404:A:SER:C	16	2.55
(1,365)	1:369:A:ALA:N	1:369:A:ALA:CA	1:369:A:ALA:C	1:370:A:MET:N	14	2.54
(1,296)	1:300:A:GLU:N	1:300:A:GLU:CA	1:300:A:GLU:C	1:301:A:GLU:N	11	2.54
(1,420)	1:440:A:ASP:N	1:440:A:ASP:CA	1:440:A:ASP:C	1:441:A:VAL:N	18	2.53
(1,325)	1:329:A:PRO:N	1:329:A:PRO:CA	1:329:A:PRO:C	1:330:A:PHE:N	7	2.53
(1,38)	1:286:A:THR:C	1:287:A:VAL:N	1:287:A:VAL:CA	1:287:A:VAL:C	20	2.53

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,455)	1:475:A:TYR:N	1:475:A:TYR:CA	1:475:A:TYR:C	1:476:A:ARG:N	9	2.52
(1,189)	1:456:A:MET:C	1:457:A:SER:N	1:457:A:SER:CA	1:457:A:SER:C	14	2.52
(1,12)	1:260:A:ASP:C	1:261:A:ILE:N	1:261:A:ILE:CA	1:261:A:ILE:C	19	2.52
(1,434)	1:454:A:TYR:N	1:454:A:TYR:CA	1:454:A:TYR:C	1:455:A:GLY:N	18	2.5
(1,398)	1:404:A:SER:N	1:404:A:SER:CA	1:404:A:SER:C	1:405:A:ARG:N	8	2.5
(1,365)	1:369:A:ALA:N	1:369:A:ALA:CA	1:369:A:ALA:C	1:370:A:MET:N	5	2.5
(1,148)	1:400:A:ASP:C	1:401:A:PHE:N	1:401:A:PHE:CA	1:401:A:PHE:C	5	2.5
(1,394)	1:400:A:ASP:N	1:400:A:ASP:CA	1:400:A:ASP:C	1:401:A:PHE:N	15	2.49
(1,393)	1:397:A:LYS:N	1:397:A:LYS:CA	1:397:A:LYS:C	1:398:A:VAL:N	14	2.49
(1,295)	1:299:A:VAL:N	1:299:A:VAL:CA	1:299:A:VAL:C	1:300:A:GLU:N	13	2.49
(1,365)	1:369:A:ALA:N	1:369:A:ALA:CA	1:369:A:ALA:C	1:370:A:MET:N	1	2.46
(1,464)	1:484:A:PRO:N	1:484:A:PRO:CA	1:484:A:PRO:C	1:485:A:GLU:N	4	2.45
(1,400)	1:406:A:LEU:N	1:406:A:LEU:CA	1:406:A:LEU:C	1:407:A:MET:N	9	2.45
(1,365)	1:369:A:ALA:N	1:369:A:ALA:CA	1:369:A:ALA:C	1:370:A:MET:N	6	2.45
(1,205)	1:474:A:ASP:C	1:475:A:TYR:N	1:475:A:TYR:CA	1:475:A:TYR:C	1	2.45
(1,50)	1:298:A:GLU:C	1:299:A:VAL:N	1:299:A:VAL:CA	1:299:A:VAL:C	5	2.44
(1,458)	1:478:A:GLU:N	1:478:A:GLU:CA	1:478:A:GLU:C	1:479:A:ARG:N	9	2.43
(1,415)	1:435:A:PHE:N	1:435:A:PHE:CA	1:435:A:PHE:C	1:436:A:SER:N	13	2.43
(1,7)	1:255:A:GLU:C	1:256:A:MET:N	1:256:A:MET:CA	1:256:A:MET:C	3	2.42
(1,271)	1:275:A:VAL:N	1:275:A:VAL:CA	1:275:A:VAL:C	1:276:A:TYR:N	2	2.41
(1,149)	1:402:A:GLY:C	1:403:A:LEU:N	1:403:A:LEU:CA	1:403:A:LEU:C	18	2.41
(1,38)	1:286:A:THR:C	1:287:A:VAL:N	1:287:A:VAL:CA	1:287:A:VAL:C	7	2.41
(1,38)	1:286:A:THR:C	1:287:A:VAL:N	1:287:A:VAL:CA	1:287:A:VAL:C	17	2.41
(1,307)	1:311:A:GLU:N	1:311:A:GLU:CA	1:311:A:GLU:C	1:312:A:ILE:N	7	2.4
(1,292)	1:296:A:THR:N	1:296:A:THR:CA	1:296:A:THR:C	1:297:A:MET:N	4	2.4
(1,466)	1:486:A:LYS:N	1:486:A:LYS:CA	1:486:A:LYS:C	1:487:A:VAL:N	20	2.39
(1,437)	1:457:A:SER:N	1:457:A:SER:CA	1:457:A:SER:C	1:458:A:PRO:N	20	2.38
(1,132)	1:383:A:LEU:C	1:384:A:ALA:N	1:384:A:ALA:CA	1:384:A:ALA:C	4	2.38
(1,478)	1:498:A:ASN:N	1:498:A:ASN:CA	1:498:A:ASN:C	1:499:A:PRO:N	20	2.37
(1,189)	1:456:A:MET:C	1:457:A:SER:N	1:457:A:SER:CA	1:457:A:SER:C	1	2.37
(1,153)	1:408:A:TYR:C	1:409:A:GLY:N	1:409:A:GLY:CA	1:409:A:GLY:C	9	2.36
(1,130)	1:381:A:ARG:C	1:382:A:ASP:N	1:382:A:ASP:CA	1:382:A:ASP:C	9	2.36
(1,189)	1:456:A:MET:C	1:457:A:SER:N	1:457:A:SER:CA	1:457:A:SER:C	5	2.35
(1,189)	1:456:A:MET:C	1:457:A:SER:N	1:457:A:SER:CA	1:457:A:SER:C	19	2.35
(1,488)	1:508:A:ILE:N	1:508:A:ILE:CA	1:508:A:ILE:C	1:509:A:HIS:N	3	2.34
(1,456)	1:476:A:ARG:N	1:476:A:ARG:CA	1:476:A:ARG:C	1:477:A:MET:N	7	2.34
(1,339)	1:343:A:LEU:N	1:343:A:LEU:CA	1:343:A:LEU:C	1:344:A:ASP:N	6	2.34
(1,292)	1:296:A:THR:N	1:296:A:THR:CA	1:296:A:THR:C	1:297:A:MET:N	13	2.33
(1,207)	1:476:A:ARG:C	1:477:A:MET:N	1:477:A:MET:CA	1:477:A:MET:C	2	2.33
(1,31)	1:279:A:VAL:C	1:280:A:TRP:N	1:280:A:TRP:CA	1:280:A:TRP:C	2	2.33
(1,374)	1:378:A:PHE:N	1:378:A:PHE:CA	1:378:A:PHE:C	1:379:A:ILE:N	14	2.32
(1,325)	1:329:A:PRO:N	1:329:A:PRO:CA	1:329:A:PRO:C	1:330:A:PHE:N	9	2.32
(1,325)	1:329:A:PRO:N	1:329:A:PRO:CA	1:329:A:PRO:C	1:330:A:PHE:N	13	2.32
(1,365)	1:369:A:ALA:N	1:369:A:ALA:CA	1:369:A:ALA:C	1:370:A:MET:N	2	2.31
(1,242)	1:515:A:MET:C	1:516:A:PHE:N	1:516:A:PHE:CA	1:516:A:PHE:C	4	2.31
(1,416)	1:436:A:SER:N	1:436:A:SER:CA	1:436:A:SER:C	1:437:A:ILE:N	15	2.3
(1,293)	1:297:A:MET:N	1:297:A:MET:CA	1:297:A:MET:C	1:298:A:GLU:N	4	2.3
(1,331)	1:335:A:GLU:N	1:335:A:GLU:CA	1:335:A:GLU:C	1:336:A:PHE:N	5	2.29
(1,461)	1:481:A:GLU:N	1:481:A:GLU:CA	1:481:A:GLU:C	1:482:A:GLY:N	8	2.28
(1,309)	1:313:A:LYS:N	1:313:A:LYS:CA	1:313:A:LYS:C	1:314:A:HIS:N	17	2.28
(1,250)	1:254:A:TRP:N	1:254:A:TRP:CA	1:254:A:TRP:C	1:255:A:GLU:N	17	2.28

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,401)	1:409:A:GLY:N	1:409:A:GLY:CA	1:409:A:GLY:C	1:410:A:ASP:N	12	2.27
(1,323)	1:327:A:GLU:N	1:327:A:GLU:CA	1:327:A:GLU:C	1:328:A:PRO:N	12	2.26
(1,252)	1:256:A:MET:N	1:256:A:MET:CA	1:256:A:MET:C	1:257:A:GLU:N	15	2.26
(1,50)	1:298:A:GLU:C	1:299:A:VAL:N	1:299:A:VAL:CA	1:299:A:VAL:C	7	2.25
(1,394)	1:400:A:ASP:N	1:400:A:ASP:CA	1:400:A:ASP:C	1:401:A:PHE:N	12	2.24
(1,27)	1:275:A:VAL:C	1:276:A:TYR:N	1:276:A:TYR:CA	1:276:A:TYR:C	18	2.24
(1,252)	1:256:A:MET:N	1:256:A:MET:CA	1:256:A:MET:C	1:257:A:GLU:N	18	2.23
(1,482)	1:502:A:ARG:N	1:502:A:ARG:CA	1:502:A:ARG:C	1:503:A:PRO:N	18	2.21
(1,434)	1:454:A:TYR:N	1:454:A:TYR:CA	1:454:A:TYR:C	1:455:A:GLY:N	6	2.2
(1,378)	1:382:A:ASP:N	1:382:A:ASP:CA	1:382:A:ASP:C	1:383:A:LEU:N	5	2.2
(1,323)	1:327:A:GLU:N	1:327:A:GLU:CA	1:327:A:GLU:C	1:328:A:PRO:N	10	2.19
(1,242)	1:515:A:MET:C	1:516:A:PHE:N	1:516:A:PHE:CA	1:516:A:PHE:C	19	2.19
(1,38)	1:286:A:THR:C	1:287:A:VAL:N	1:287:A:VAL:CA	1:287:A:VAL:C	13	2.19
(1,374)	1:378:A:PHE:N	1:378:A:PHE:CA	1:378:A:PHE:C	1:379:A:ILE:N	7	2.18
(1,471)	1:491:A:MET:N	1:491:A:MET:CA	1:491:A:MET:C	1:492:A:ARG:N	1	2.16
(1,457)	1:477:A:MET:N	1:477:A:MET:CA	1:477:A:MET:C	1:478:A:GLU:N	12	2.16
(1,456)	1:476:A:ARG:N	1:476:A:ARG:CA	1:476:A:ARG:C	1:477:A:MET:N	3	2.16
(1,295)	1:299:A:VAL:N	1:299:A:VAL:CA	1:299:A:VAL:C	1:300:A:GLU:N	5	2.16
(1,293)	1:297:A:MET:N	1:297:A:MET:CA	1:297:A:MET:C	1:298:A:GLU:N	10	2.15
(1,283)	1:287:A:VAL:N	1:287:A:VAL:CA	1:287:A:VAL:C	1:288:A:ALA:N	11	2.15
(1,151)	1:404:A:SER:C	1:405:A:ARG:N	1:405:A:ARG:CA	1:405:A:ARG:C	7	2.15
(1,365)	1:369:A:ALA:N	1:369:A:ALA:CA	1:369:A:ALA:C	1:370:A:MET:N	17	2.14
(1,394)	1:400:A:ASP:N	1:400:A:ASP:CA	1:400:A:ASP:C	1:401:A:PHE:N	11	2.13
(1,371)	1:375:A:LYS:N	1:375:A:LYS:CA	1:375:A:LYS:C	1:376:A:LYS:N	18	2.13
(1,296)	1:300:A:GLU:N	1:300:A:GLU:CA	1:300:A:GLU:C	1:301:A:GLU:N	15	2.13
(1,98)	1:349:A:CYS:C	1:350:A:ASN:N	1:350:A:ASN:CA	1:350:A:ASN:C	1	2.13
(1,132)	1:383:A:LEU:C	1:384:A:ALA:N	1:384:A:ALA:CA	1:384:A:ALA:C	19	2.12
(1,482)	1:502:A:ARG:N	1:502:A:ARG:CA	1:502:A:ARG:C	1:503:A:PRO:N	5	2.1
(1,414)	1:434:A:LYS:N	1:434:A:LYS:CA	1:434:A:LYS:C	1:435:A:PHE:N	4	2.1
(1,295)	1:299:A:VAL:N	1:299:A:VAL:CA	1:299:A:VAL:C	1:300:A:GLU:N	11	2.1
(1,494)	1:514:A:THR:N	1:514:A:THR:CA	1:514:A:THR:C	1:515:A:MET:N	17	2.08
(1,464)	1:484:A:PRO:N	1:484:A:PRO:CA	1:484:A:PRO:C	1:485:A:GLU:N	19	2.08
(1,31)	1:279:A:VAL:C	1:280:A:TRP:N	1:280:A:TRP:CA	1:280:A:TRP:C	1	2.08
(1,31)	1:279:A:VAL:C	1:280:A:TRP:N	1:280:A:TRP:CA	1:280:A:TRP:C	12	2.08
(1,283)	1:287:A:VAL:N	1:287:A:VAL:CA	1:287:A:VAL:C	1:288:A:ALA:N	9	2.07
(1,50)	1:298:A:GLU:C	1:299:A:VAL:N	1:299:A:VAL:CA	1:299:A:VAL:C	14	2.07
(1,30)	1:278:A:GLY:C	1:279:A:VAL:N	1:279:A:VAL:CA	1:279:A:VAL:C	12	2.07
(1,12)	1:260:A:ASP:C	1:261:A:ILE:N	1:261:A:ILE:CA	1:261:A:ILE:C	18	2.07
(1,485)	1:505:A:PHE:N	1:505:A:PHE:CA	1:505:A:PHE:C	1:506:A:ALA:N	14	2.06
(1,395)	1:401:A:PHE:N	1:401:A:PHE:CA	1:401:A:PHE:C	1:402:A:GLY:N	10	2.06
(1,464)	1:484:A:PRO:N	1:484:A:PRO:CA	1:484:A:PRO:C	1:485:A:GLU:N	15	2.05
(1,409)	1:429:A:SER:N	1:429:A:SER:CA	1:429:A:SER:C	1:430:A:LEU:N	10	2.05
(1,2)	1:250:A:ASN:C	1:251:A:TYR:N	1:251:A:TYR:CA	1:251:A:TYR:C	16	2.04
(1,485)	1:505:A:PHE:N	1:505:A:PHE:CA	1:505:A:PHE:C	1:506:A:ALA:N	19	2.03
(1,189)	1:456:A:MET:C	1:457:A:SER:N	1:457:A:SER:CA	1:457:A:SER:C	15	2.02
(1,124)	1:375:A:LYS:C	1:376:A:LYS:N	1:376:A:LYS:CA	1:376:A:LYS:C	14	2.01
(1,84)	1:335:A:GLU:C	1:336:A:PHE:N	1:336:A:PHE:CA	1:336:A:PHE:C	7	2.01
(1,395)	1:401:A:PHE:N	1:401:A:PHE:CA	1:401:A:PHE:C	1:402:A:GLY:N	6	2.0
(1,494)	1:514:A:THR:N	1:514:A:THR:CA	1:514:A:THR:C	1:515:A:MET:N	3	1.98
(1,478)	1:498:A:ASN:N	1:498:A:ASN:CA	1:498:A:ASN:C	1:499:A:PRO:N	7	1.98
(1,294)	1:298:A:GLU:N	1:298:A:GLU:CA	1:298:A:GLU:C	1:299:A:VAL:N	9	1.97

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,38)	1:286:A:THR:C	1:287:A:VAL:N	1:287:A:VAL:CA	1:287:A:VAL:C	1	1.97
(1,479)	1:499:A:PRO:N	1:499:A:PRO:CA	1:499:A:PRO:C	1:500:A:SER:N	14	1.96
(1,402)	1:412:A:TYR:N	1:412:A:TYR:CA	1:412:A:TYR:C	1:413:A:THR:N	18	1.96
(1,398)	1:404:A:SER:N	1:404:A:SER:CA	1:404:A:SER:C	1:405:A:ARG:N	15	1.96
(1,205)	1:474:A:ASP:C	1:475:A:TYR:N	1:475:A:TYR:CA	1:475:A:TYR:C	12	1.96
(1,64)	1:312:A:ILE:C	1:313:A:LYS:N	1:313:A:LYS:CA	1:313:A:LYS:C	12	1.96
(1,295)	1:299:A:VAL:N	1:299:A:VAL:CA	1:299:A:VAL:C	1:300:A:GLU:N	14	1.95
(1,130)	1:381:A:ARG:C	1:382:A:ASP:N	1:382:A:ASP:CA	1:382:A:ASP:C	18	1.94
(1,155)	1:410:A:ASP:C	1:411:A:THR:N	1:411:A:THR:CA	1:411:A:THR:C	5	1.93
(1,495)	1:515:A:MET:N	1:515:A:MET:CA	1:515:A:MET:C	1:516:A:PHE:N	8	1.91
(1,227)	1:499:A:PRO:C	1:500:A:SER:N	1:500:A:SER:CA	1:500:A:SER:C	2	1.91
(1,50)	1:298:A:GLU:C	1:299:A:VAL:N	1:299:A:VAL:CA	1:299:A:VAL:C	11	1.91
(1,7)	1:255:A:GLU:C	1:256:A:MET:N	1:256:A:MET:CA	1:256:A:MET:C	12	1.91
(1,382)	1:386:A:ARG:N	1:386:A:ARG:CA	1:386:A:ARG:C	1:387:A:ASN:N	4	1.9
(1,295)	1:299:A:VAL:N	1:299:A:VAL:CA	1:299:A:VAL:C	1:300:A:GLU:N	10	1.9
(1,287)	1:291:A:THR:N	1:291:A:THR:CA	1:291:A:THR:C	1:292:A:LEU:N	19	1.9
(1,409)	1:429:A:SER:N	1:429:A:SER:CA	1:429:A:SER:C	1:430:A:LEU:N	20	1.89
(1,339)	1:343:A:LEU:N	1:343:A:LEU:CA	1:343:A:LEU:C	1:344:A:ASP:N	4	1.89
(1,222)	1:493:A:ALA:C	1:494:A:CYS:N	1:494:A:CYS:CA	1:494:A:CYS:C	15	1.89
(1,38)	1:286:A:THR:C	1:287:A:VAL:N	1:287:A:VAL:CA	1:287:A:VAL:C	3	1.89
(1,64)	1:312:A:ILE:C	1:313:A:LYS:N	1:313:A:LYS:CA	1:313:A:LYS:C	6	1.88
(1,325)	1:329:A:PRO:N	1:329:A:PRO:CA	1:329:A:PRO:C	1:330:A:PHE:N	18	1.87
(1,53)	1:301:A:GLU:C	1:302:A:PHE:N	1:302:A:PHE:CA	1:302:A:PHE:C	20	1.87
(1,488)	1:508:A:ILE:N	1:508:A:ILE:CA	1:508:A:ILE:C	1:509:A:HIS:N	18	1.85
(1,412)	1:432:A:TYR:N	1:432:A:TYR:CA	1:432:A:TYR:C	1:433:A:ASN:N	13	1.85
(1,365)	1:369:A:ALA:N	1:369:A:ALA:CA	1:369:A:ALA:C	1:370:A:MET:N	20	1.85
(1,274)	1:278:A:GLY:N	1:278:A:GLY:CA	1:278:A:GLY:C	1:279:A:VAL:N	14	1.85
(1,271)	1:275:A:VAL:N	1:275:A:VAL:CA	1:275:A:VAL:C	1:276:A:TYR:N	4	1.85
(1,3)	1:251:A:TYR:C	1:252:A:ASP:N	1:252:A:ASP:CA	1:252:A:ASP:C	8	1.85
(1,464)	1:484:A:PRO:N	1:484:A:PRO:CA	1:484:A:PRO:C	1:485:A:GLU:N	1	1.84
(1,456)	1:476:A:ARG:N	1:476:A:ARG:CA	1:476:A:ARG:C	1:477:A:MET:N	12	1.84
(1,294)	1:298:A:GLU:N	1:298:A:GLU:CA	1:298:A:GLU:C	1:299:A:VAL:N	2	1.84
(1,38)	1:286:A:THR:C	1:287:A:VAL:N	1:287:A:VAL:CA	1:287:A:VAL:C	15	1.84
(1,285)	1:289:A:VAL:N	1:289:A:VAL:CA	1:289:A:VAL:C	1:290:A:LYS:N	12	1.83
(1,38)	1:286:A:THR:C	1:287:A:VAL:N	1:287:A:VAL:CA	1:287:A:VAL:C	6	1.83
(1,401)	1:409:A:GLY:N	1:409:A:GLY:CA	1:409:A:GLY:C	1:410:A:ASP:N	15	1.82
(1,326)	1:330:A:PHE:N	1:330:A:PHE:CA	1:330:A:PHE:C	1:331:A:TYR:N	19	1.82
(1,151)	1:404:A:SER:C	1:405:A:ARG:N	1:405:A:ARG:CA	1:405:A:ARG:C	20	1.82
(1,398)	1:404:A:SER:N	1:404:A:SER:CA	1:404:A:SER:C	1:405:A:ARG:N	7	1.81
(1,283)	1:287:A:VAL:N	1:287:A:VAL:CA	1:287:A:VAL:C	1:288:A:ALA:N	19	1.81
(1,414)	1:434:A:LYS:N	1:434:A:LYS:CA	1:434:A:LYS:C	1:435:A:PHE:N	14	1.8
(1,336)	1:340:A:GLY:N	1:340:A:GLY:CA	1:340:A:GLY:C	1:341:A:ASN:N	4	1.8
(1,293)	1:297:A:MET:N	1:297:A:MET:CA	1:297:A:MET:C	1:298:A:GLU:N	5	1.8
(1,269)	1:273:A:GLY:N	1:273:A:GLY:CA	1:273:A:GLY:C	1:274:A:GLU:N	15	1.8
(1,403)	1:423:A:LYS:N	1:423:A:LYS:CA	1:423:A:LYS:C	1:424:A:TRP:N	15	1.79
(1,339)	1:343:A:LEU:N	1:343:A:LEU:CA	1:343:A:LEU:C	1:344:A:ASP:N	2	1.79
(1,296)	1:300:A:GLU:N	1:300:A:GLU:CA	1:300:A:GLU:C	1:301:A:GLU:N	18	1.79
(1,38)	1:286:A:THR:C	1:287:A:VAL:N	1:287:A:VAL:CA	1:287:A:VAL:C	5	1.79
(1,296)	1:300:A:GLU:N	1:300:A:GLU:CA	1:300:A:GLU:C	1:301:A:GLU:N	6	1.77
(1,401)	1:409:A:GLY:N	1:409:A:GLY:CA	1:409:A:GLY:C	1:410:A:ASP:N	8	1.75
(1,373)	1:377:A:ASN:N	1:377:A:ASN:CA	1:377:A:ASN:C	1:378:A:PHE:N	3	1.75

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,339)	1:343:A:LEU:N	1:343:A:LEU:CA	1:343:A:LEU:C	1:344:A:ASP:N	7	1.75
(1,269)	1:273:A:GLY:N	1:273:A:GLY:CA	1:273:A:GLY:C	1:274:A:GLU:N	10	1.75
(1,414)	1:434:A:LYS:N	1:434:A:LYS:CA	1:434:A:LYS:C	1:435:A:PHE:N	10	1.72
(1,412)	1:432:A:TYR:N	1:432:A:TYR:CA	1:432:A:TYR:C	1:433:A:ASN:N	4	1.72
(1,397)	1:403:A:LEU:N	1:403:A:LEU:CA	1:403:A:LEU:C	1:404:A:SER:N	11	1.72
(1,53)	1:301:A:GLU:C	1:302:A:PHE:N	1:302:A:PHE:CA	1:302:A:PHE:C	10	1.72
(1,38)	1:286:A:THR:C	1:287:A:VAL:N	1:287:A:VAL:CA	1:287:A:VAL:C	12	1.72
(1,478)	1:498:A:ASN:N	1:498:A:ASN:CA	1:498:A:ASN:C	1:499:A:PRO:N	9	1.71
(1,365)	1:369:A:ALA:N	1:369:A:ALA:CA	1:369:A:ALA:C	1:370:A:MET:N	9	1.71
(1,43)	1:291:A:THR:C	1:292:A:LEU:N	1:292:A:LEU:CA	1:292:A:LEU:C	19	1.69
(1,323)	1:327:A:GLU:N	1:327:A:GLU:CA	1:327:A:GLU:C	1:328:A:PRO:N	11	1.68
(1,38)	1:286:A:THR:C	1:287:A:VAL:N	1:287:A:VAL:CA	1:287:A:VAL:C	16	1.67
(1,494)	1:514:A:THR:N	1:514:A:THR:CA	1:514:A:THR:C	1:515:A:MET:N	6	1.64
(1,409)	1:429:A:SER:N	1:429:A:SER:CA	1:429:A:SER:C	1:430:A:LEU:N	16	1.63
(1,323)	1:327:A:GLU:N	1:327:A:GLU:CA	1:327:A:GLU:C	1:328:A:PRO:N	6	1.63
(1,314)	1:318:A:VAL:N	1:318:A:VAL:CA	1:318:A:VAL:C	1:319:A:GLN:N	20	1.63
(1,157)	1:423:A:LYS:C	1:424:A:TRP:N	1:424:A:TRP:CA	1:424:A:TRP:C	13	1.63
(1,155)	1:410:A:ASP:C	1:411:A:THR:N	1:411:A:THR:CA	1:411:A:THR:C	8	1.63
(1,295)	1:299:A:VAL:N	1:299:A:VAL:CA	1:299:A:VAL:C	1:300:A:GLU:N	15	1.62
(1,283)	1:287:A:VAL:N	1:287:A:VAL:CA	1:287:A:VAL:C	1:288:A:ALA:N	13	1.62
(1,223)	1:494:A:CYS:C	1:495:A:TRP:N	1:495:A:TRP:CA	1:495:A:TRP:C	15	1.62
(1,9)	1:257:A:GLU:C	1:258:A:ARG:N	1:258:A:ARG:CA	1:258:A:ARG:C	14	1.62
(1,494)	1:514:A:THR:N	1:514:A:THR:CA	1:514:A:THR:C	1:515:A:MET:N	15	1.61
(1,376)	1:380:A:HIS:N	1:380:A:HIS:CA	1:380:A:HIS:C	1:381:A:ARG:N	7	1.61
(1,314)	1:318:A:VAL:N	1:318:A:VAL:CA	1:318:A:VAL:C	1:319:A:GLN:N	7	1.61
(1,297)	1:301:A:GLU:N	1:301:A:GLU:CA	1:301:A:GLU:C	1:302:A:PHE:N	5	1.61
(1,189)	1:456:A:MET:C	1:457:A:SER:N	1:457:A:SER:CA	1:457:A:SER:C	9	1.61
(1,84)	1:335:A:GLU:C	1:336:A:PHE:N	1:336:A:PHE:CA	1:336:A:PHE:C	12	1.61
(1,283)	1:287:A:VAL:N	1:287:A:VAL:CA	1:287:A:VAL:C	1:288:A:ALA:N	12	1.59
(1,267)	1:271:A:GLN:N	1:271:A:GLN:CA	1:271:A:GLN:C	1:272:A:TYR:N	13	1.59
(1,95)	1:346:A:LEU:C	1:347:A:ARG:N	1:347:A:ARG:CA	1:347:A:ARG:C	17	1.58
(1,456)	1:476:A:ARG:N	1:476:A:ARG:CA	1:476:A:ARG:C	1:477:A:MET:N	6	1.57
(1,420)	1:440:A:ASP:N	1:440:A:ASP:CA	1:440:A:ASP:C	1:441:A:VAL:N	7	1.57
(1,396)	1:402:A:GLY:N	1:402:A:GLY:CA	1:402:A:GLY:C	1:403:A:LEU:N	10	1.57
(1,309)	1:313:A:LYS:N	1:313:A:LYS:CA	1:313:A:LYS:C	1:314:A:HIS:N	6	1.57
(1,143)	1:394:A:HIS:C	1:395:A:LEU:N	1:395:A:LEU:CA	1:395:A:LEU:C	20	1.57
(1,459)	1:479:A:ARG:N	1:479:A:ARG:CA	1:479:A:ARG:C	1:480:A:PRO:N	13	1.56
(1,458)	1:478:A:GLU:N	1:478:A:GLU:CA	1:478:A:GLU:C	1:479:A:ARG:N	4	1.56
(1,378)	1:382:A:ASP:N	1:382:A:ASP:CA	1:382:A:ASP:C	1:383:A:LEU:N	19	1.56
(1,374)	1:378:A:PHE:N	1:378:A:PHE:CA	1:378:A:PHE:C	1:379:A:ILE:N	12	1.56
(1,365)	1:369:A:ALA:N	1:369:A:ALA:CA	1:369:A:ALA:C	1:370:A:MET:N	15	1.56
(1,278)	1:282:A:LYS:N	1:282:A:LYS:CA	1:282:A:LYS:C	1:283:A:TYR:N	16	1.56
(1,275)	1:279:A:VAL:N	1:279:A:VAL:CA	1:279:A:VAL:C	1:280:A:TRP:N	19	1.56
(1,460)	1:480:A:PRO:N	1:480:A:PRO:CA	1:480:A:PRO:C	1:481:A:GLU:N	2	1.55
(1,150)	1:403:A:LEU:C	1:404:A:SER:N	1:404:A:SER:CA	1:404:A:SER:C	1	1.55
(1,293)	1:297:A:MET:N	1:297:A:MET:CA	1:297:A:MET:C	1:298:A:GLU:N	7	1.54
(1,204)	1:473:A:LYS:C	1:474:A:ASP:N	1:474:A:ASP:CA	1:474:A:ASP:C	9	1.54
(1,464)	1:484:A:PRO:N	1:484:A:PRO:CA	1:484:A:PRO:C	1:485:A:GLU:N	17	1.53
(1,357)	1:361:A:TYR:N	1:361:A:TYR:CA	1:361:A:TYR:C	1:362:A:MET:N	19	1.53
(1,197)	1:466:A:GLN:C	1:467:A:VAL:N	1:467:A:VAL:CA	1:467:A:VAL:C	10	1.53
(1,8)	1:256:A:MET:C	1:257:A:GLU:N	1:257:A:GLU:CA	1:257:A:GLU:C	17	1.53

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,197)	1:466:A:GLN:C	1:467:A:VAL:N	1:467:A:VAL:CA	1:467:A:VAL:C	8	1.52
(1,378)	1:382:A:ASP:N	1:382:A:ASP:CA	1:382:A:ASP:C	1:383:A:LEU:N	20	1.51
(1,366)	1:370:A:MET:N	1:370:A:MET:CA	1:370:A:MET:C	1:371:A:GLU:N	11	1.51
(1,365)	1:369:A:ALA:N	1:369:A:ALA:CA	1:369:A:ALA:C	1:370:A:MET:N	12	1.51
(1,271)	1:275:A:VAL:N	1:275:A:VAL:CA	1:275:A:VAL:C	1:276:A:TYR:N	18	1.51
(1,8)	1:256:A:MET:C	1:257:A:GLU:N	1:257:A:GLU:CA	1:257:A:GLU:C	14	1.51
(1,483)	1:503:A:PRO:N	1:503:A:PRO:CA	1:503:A:PRO:C	1:504:A:SER:N	17	1.5
(1,367)	1:371:A:GLU:N	1:371:A:GLU:CA	1:371:A:GLU:C	1:372:A:TYR:N	3	1.5
(1,7)	1:255:A:GLU:C	1:256:A:MET:N	1:256:A:MET:CA	1:256:A:MET:C	16	1.5
(1,456)	1:476:A:ARG:N	1:476:A:ARG:CA	1:476:A:ARG:C	1:477:A:MET:N	17	1.49
(1,403)	1:423:A:LYS:N	1:423:A:LYS:CA	1:423:A:LYS:C	1:424:A:TRP:N	20	1.49
(1,31)	1:279:A:VAL:C	1:280:A:TRP:N	1:280:A:TRP:CA	1:280:A:TRP:C	13	1.47
(1,483)	1:503:A:PRO:N	1:503:A:PRO:CA	1:503:A:PRO:C	1:504:A:SER:N	19	1.46
(1,295)	1:299:A:VAL:N	1:299:A:VAL:CA	1:299:A:VAL:C	1:300:A:GLU:N	12	1.46
(1,146)	1:397:A:LYS:C	1:398:A:VAL:N	1:398:A:VAL:CA	1:398:A:VAL:C	17	1.46
(1,357)	1:361:A:TYR:N	1:361:A:TYR:CA	1:361:A:TYR:C	1:362:A:MET:N	12	1.44
(1,339)	1:343:A:LEU:N	1:343:A:LEU:CA	1:343:A:LEU:C	1:344:A:ASP:N	17	1.44
(1,296)	1:300:A:GLU:N	1:300:A:GLU:CA	1:300:A:GLU:C	1:301:A:GLU:N	17	1.44
(1,283)	1:287:A:VAL:N	1:287:A:VAL:CA	1:287:A:VAL:C	1:288:A:ALA:N	20	1.44
(1,357)	1:361:A:TYR:N	1:361:A:TYR:CA	1:361:A:TYR:C	1:362:A:MET:N	20	1.43
(1,242)	1:515:A:MET:C	1:516:A:PHE:N	1:516:A:PHE:CA	1:516:A:PHE:C	9	1.43
(1,38)	1:286:A:THR:C	1:287:A:VAL:N	1:287:A:VAL:CA	1:287:A:VAL:C	18	1.43
(1,471)	1:491:A:MET:N	1:491:A:MET:CA	1:491:A:MET:C	1:492:A:ARG:N	19	1.42
(1,295)	1:299:A:VAL:N	1:299:A:VAL:CA	1:299:A:VAL:C	1:300:A:GLU:N	17	1.42
(1,398)	1:404:A:SER:N	1:404:A:SER:CA	1:404:A:SER:C	1:405:A:ARG:N	2	1.41
(1,394)	1:400:A:ASP:N	1:400:A:ASP:CA	1:400:A:ASP:C	1:401:A:PHE:N	16	1.41
(1,292)	1:296:A:THR:N	1:296:A:THR:CA	1:296:A:THR:C	1:297:A:MET:N	18	1.4
(1,267)	1:271:A:GLN:N	1:271:A:GLN:CA	1:271:A:GLN:C	1:272:A:TYR:N	18	1.4
(1,204)	1:473:A:LYS:C	1:474:A:ASP:N	1:474:A:ASP:CA	1:474:A:ASP:C	20	1.4
(1,197)	1:466:A:GLN:C	1:467:A:VAL:N	1:467:A:VAL:CA	1:467:A:VAL:C	15	1.39
(1,402)	1:412:A:TYR:N	1:412:A:TYR:CA	1:412:A:TYR:C	1:413:A:THR:N	7	1.38
(1,50)	1:298:A:GLU:C	1:299:A:VAL:N	1:299:A:VAL:CA	1:299:A:VAL:C	8	1.38
(1,382)	1:386:A:ARG:N	1:386:A:ARG:CA	1:386:A:ARG:C	1:387:A:ASN:N	10	1.37
(1,362)	1:366:A:ILE:N	1:366:A:ILE:CA	1:366:A:ILE:C	1:367:A:SER:N	6	1.37
(1,495)	1:515:A:MET:N	1:515:A:MET:CA	1:515:A:MET:C	1:516:A:PHE:N	10	1.36
(1,407)	1:427:A:PRO:N	1:427:A:PRO:CA	1:427:A:PRO:C	1:428:A:GLU:N	7	1.36
(1,374)	1:378:A:PHE:N	1:378:A:PHE:CA	1:378:A:PHE:C	1:379:A:ILE:N	15	1.35
(1,323)	1:327:A:GLU:N	1:327:A:GLU:CA	1:327:A:GLU:C	1:328:A:PRO:N	15	1.35
(1,43)	1:291:A:THR:C	1:292:A:LEU:N	1:292:A:LEU:CA	1:292:A:LEU:C	13	1.35
(1,252)	1:256:A:MET:N	1:256:A:MET:CA	1:256:A:MET:C	1:257:A:GLU:N	14	1.34
(1,467)	1:487:A:VAL:N	1:487:A:VAL:CA	1:487:A:VAL:C	1:488:A:TYR:N	4	1.33
(1,403)	1:423:A:LYS:N	1:423:A:LYS:CA	1:423:A:LYS:C	1:424:A:TRP:N	6	1.33
(1,403)	1:423:A:LYS:N	1:423:A:LYS:CA	1:423:A:LYS:C	1:424:A:TRP:N	9	1.33
(1,295)	1:299:A:VAL:N	1:299:A:VAL:CA	1:299:A:VAL:C	1:300:A:GLU:N	7	1.33
(1,1)	1:249:A:PRO:C	1:250:A:ASN:N	1:250:A:ASN:CA	1:250:A:ASN:C	14	1.33
(1,366)	1:370:A:MET:N	1:370:A:MET:CA	1:370:A:MET:C	1:371:A:GLU:N	7	1.32
(1,283)	1:287:A:VAL:N	1:287:A:VAL:CA	1:287:A:VAL:C	1:288:A:ALA:N	18	1.32
(1,31)	1:279:A:VAL:C	1:280:A:TRP:N	1:280:A:TRP:CA	1:280:A:TRP:C	8	1.32
(1,409)	1:429:A:SER:N	1:429:A:SER:CA	1:429:A:SER:C	1:430:A:LEU:N	4	1.31
(1,483)	1:503:A:PRO:N	1:503:A:PRO:CA	1:503:A:PRO:C	1:504:A:SER:N	5	1.3
(1,393)	1:397:A:LYS:N	1:397:A:LYS:CA	1:397:A:LYS:C	1:398:A:VAL:N	7	1.3

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,292)	1:296:A:THR:N	1:296:A:THR:CA	1:296:A:THR:C	1:297:A:MET:N	10	1.3
(1,31)	1:279:A:VAL:C	1:280:A:TRP:N	1:280:A:TRP:CA	1:280:A:TRP:C	7	1.3
(1,283)	1:287:A:VAL:N	1:287:A:VAL:CA	1:287:A:VAL:C	1:288:A:ALA:N	16	1.29
(1,494)	1:514:A:THR:N	1:514:A:THR:CA	1:514:A:THR:C	1:515:A:MET:N	11	1.28
(1,488)	1:508:A:ILE:N	1:508:A:ILE:CA	1:508:A:ILE:C	1:509:A:HIS:N	5	1.28
(1,269)	1:273:A:GLY:N	1:273:A:GLY:CA	1:273:A:GLY:C	1:274:A:GLU:N	5	1.28
(1,482)	1:502:A:ARG:N	1:502:A:ARG:CA	1:502:A:ARG:C	1:503:A:PRO:N	14	1.27
(1,293)	1:297:A:MET:N	1:297:A:MET:CA	1:297:A:MET:C	1:298:A:GLU:N	3	1.27
(1,246)	1:250:A:ASN:N	1:250:A:ASN:CA	1:250:A:ASN:C	1:251:A:TYR:N	19	1.27
(1,95)	1:346:A:LEU:C	1:347:A:ARG:N	1:347:A:ARG:CA	1:347:A:ARG:C	8	1.27
(1,357)	1:361:A:TYR:N	1:361:A:TYR:CA	1:361:A:TYR:C	1:362:A:MET:N	17	1.26
(1,457)	1:477:A:MET:N	1:477:A:MET:CA	1:477:A:MET:C	1:478:A:GLU:N	13	1.25
(1,365)	1:369:A:ALA:N	1:369:A:ALA:CA	1:369:A:ALA:C	1:370:A:MET:N	13	1.25
(1,371)	1:375:A:LYS:N	1:375:A:LYS:CA	1:375:A:LYS:C	1:376:A:LYS:N	14	1.24
(1,339)	1:343:A:LEU:N	1:343:A:LEU:CA	1:343:A:LEU:C	1:344:A:ASP:N	18	1.24
(1,336)	1:340:A:GLY:N	1:340:A:GLY:CA	1:340:A:GLY:C	1:341:A:ASN:N	19	1.24
(1,292)	1:296:A:THR:N	1:296:A:THR:CA	1:296:A:THR:C	1:297:A:MET:N	20	1.24
(1,412)	1:432:A:TYR:N	1:432:A:TYR:CA	1:432:A:TYR:C	1:433:A:ASN:N	19	1.23
(1,150)	1:403:A:LEU:C	1:404:A:SER:N	1:404:A:SER:CA	1:404:A:SER:C	19	1.23
(1,477)	1:497:A:TRP:N	1:497:A:TRP:CA	1:497:A:TRP:C	1:498:A:ASN:N	13	1.22
(1,345)	1:349:A:CYS:N	1:349:A:CYS:CA	1:349:A:CYS:C	1:350:A:ASN:N	1	1.22
(1,50)	1:298:A:GLU:C	1:299:A:VAL:N	1:299:A:VAL:CA	1:299:A:VAL:C	17	1.21
(1,459)	1:479:A:ARG:N	1:479:A:ARG:CA	1:479:A:ARG:C	1:480:A:PRO:N	1	1.2
(1,434)	1:454:A:TYR:N	1:454:A:TYR:CA	1:454:A:TYR:C	1:455:A:GLY:N	4	1.2
(1,287)	1:291:A:THR:N	1:291:A:THR:CA	1:291:A:THR:C	1:292:A:LEU:N	13	1.2
(1,292)	1:296:A:THR:N	1:296:A:THR:CA	1:296:A:THR:C	1:297:A:MET:N	5	1.19
(1,149)	1:402:A:GLY:C	1:403:A:LEU:N	1:403:A:LEU:CA	1:403:A:LEU:C	8	1.19
(1,453)	1:473:A:LYS:N	1:473:A:LYS:CA	1:473:A:LYS:C	1:474:A:ASP:N	17	1.18
(1,398)	1:404:A:SER:N	1:404:A:SER:CA	1:404:A:SER:C	1:405:A:ARG:N	6	1.17
(1,314)	1:318:A:VAL:N	1:318:A:VAL:CA	1:318:A:VAL:C	1:319:A:GLN:N	9	1.16
(1,312)	1:316:A:ASN:N	1:316:A:ASN:CA	1:316:A:ASN:C	1:317:A:LEU:N	11	1.16
(1,283)	1:287:A:VAL:N	1:287:A:VAL:CA	1:287:A:VAL:C	1:288:A:ALA:N	14	1.16
(1,218)	1:489:A:GLU:C	1:490:A:LEU:N	1:490:A:LEU:CA	1:490:A:LEU:C	18	1.16
(1,11)	1:259:A:THR:C	1:260:A:ASP:N	1:260:A:ASP:CA	1:260:A:ASP:C	9	1.16
(1,325)	1:329:A:PRO:N	1:329:A:PRO:CA	1:329:A:PRO:C	1:330:A:PHE:N	12	1.15
(1,204)	1:473:A:LYS:C	1:474:A:ASP:N	1:474:A:ASP:CA	1:474:A:ASP:C	13	1.15
(1,464)	1:484:A:PRO:N	1:484:A:PRO:CA	1:484:A:PRO:C	1:485:A:GLU:N	2	1.14
(1,314)	1:318:A:VAL:N	1:318:A:VAL:CA	1:318:A:VAL:C	1:319:A:GLN:N	15	1.14
(1,473)	1:493:A:ALA:N	1:493:A:ALA:CA	1:493:A:ALA:C	1:494:A:CYS:N	18	1.13
(1,437)	1:457:A:SER:N	1:457:A:SER:CA	1:457:A:SER:C	1:458:A:PRO:N	8	1.13
(1,202)	1:471:A:LEU:C	1:472:A:GLU:N	1:472:A:GLU:CA	1:472:A:GLU:C	14	1.13
(1,154)	1:409:A:GLY:C	1:410:A:ASP:N	1:410:A:ASP:CA	1:410:A:ASP:C	12	1.13
(1,16)	1:264:A:LYS:C	1:265:A:HIS:N	1:265:A:HIS:CA	1:265:A:HIS:C	18	1.13
(1,377)	1:381:A:ARG:N	1:381:A:ARG:CA	1:381:A:ARG:C	1:382:A:ASP:N	7	1.11
(1,376)	1:380:A:HIS:N	1:380:A:HIS:CA	1:380:A:HIS:C	1:381:A:ARG:N	13	1.11
(1,331)	1:335:A:GLU:N	1:335:A:GLU:CA	1:335:A:GLU:C	1:336:A:PHE:N	17	1.11
(1,197)	1:466:A:GLN:C	1:467:A:VAL:N	1:467:A:VAL:CA	1:467:A:VAL:C	13	1.11
(1,405)	1:425:A:THR:N	1:425:A:THR:CA	1:425:A:THR:C	1:426:A:ALA:N	2	1.1
(1,331)	1:335:A:GLU:N	1:335:A:GLU:CA	1:335:A:GLU:C	1:336:A:PHE:N	7	1.1
(1,64)	1:312:A:ILE:C	1:313:A:LYS:N	1:313:A:LYS:CA	1:313:A:LYS:C	2	1.09
(1,2)	1:250:A:ASN:C	1:251:A:TYR:N	1:251:A:TYR:CA	1:251:A:TYR:C	19	1.09

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,494)	1:514:A:THR:N	1:514:A:THR:CA	1:514:A:THR:C	1:515:A:MET:N	13	1.08
(1,28)	1:276:A:TYR:C	1:277:A:GLU:N	1:277:A:GLU:CA	1:277:A:GLU:C	12	1.08
(1,434)	1:454:A:TYR:N	1:454:A:TYR:CA	1:454:A:TYR:C	1:455:A:GLY:N	12	1.07
(1,326)	1:330:A:PHE:N	1:330:A:PHE:CA	1:330:A:PHE:C	1:331:A:TYR:N	6	1.06
(1,283)	1:287:A:VAL:N	1:287:A:VAL:CA	1:287:A:VAL:C	1:288:A:ALA:N	2	1.06
(1,323)	1:327:A:GLU:N	1:327:A:GLU:CA	1:327:A:GLU:C	1:328:A:PRO:N	13	1.05
(1,293)	1:297:A:MET:N	1:297:A:MET:CA	1:297:A:MET:C	1:298:A:GLU:N	9	1.05
(1,179)	1:446:A:VAL:C	1:447:A:LEU:N	1:447:A:LEU:CA	1:447:A:LEU:C	12	1.05
(1,473)	1:493:A:ALA:N	1:493:A:ALA:CA	1:493:A:ALA:C	1:494:A:CYS:N	10	1.04
(1,295)	1:299:A:VAL:N	1:299:A:VAL:CA	1:299:A:VAL:C	1:300:A:GLU:N	3	1.03
(1,242)	1:515:A:MET:C	1:516:A:PHE:N	1:516:A:PHE:CA	1:516:A:PHE:C	5	1.03
(1,16)	1:264:A:LYS:C	1:265:A:HIS:N	1:265:A:HIS:CA	1:265:A:HIS:C	5	1.03
(1,441)	1:461:A:GLY:N	1:461:A:GLY:CA	1:461:A:GLY:C	1:462:A:ILE:N	9	1.02
(1,305)	1:309:A:LEU:N	1:309:A:LEU:CA	1:309:A:LEU:C	1:310:A:LYS:N	12	1.02
(1,312)	1:316:A:ASN:N	1:316:A:ASN:CA	1:316:A:ASN:C	1:317:A:LEU:N	16	1.01
(1,376)	1:380:A:HIS:N	1:380:A:HIS:CA	1:380:A:HIS:C	1:381:A:ARG:N	2	1.0
(1,323)	1:327:A:GLU:N	1:327:A:GLU:CA	1:327:A:GLU:C	1:328:A:PRO:N	8	1.0
(1,307)	1:311:A:GLU:N	1:311:A:GLU:CA	1:311:A:GLU:C	1:312:A:ILE:N	11	1.0