



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 10:08 PM UTC

PDB ID : 2NDH / pdb_00002ndh
BMRB ID : 26061
Title : NMR solution structure of MAL/TIRAP TIR domain (C116A)
Authors : Lavrencic, P.; Mobli, M.
Deposited on : 2016-05-27

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

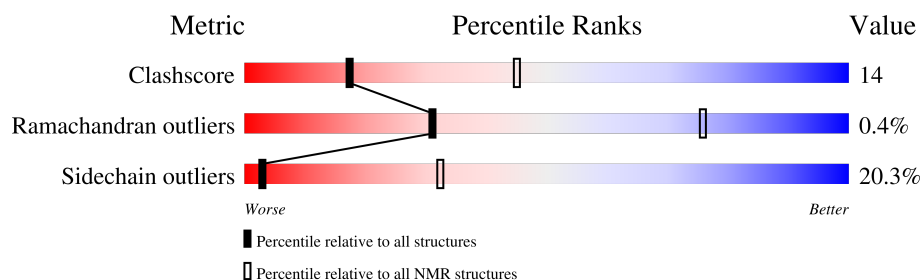
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 68%.

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	143	

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 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:84-A:122, A:134-A:192, A:197-A:221 (123)	1.66	3

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

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

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2179 atoms, of which 1079 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Toll/interleukin-1 receptor domain-containing adapter protein.

Mol	Chain	Residues	Atoms						Trace
1	A	143	Total	C	H	N	O	S	0
			2179	694	1079	187	210	9	

There is a discrepancy between the modelled and reference sequences:

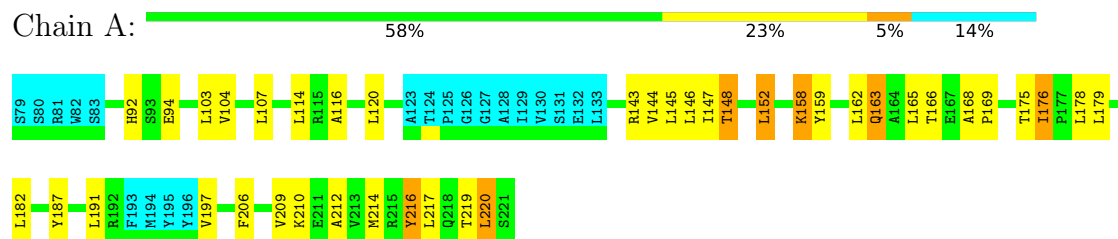
Chain	Residue	Modelled	Actual	Comment	Reference
A	116	ALA	CYS	engineered mutation	UNP P58753

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: Toll/interleukin-1 receptor domain-containing adapter protein

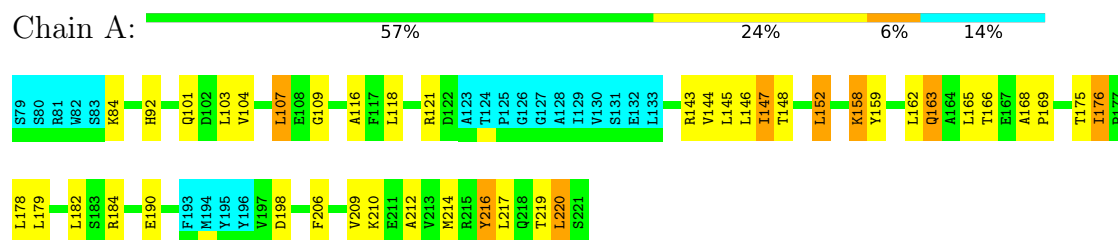


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

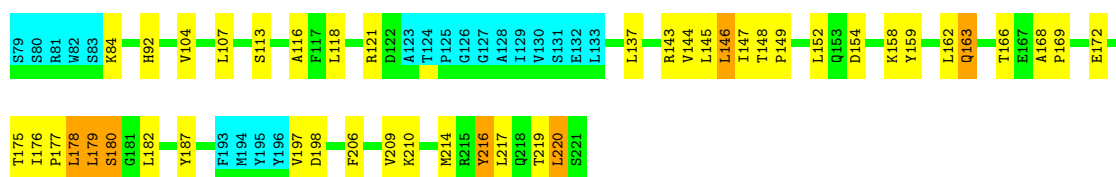
- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



4.2.2 Score per residue for model 2

- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein

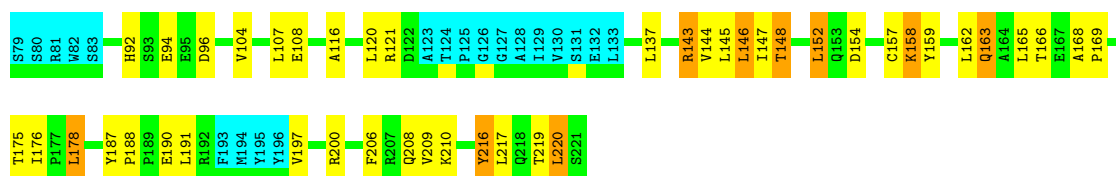




4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein

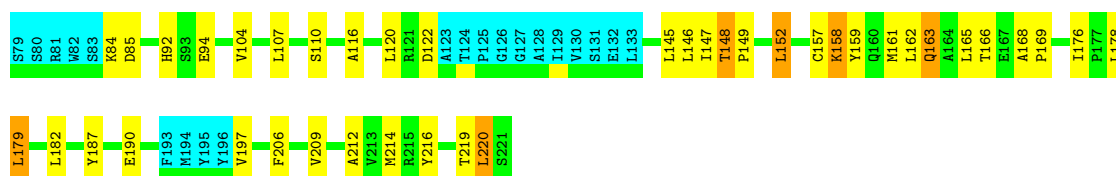
Chain A: 



4.2.4 Score per residue for model 4

- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein

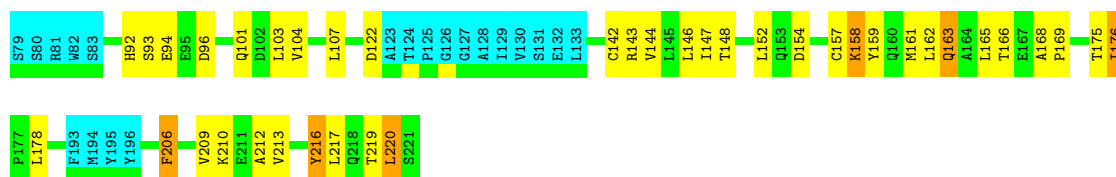
Chain A: 



4.2.5 Score per residue for model 5

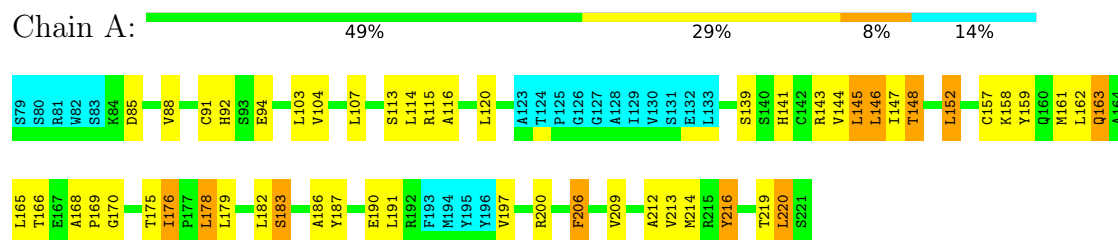
- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein

Chain A: 

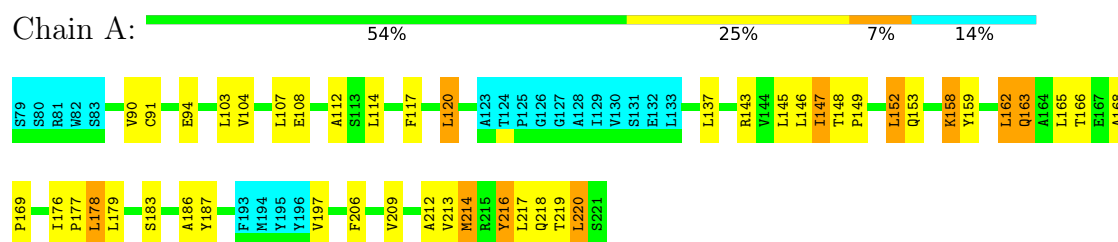


4.2.6 Score per residue for model 6

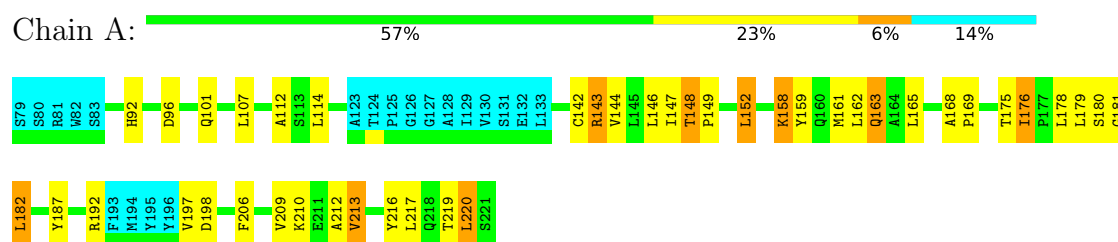
- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



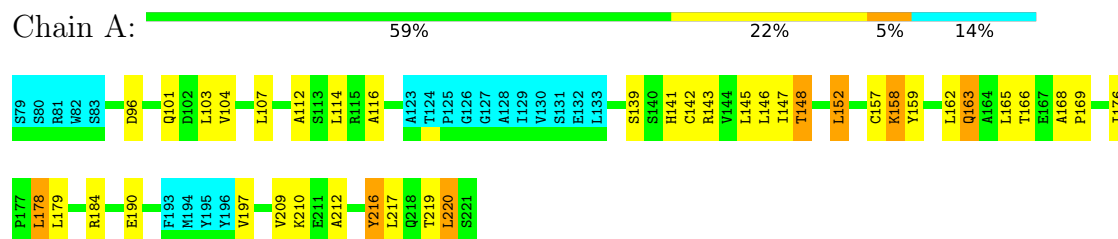
- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein

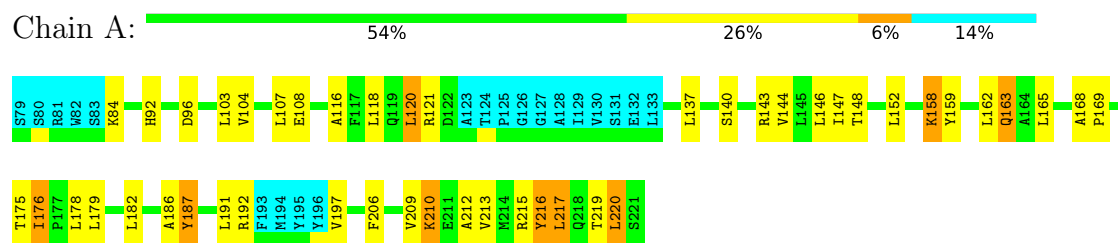


- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



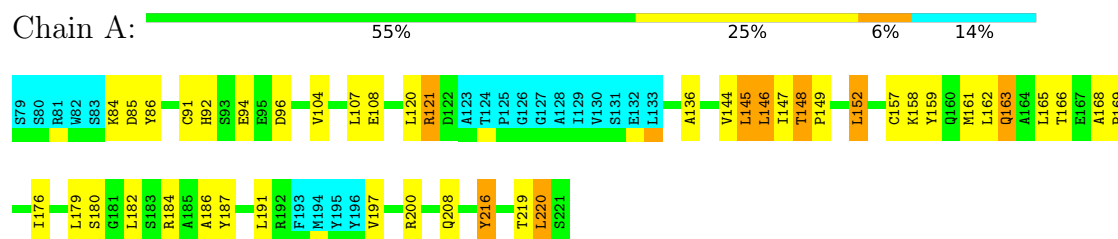
4.2.10 Score per residue for model 10

- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



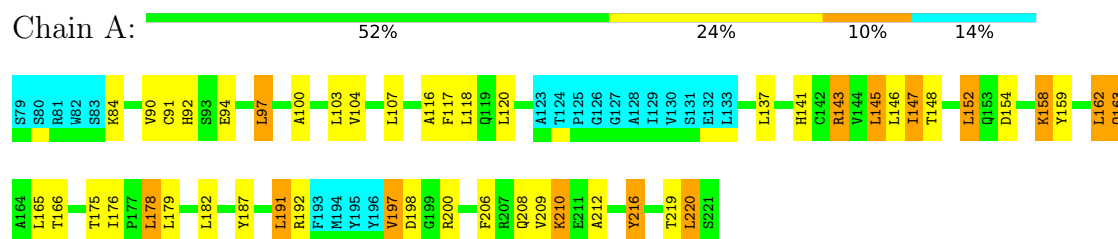
4.2.11 Score per residue for model 11

- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



4.2.12 Score per residue for model 12

- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



4.2.13 Score per residue for model 13

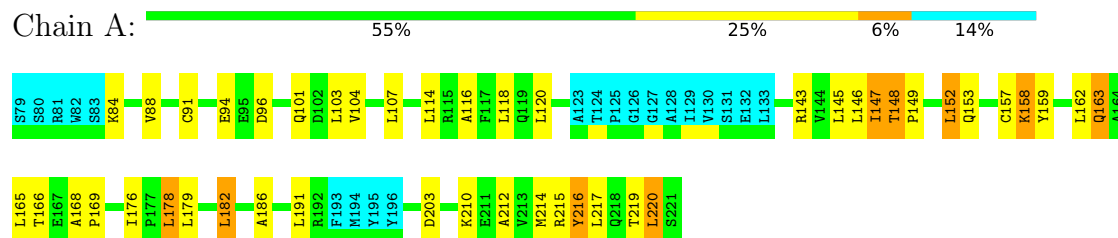
- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein





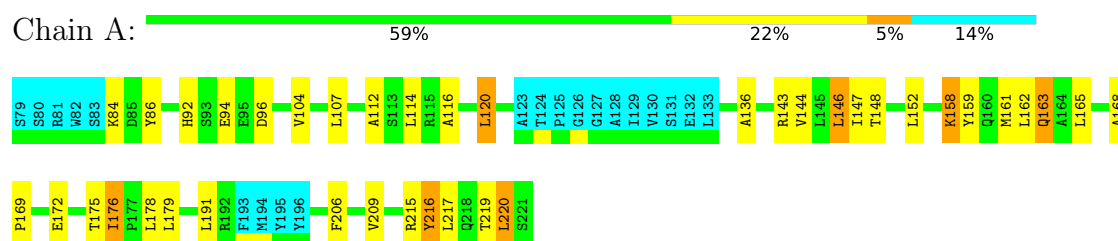
4.2.14 Score per residue for model 14

- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



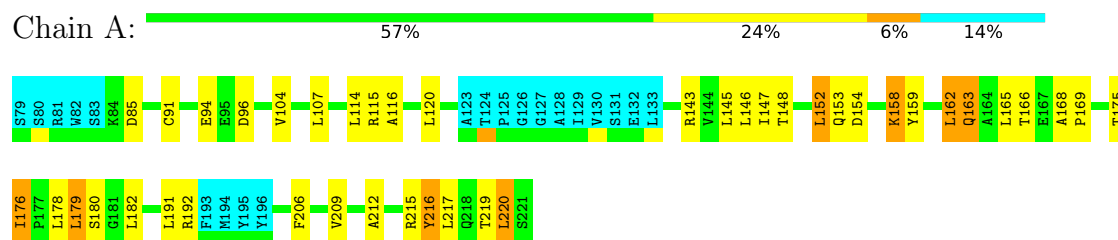
4.2.15 Score per residue for model 15

- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



4.2.16 Score per residue for model 16

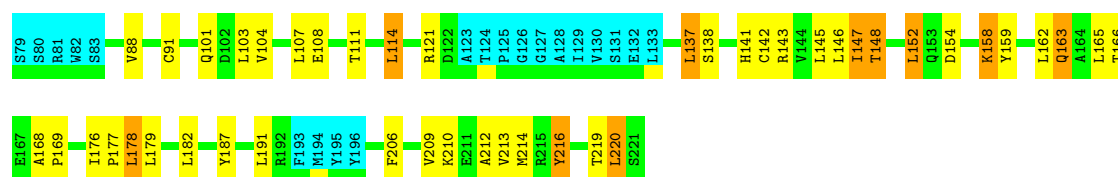
- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



4.2.17 Score per residue for model 17

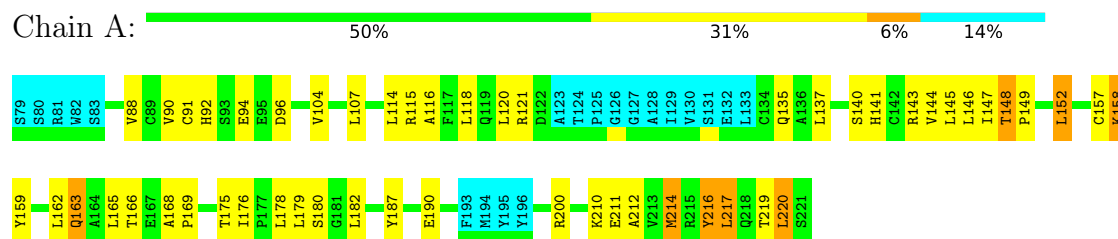
- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein





4.2.18 Score per residue for model 18

- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



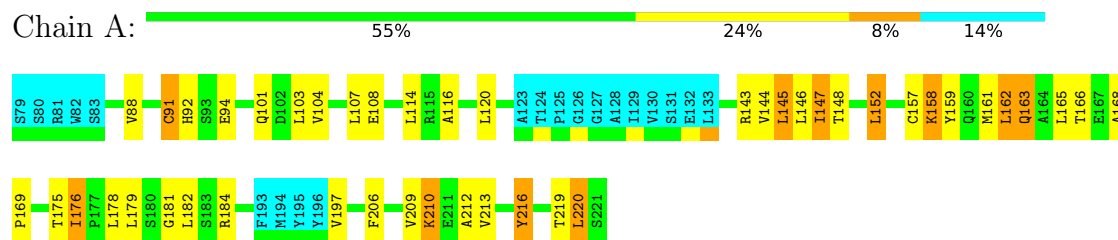
4.2.19 Score per residue for model 19

- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



4.2.20 Score per residue for model 20

- Molecule 1: Toll/interleukin-1 receptor domain-containing adapter protein



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
CYANA	structure solution	2.1
CYANA	refinement	2.1

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	1185
Number of shifts mapped to atoms	1185
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	68%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	944	933	933	26±5
All	All	18880	18660	18660	511

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:VAL:HG23	1:A:116:ALA:HB3	0.86	1.47	15	11
1:A:112:ALA:HB1	1:A:114:LEU:HD13	0.83	1.49	7	3
1:A:162:LEU:C	1:A:162:LEU:HD22	0.81	1.99	20	1
1:A:179:LEU:HD12	1:A:182:LEU:HD12	0.80	1.53	12	1
1:A:137:LEU:HD22	1:A:137:LEU:C	0.80	2.01	17	1
1:A:176:ILE:HD13	1:A:212:ALA:HB3	0.79	1.55	8	9
1:A:144:VAL:HG13	1:A:176:ILE:HD11	0.78	1.54	10	9
1:A:145:LEU:HD21	1:A:147:ILE:HD11	0.76	1.56	7	3
1:A:219:THR:HG23	1:A:220:LEU:HD23	0.71	1.63	15	5
1:A:182:LEU:HD12	1:A:187:TYR:CE1	0.67	2.25	8	2
1:A:216:TYR:O	1:A:219:THR:HG22	0.66	1.90	14	20
1:A:182:LEU:HD13	1:A:187:TYR:CZ	0.66	2.25	19	1
1:A:94:GLU:O	1:A:97:LEU:HD23	0.65	1.92	12	1
1:A:137:LEU:HD12	1:A:143:ARG:HD3	0.65	1.68	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:176:ILE:HD13	1:A:212:ALA:HB1	0.64	1.68	12	6
1:A:176:ILE:HD13	1:A:212:ALA:CB	0.64	2.22	18	4
1:A:179:LEU:HD12	1:A:182:LEU:HD13	0.64	1.69	17	1
1:A:94:GLU:CB	1:A:120:LEU:HD21	0.63	2.23	15	7
1:A:88:VAL:CG2	1:A:114:LEU:HD21	0.63	2.24	18	3
1:A:159:TYR:O	1:A:162:LEU:HD22	0.62	1.95	7	15
1:A:88:VAL:CG2	1:A:114:LEU:HD11	0.62	2.25	20	2
1:A:162:LEU:HD13	1:A:163:GLN:N	0.62	2.09	20	1
1:A:187:TYR:CE2	1:A:197:VAL:HG21	0.61	2.30	4	3
1:A:143:ARG:HB2	1:A:175:THR:HG22	0.61	1.73	19	12
1:A:191:LEU:HD23	1:A:197:VAL:CG1	0.61	2.26	11	1
1:A:178:LEU:O	1:A:179:LEU:HD23	0.61	1.95	8	1
1:A:137:LEU:C	1:A:137:LEU:CD2	0.61	2.74	17	1
1:A:165:LEU:HD13	1:A:190:GLU:CB	0.61	2.26	3	2
1:A:86:TYR:CZ	1:A:136:ALA:HB1	0.61	2.31	15	2
1:A:159:TYR:O	1:A:162:LEU:HD23	0.60	1.96	4	4
1:A:181:GLY:C	1:A:182:LEU:HD23	0.60	2.22	8	1
1:A:143:ARG:CB	1:A:175:THR:HG22	0.59	2.27	16	7
1:A:104:VAL:HG22	1:A:108:GLU:HG3	0.59	1.75	17	6
1:A:149:PRO:O	1:A:186:ALA:HB1	0.59	1.98	11	1
1:A:182:LEU:HD21	1:A:186:ALA:HB3	0.59	1.74	14	1
1:A:187:TYR:HB2	1:A:191:LEU:HD21	0.59	1.75	12	1
1:A:145:LEU:HD12	1:A:175:THR:CB	0.59	2.28	19	1
1:A:88:VAL:HG23	1:A:114:LEU:HD11	0.59	1.74	20	1
1:A:179:LEU:HB3	1:A:182:LEU:HD11	0.59	1.75	8	1
1:A:162:LEU:C	1:A:162:LEU:HD12	0.58	2.24	4	3
1:A:182:LEU:HD22	1:A:187:TYR:CE1	0.58	2.33	19	4
1:A:187:TYR:CZ	1:A:197:VAL:HG21	0.58	2.32	7	2
1:A:162:LEU:HD12	1:A:162:LEU:C	0.58	2.24	5	1
1:A:176:ILE:CD1	1:A:212:ALA:HB1	0.58	2.29	12	6
1:A:91:CYS:O	1:A:145:LEU:HD23	0.57	1.99	18	3
1:A:178:LEU:C	1:A:179:LEU:HD23	0.57	2.24	8	1
1:A:182:LEU:HD21	1:A:186:ALA:CB	0.57	2.29	14	1
1:A:145:LEU:HD12	1:A:175:THR:OG1	0.57	1.99	18	2
1:A:159:TYR:O	1:A:162:LEU:HD12	0.57	2.00	20	1
1:A:165:LEU:HD13	1:A:190:GLU:HG2	0.57	1.77	18	1
1:A:165:LEU:HD13	1:A:190:GLU:HB3	0.57	1.77	9	4
1:A:147:ILE:HD12	1:A:152:LEU:CB	0.56	2.30	20	3
1:A:149:PRO:HB3	1:A:179:LEU:HD21	0.56	1.77	4	1
1:A:149:PRO:HA	1:A:152:LEU:HD22	0.56	1.77	7	1
1:A:181:GLY:O	1:A:182:LEU:HD22	0.56	2.00	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:CYS:O	1:A:145:LEU:HD22	0.56	2.00	11	1
1:A:91:CYS:O	1:A:145:LEU:HD12	0.56	2.01	7	3
1:A:182:LEU:HD12	1:A:187:TYR:CD1	0.56	2.35	11	2
1:A:112:ALA:HB1	1:A:114:LEU:CD1	0.56	2.31	8	3
1:A:88:VAL:HG21	1:A:114:LEU:HD21	0.56	1.78	18	2
1:A:148:THR:O	1:A:152:LEU:HD23	0.56	2.01	17	3
1:A:178:LEU:HD23	1:A:212:ALA:HB2	0.55	1.78	9	1
1:A:216:TYR:CD2	1:A:217:LEU:HD22	0.55	2.36	19	2
1:A:114:LEU:HD23	1:A:115:ARG:N	0.55	2.16	6	3
1:A:179:LEU:HD23	1:A:182:LEU:HG	0.55	1.77	20	1
1:A:104:VAL:CG2	1:A:116:ALA:HB3	0.54	2.32	12	6
1:A:216:TYR:CE1	1:A:217:LEU:HD23	0.54	2.36	5	4
1:A:162:LEU:C	1:A:162:LEU:CD2	0.54	2.73	20	1
1:A:178:LEU:HD11	1:A:208:GLN:OE1	0.54	2.01	3	1
1:A:182:LEU:O	1:A:182:LEU:HD12	0.54	2.01	6	1
1:A:148:THR:O	1:A:152:LEU:HD22	0.54	2.02	14	8
1:A:192:ARG:HB3	1:A:197:VAL:HG13	0.54	1.79	10	1
1:A:86:TYR:CE2	1:A:136:ALA:HB1	0.54	2.36	11	2
1:A:94:GLU:HB3	1:A:120:LEU:HD21	0.54	1.78	15	1
1:A:179:LEU:HD13	1:A:180:SER:N	0.54	2.18	2	1
1:A:178:LEU:HD23	1:A:209:VAL:HG23	0.54	1.79	6	1
1:A:94:GLU:HB2	1:A:120:LEU:HD21	0.54	1.80	11	1
1:A:179:LEU:HD22	1:A:197:VAL:HG11	0.54	1.80	20	1
1:A:179:LEU:HD21	1:A:182:LEU:O	0.54	2.03	14	1
1:A:149:PRO:CB	1:A:182:LEU:HD12	0.54	2.33	19	1
1:A:181:GLY:C	1:A:182:LEU:HD22	0.54	2.28	20	1
1:A:149:PRO:HB3	1:A:179:LEU:HD11	0.53	1.79	2	1
1:A:158:LYS:HE3	1:A:165:LEU:HD12	0.53	1.79	7	12
1:A:182:LEU:HD23	1:A:187:TYR:CE1	0.53	2.39	2	1
1:A:177:PRO:O	1:A:178:LEU:HD22	0.53	2.04	19	1
1:A:179:LEU:HD11	1:A:200:ARG:HA	0.53	1.81	6	1
1:A:94:GLU:CG	1:A:120:LEU:HD21	0.53	2.34	3	4
1:A:137:LEU:HD11	1:A:143:ARG:NE	0.53	2.19	12	1
1:A:178:LEU:C	1:A:179:LEU:HD22	0.53	2.28	7	3
1:A:191:LEU:HD23	1:A:197:VAL:HG11	0.52	1.81	11	1
1:A:179:LEU:HD12	1:A:182:LEU:HB2	0.52	1.80	10	1
1:A:103:LEU:HD22	1:A:210:LYS:HB2	0.52	1.79	12	1
1:A:152:LEU:HD12	1:A:152:LEU:O	0.52	2.05	11	4
1:A:179:LEU:HB2	1:A:182:LEU:HD13	0.52	1.81	16	2
1:A:91:CYS:O	1:A:145:LEU:HD13	0.52	2.05	20	2
1:A:144:VAL:HG12	1:A:146:LEU:CD2	0.52	2.35	15	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:143:ARG:O	1:A:176:ILE:HG22	0.52	2.05	17	5
1:A:152:LEU:HD23	1:A:153:GLN:N	0.51	2.20	7	1
1:A:103:LEU:HD11	1:A:213:VAL:HG11	0.51	1.83	7	2
1:A:179:LEU:CB	1:A:182:LEU:HD13	0.51	2.35	16	1
1:A:178:LEU:O	1:A:179:LEU:HD22	0.51	2.06	9	3
1:A:137:LEU:HD12	1:A:143:ARG:NE	0.51	2.20	18	1
1:A:145:LEU:CD2	1:A:147:ILE:HD11	0.50	2.36	14	1
1:A:206:PHE:O	1:A:209:VAL:HG22	0.50	2.07	3	7
1:A:162:LEU:HD23	1:A:163:GLN:N	0.50	2.22	12	15
1:A:104:VAL:HG22	1:A:108:GLU:CG	0.49	2.36	7	1
1:A:145:LEU:HD23	1:A:177:PRO:HB3	0.49	1.84	2	1
1:A:103:LEU:HD13	1:A:209:VAL:CG1	0.49	2.37	9	1
1:A:188:PRO:HG2	1:A:191:LEU:HD13	0.49	1.85	3	1
1:A:219:THR:CG2	1:A:220:LEU:HD23	0.49	2.37	10	5
1:A:149:PRO:HD3	1:A:179:LEU:HD12	0.49	1.83	18	1
1:A:182:LEU:HD23	1:A:187:TYR:CD1	0.49	2.43	2	1
1:A:162:LEU:HD12	1:A:163:GLN:N	0.49	2.23	5	4
1:A:162:LEU:HD13	1:A:163:GLN:H	0.49	1.65	20	1
1:A:158:LYS:HA	1:A:161:MET:HE2	0.48	1.85	5	4
1:A:178:LEU:HD22	1:A:198:ASP:HB3	0.48	1.84	12	1
1:A:217:LEU:HD13	1:A:220:LEU:HD23	0.48	1.83	19	2
1:A:217:LEU:HD12	1:A:218:GLN:N	0.48	2.24	7	1
1:A:214:MET:HE3	1:A:217:LEU:HD13	0.48	1.85	18	1
1:A:178:LEU:CD2	1:A:212:ALA:HB2	0.48	2.39	9	1
1:A:178:LEU:C	1:A:178:LEU:HD13	0.47	2.34	20	6
1:A:187:TYR:CE2	1:A:197:VAL:HG11	0.47	2.44	6	1
1:A:118:LEU:HD12	1:A:120:LEU:HD13	0.47	1.85	12	1
1:A:103:LEU:HD12	1:A:104:VAL:N	0.47	2.24	1	2
1:A:137:LEU:HD13	1:A:143:ARG:NH1	0.47	2.25	7	1
1:A:145:LEU:HD12	1:A:175:THR:HB	0.47	1.85	19	2
1:A:143:ARG:HB3	1:A:175:THR:HG22	0.47	1.86	18	2
1:A:176:ILE:HG23	1:A:176:ILE:O	0.47	2.10	12	6
1:A:114:LEU:HD22	1:A:216:TYR:OH	0.47	2.09	19	1
1:A:219:THR:CG2	1:A:220:LEU:HD22	0.46	2.40	19	15
1:A:210:LYS:O	1:A:213:VAL:HG12	0.46	2.10	8	5
1:A:137:LEU:HD22	1:A:138:SER:N	0.46	2.24	17	1
1:A:103:LEU:HD13	1:A:209:VAL:HG11	0.46	1.87	9	1
1:A:152:LEU:CD2	1:A:179:LEU:HD11	0.46	2.41	11	1
1:A:177:PRO:HG2	1:A:197:VAL:HG12	0.46	1.88	7	1
1:A:179:LEU:HD23	1:A:197:VAL:HB	0.46	1.87	12	1
1:A:177:PRO:HG3	1:A:191:LEU:HD22	0.46	1.88	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:147:ILE:HD12	1:A:152:LEU:HB2	0.46	1.88	20	2
1:A:187:TYR:CD2	1:A:191:LEU:HD12	0.46	2.45	17	1
1:A:182:LEU:HD22	1:A:187:TYR:CD2	0.45	2.46	10	1
1:A:213:VAL:O	1:A:217:LEU:HD12	0.45	2.11	10	1
1:A:103:LEU:HD13	1:A:103:LEU:O	0.45	2.11	6	1
1:A:187:TYR:OH	1:A:197:VAL:HG21	0.45	2.12	3	1
1:A:206:PHE:O	1:A:209:VAL:HG12	0.45	2.12	10	8
1:A:161:MET:HE3	1:A:165:LEU:HD21	0.45	1.89	6	2
1:A:192:ARG:HG3	1:A:197:VAL:HG22	0.45	1.88	8	1
1:A:178:LEU:HD13	1:A:179:LEU:N	0.45	2.26	14	2
1:A:90:VAL:HG12	1:A:117:PHE:O	0.45	2.11	7	2
1:A:183:SER:OG	1:A:186:ALA:HB2	0.45	2.12	7	1
1:A:178:LEU:HD13	1:A:198:ASP:HB2	0.45	1.88	19	1
1:A:103:LEU:HD13	1:A:103:LEU:C	0.45	2.37	6	1
1:A:182:LEU:HD11	1:A:186:ALA:HB3	0.45	1.89	14	1
1:A:103:LEU:HD21	1:A:213:VAL:HG11	0.45	1.88	19	1
1:A:137:LEU:HD12	1:A:143:ARG:CD	0.44	2.41	10	1
1:A:149:PRO:CB	1:A:182:LEU:HD23	0.44	2.41	14	1
1:A:179:LEU:HD23	1:A:197:VAL:CG1	0.44	2.43	12	1
1:A:182:LEU:HD13	1:A:187:TYR:OH	0.44	2.12	19	1
1:A:219:THR:HG23	1:A:220:LEU:HD22	0.43	1.90	11	15
1:A:161:MET:HE3	1:A:165:LEU:HD11	0.43	1.90	5	5
1:A:168:ALA:HB1	1:A:169:PRO:HD2	0.43	1.90	17	19
1:A:182:LEU:HD23	1:A:186:ALA:HB1	0.43	1.90	10	1
1:A:94:GLU:HG3	1:A:120:LEU:HD21	0.43	1.90	20	3
1:A:179:LEU:HD12	1:A:182:LEU:CD1	0.43	2.42	17	1
1:A:149:PRO:HB3	1:A:182:LEU:HD12	0.43	1.91	19	1
1:A:183:SER:CB	1:A:186:ALA:HB2	0.43	2.44	6	1
1:A:179:LEU:CD2	1:A:182:LEU:HD13	0.43	2.44	4	1
1:A:86:TYR:OH	1:A:136:ALA:HB1	0.43	2.14	15	1
1:A:179:LEU:HD12	1:A:182:LEU:HG	0.42	1.91	1	1
1:A:137:LEU:HD21	1:A:143:ARG:NH1	0.42	2.29	2	1
1:A:90:VAL:HG21	1:A:100:ALA:HB1	0.42	1.91	12	1
1:A:180:SER:C	1:A:182:LEU:HD22	0.42	2.39	11	1
1:A:182:LEU:HD13	1:A:187:TYR:CE1	0.42	2.50	6	1
1:A:179:LEU:HB3	1:A:182:LEU:HD23	0.42	1.91	20	1
1:A:178:LEU:HD22	1:A:198:ASP:O	0.42	2.14	2	1
1:A:103:LEU:C	1:A:103:LEU:HD12	0.42	2.40	14	3
1:A:210:LYS:HG2	1:A:211:GLU:N	0.42	2.29	18	1
1:A:104:VAL:HG22	1:A:108:GLU:HG2	0.42	1.90	7	1
1:A:149:PRO:HB3	1:A:182:LEU:HD22	0.42	1.92	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:144:VAL:HG12	1:A:146:LEU:HD22	0.41	1.91	2	1
1:A:162:LEU:HD23	1:A:163:GLN:H	0.41	1.75	6	9
1:A:182:LEU:HD23	1:A:183:SER:H	0.41	1.76	19	1
1:A:162:LEU:HD22	1:A:162:LEU:O	0.41	2.13	20	1
1:A:179:LEU:HD23	1:A:197:VAL:CB	0.41	2.45	12	1
1:A:178:LEU:HG	1:A:209:VAL:HG12	0.41	1.92	8	1
1:A:118:LEU:HD13	1:A:120:LEU:HD13	0.41	1.91	10	1
1:A:176:ILE:HD12	1:A:212:ALA:HB1	0.41	1.91	16	1
1:A:178:LEU:HD21	1:A:208:GLN:OE1	0.41	2.16	19	1
1:A:214:MET:HE2	1:A:217:LEU:HD21	0.41	1.91	7	1
1:A:144:VAL:HG12	1:A:146:LEU:HD23	0.41	1.92	11	1
1:A:216:TYR:CD1	1:A:217:LEU:HD23	0.41	2.51	14	1
1:A:165:LEU:HD13	1:A:190:GLU:CG	0.41	2.44	18	1
1:A:103:LEU:O	1:A:107:LEU:HD22	0.41	2.16	1	1
1:A:112:ALA:O	1:A:114:LEU:HD12	0.40	2.15	9	1
1:A:118:LEU:HD12	1:A:118:LEU:O	0.40	2.16	14	1
1:A:217:LEU:HD22	1:A:217:LEU:H	0.40	1.76	8	1
1:A:162:LEU:C	1:A:162:LEU:CD1	0.40	2.94	5	1
1:A:90:VAL:HG23	1:A:144:VAL:O	0.40	2.16	18	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	122/143 (85%)	106±2 (87±2%)	15±2 (13±2%)	0±1 (0±1%)	31	76
All	All	2440/2860 (85%)	2121 (87%)	309 (13%)	10 (0%)	31	76

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

Mol	Chain	Res	Type	Models (Total)
1	A	206	PHE	2
1	A	184	ARG	2
1	A	109	GLY	1

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Mol	Chain	Res	Type	Models (Total)
1	A	170	GLY	1
1	A	197	VAL	1
1	A	121	ARG	1
1	A	192	ARG	1
1	A	183	SER	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	103/119 (87%)	82±2 (80±2%)	21±2 (20±2%)	3	32
All	All	2060/2380 (87%)	1642 (80%)	418 (20%)	3	32

All 65 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	107	LEU	20
1	A	146	LEU	20
1	A	147	ILE	20
1	A	148	THR	20
1	A	152	LEU	20
1	A	158	LYS	20
1	A	163	GLN	20
1	A	220	LEU	20
1	A	216	TYR	18
1	A	166	THR	17
1	A	92	HIS	14
1	A	176	ILE	13
1	A	178	LEU	12
1	A	214	MET	10
1	A	96	ASP	10
1	A	157	CYS	10
1	A	84	LYS	9
1	A	121	ARG	9
1	A	145	LEU	9
1	A	210	LYS	9

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Mol	Chain	Res	Type	Models (Total)
1	A	101	GLN	8
1	A	154	ASP	7
1	A	191	LEU	7
1	A	141	HIS	5
1	A	217	LEU	5
1	A	118	LEU	4
1	A	180	SER	4
1	A	200	ARG	4
1	A	85	ASP	4
1	A	142	CYS	4
1	A	120	LEU	4
1	A	162	LEU	4
1	A	215	ARG	4
1	A	184	ARG	3
1	A	113	SER	3
1	A	179	LEU	3
1	A	143	ARG	3
1	A	182	LEU	3
1	A	153	GLN	3
1	A	190	GLU	2
1	A	198	ASP	2
1	A	172	GLU	2
1	A	137	LEU	2
1	A	94	GLU	2
1	A	139	SER	2
1	A	183	SER	2
1	A	140	SER	2
1	A	208	GLN	2
1	A	135	GLN	2
1	A	110	SER	1
1	A	93	SER	1
1	A	122	ASP	1
1	A	213	VAL	1
1	A	108	GLU	1
1	A	187	TYR	1
1	A	97	LEU	1
1	A	192	ARG	1
1	A	197	VAL	1
1	A	221	SER	1
1	A	203	ASP	1
1	A	111	THR	1
1	A	114	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	167	GLU	1
1	A	91	CYS	1
1	A	103	LEU	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 68% for the well-defined parts and 63% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1185
Number of shifts mapped to atoms	1185
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	116	-0.31 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	109	0.41 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	107	0.01 ± 0.12	None needed (< 0.5 ppm)
^{15}N	100	0.18 ± 0.26	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 68%, i.e. 1115 atoms were assigned a chemical shift out of a possible 1633. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	507/610 (83%)	203/248 (82%)	209/246 (85%)	95/116 (82%)
Sidechain	570/922 (62%)	397/603 (66%)	170/284 (60%)	3/35 (9%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	38/101 (38%)	23/49 (47%)	14/49 (29%)	1/3 (33%)
Overall	1115/1633 (68%)	623/900 (69%)	393/579 (68%)	99/154 (64%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 63%, i.e. 1185 atoms were assigned a chemical shift out of a possible 1891. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	538/710 (76%)	215/289 (74%)	223/286 (78%)	100/135 (74%)
Sidechain	609/1040 (59%)	424/682 (62%)	182/320 (57%)	3/38 (8%)
Aromatic	38/141 (27%)	23/68 (34%)	14/69 (20%)	1/4 (25%)
Overall	1185/1891 (63%)	662/1039 (64%)	419/675 (62%)	104/177 (59%)

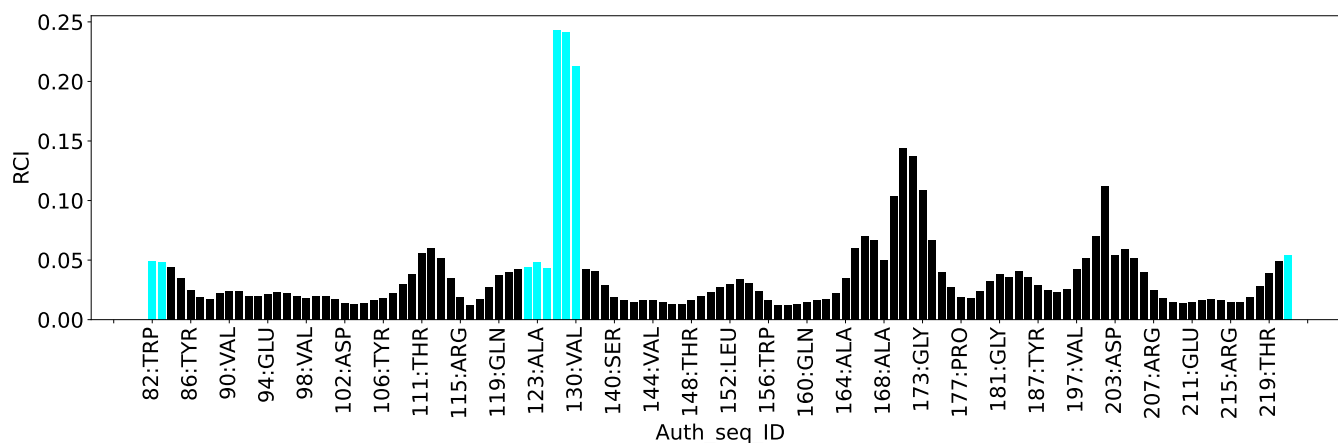
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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	1268
Intra-residue ($ i-j =0$)	313
Sequential ($ i-j =1$)	397
Medium range ($ i-j >1$ and $ i-j <5$)	286
Long range ($ i-j \geq 5$)	272
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	216
Number of unmapped restraints	0
Number of restraints per residue	10.4
Number of long range restraints per residue ¹	1.9

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)	5.0	0.2
0.2-0.5 (Medium)	2.7	0.46
>0.5 (Large)	None	None

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)	18.6	7.25
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis

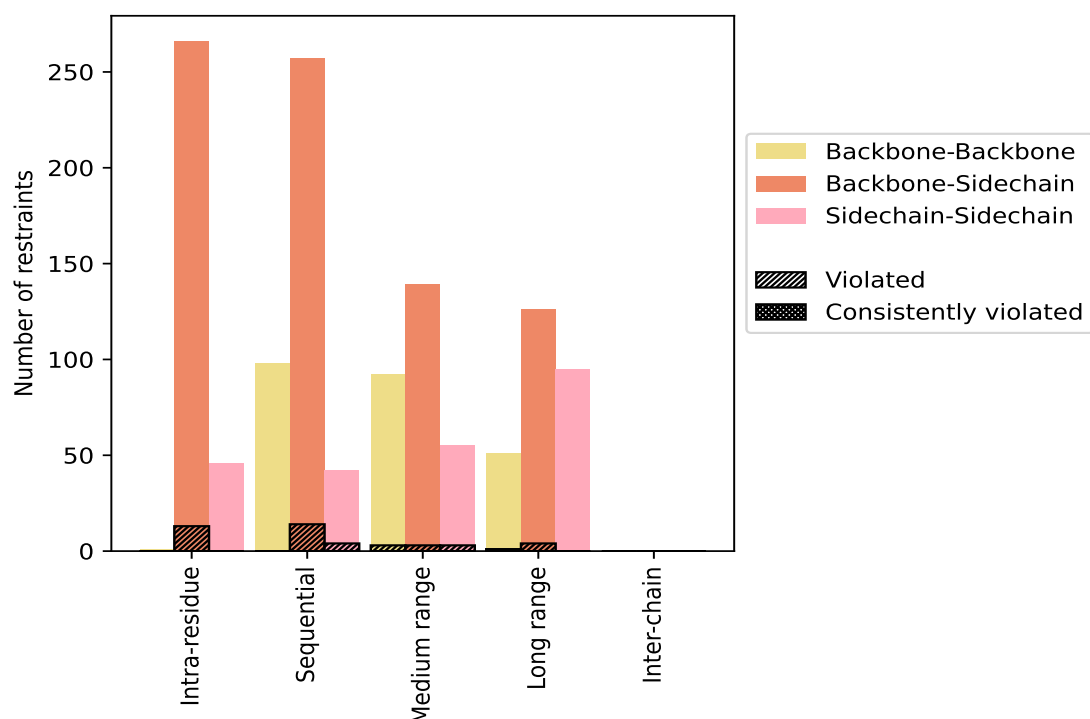
9.1 Summary of distance violations

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 ($i-j =0$)	313	24.7	13	4.2	1.0	0	0.0	0.0
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	266	21.0	13	4.9	1.0	0	0.0	0.0
Sidechain-Sidechain	46	3.6	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	397	31.3	18	4.5	1.4	0	0.0	0.0
Backbone-Backbone	98	7.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	257	20.3	14	5.4	1.1	0	0.0	0.0
Sidechain-Sidechain	42	3.3	4	9.5	0.3	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	286	22.6	9	3.1	0.7	0	0.0	0.0
Backbone-Backbone	92	7.3	3	3.3	0.2	0	0.0	0.0
Backbone-Sidechain	139	11.0	3	2.2	0.2	0	0.0	0.0
Sidechain-Sidechain	55	4.3	3	5.5	0.2	0	0.0	0.0
Long range ($i-j \geq 5$)	272	21.5	5	1.8	0.4	1	0.4	0.1
Backbone-Backbone	51	4.0	1	2.0	0.1	1	2.0	0.1
Backbone-Sidechain	126	9.9	4	3.2	0.3	0	0.0	0.0
Sidechain-Sidechain	95	7.5	0	0.0	0.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1268	100.0	45	3.5	3.5	1	0.1	0.1
Backbone-Backbone	242	19.1	4	1.7	0.3	1	0.4	0.1
Backbone-Sidechain	788	62.1	34	4.3	2.7	0	0.0	0.0
Sidechain-Sidechain	238	18.8	7	2.9	0.6	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	1	1	0	2	0	4	0.19	0.36	0.1	0.16
2	2	2	0	2	0	6	0.18	0.33	0.08	0.14
3	2	1	0	2	0	5	0.19	0.32	0.08	0.14
4	2	3	0	2	0	7	0.18	0.35	0.08	0.17
5	1	2	0	2	0	5	0.19	0.33	0.08	0.18
6	3	0	1	2	0	6	0.24	0.45	0.13	0.23
7	2	5	1	1	0	9	0.18	0.38	0.09	0.14
8	2	5	0	2	0	9	0.18	0.35	0.08	0.15
9	3	3	4	1	0	11	0.18	0.45	0.1	0.14
10	3	7	1	2	0	13	0.18	0.38	0.09	0.14

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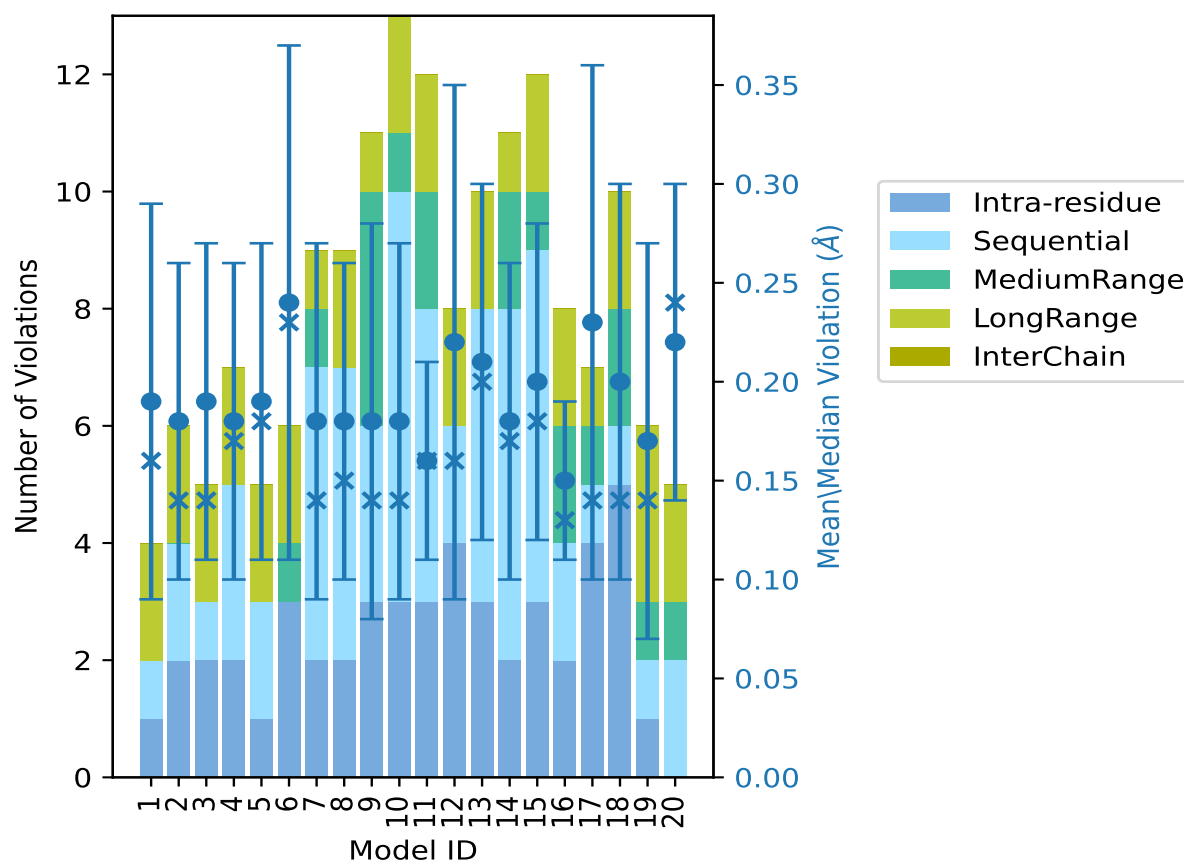
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	3	5	2	2	0	12	0.16	0.3	0.05	0.16
12	4	2	0	2	0	8	0.22	0.46	0.13	0.16
13	3	5	0	2	0	10	0.21	0.38	0.09	0.2
14	2	6	2	1	0	11	0.18	0.38	0.08	0.17
15	3	6	1	2	0	12	0.2	0.38	0.08	0.18
16	2	2	2	2	0	8	0.15	0.21	0.04	0.13
17	4	1	1	1	0	7	0.23	0.45	0.13	0.14
18	5	1	2	2	0	10	0.2	0.45	0.1	0.14
19	1	1	1	3	0	6	0.17	0.38	0.1	0.14
20	0	2	1	2	0	5	0.22	0.35	0.08	0.24

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

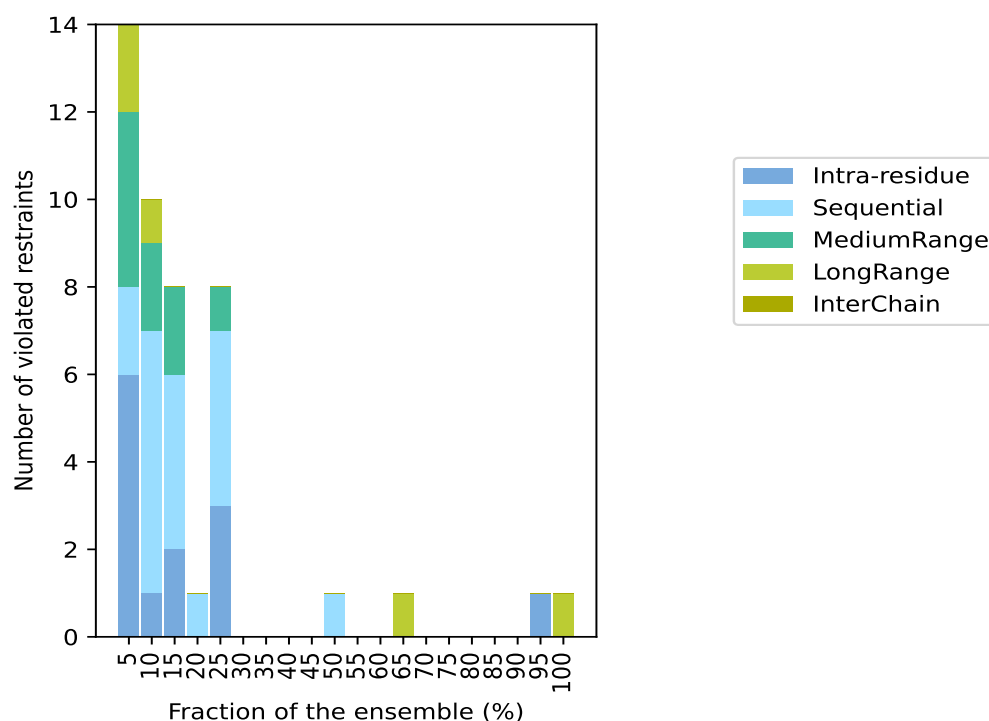
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1223(IR:300, SQ:379, MR:277, LR:267, IC:0) restraints are 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	%
6	2	4	2	0	14	1	5.0
1	6	2	1	0	10	2	10.0
2	4	2	0	0	8	3	15.0
0	1	0	0	0	1	4	20.0
3	4	1	0	0	8	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	1	0	0	0	1	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	1	0	1	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	0	0	0	18	90.0
1	0	0	0	0	1	19	95.0
0	0	0	1	0	1	20	100.0

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

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

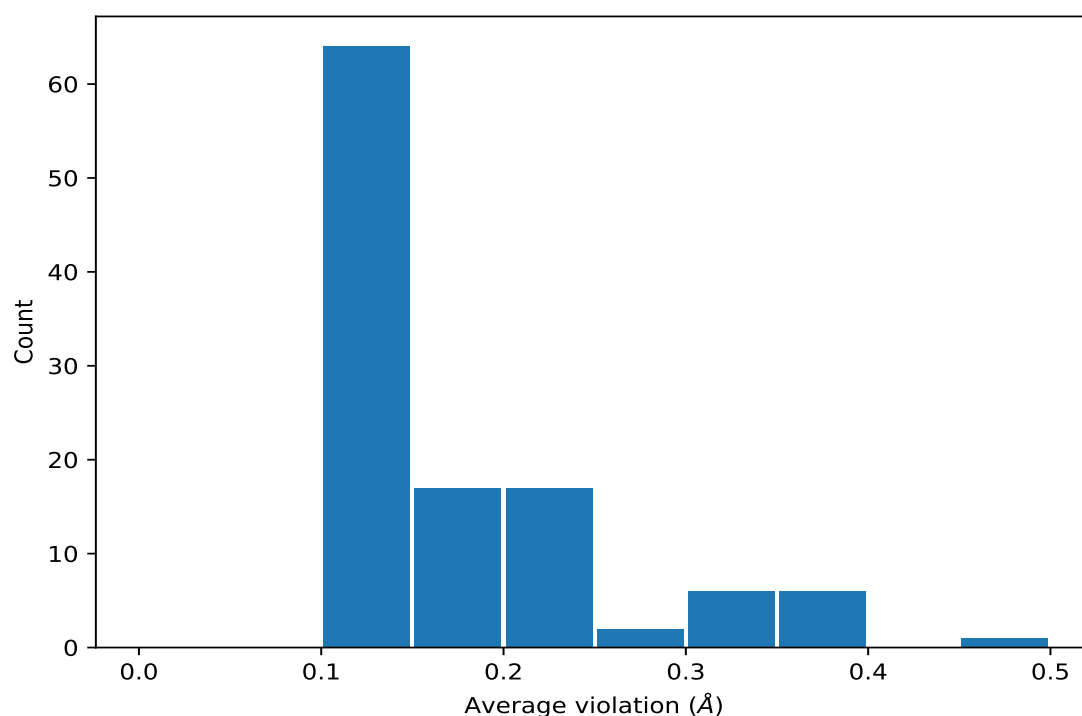
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,616)	1:162:A:LEU:HA	1:167:A:GLU:H	20	0.13	0.04	0.11
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD11	19	0.13	0.01	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD12	19	0.13	0.01	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD13	19	0.13	0.01	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD21	19	0.13	0.01	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD22	19	0.13	0.01	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD23	19	0.13	0.01	0.14
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG21	13	0.33	0.04	0.33
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG22	13	0.33	0.04	0.33
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG23	13	0.33	0.04	0.33
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD11	10	0.15	0.03	0.15
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD12	10	0.15	0.03	0.15
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD13	10	0.15	0.03	0.15
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD21	10	0.15	0.03	0.15
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD22	10	0.15	0.03	0.15
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD23	10	0.15	0.03	0.15

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,814)	1:141:A:HIS:HA	1:141:A:HIS:HE1	5	0.45	0.0	0.45
(1,1267)	1:220:A:LEU:HD11	1:221:A:SER:H	5	0.38	0.0	0.38
(1,1267)	1:220:A:LEU:HD12	1:221:A:SER:H	5	0.38	0.0	0.38
(1,1267)	1:220:A:LEU:HD13	1:221:A:SER:H	5	0.38	0.0	0.38
(1,1267)	1:220:A:LEU:HD21	1:221:A:SER:H	5	0.38	0.0	0.38
(1,1267)	1:220:A:LEU:HD22	1:221:A:SER:H	5	0.38	0.0	0.38
(1,1267)	1:220:A:LEU:HD23	1:221:A:SER:H	5	0.38	0.0	0.38
(1,852)	1:141:A:HIS:H	1:141:A:HIS:HD2	5	0.32	0.0	0.32
(1,256)	1:220:A:LEU:HD21	1:221:A:SER:H	5	0.24	0.0	0.24
(1,256)	1:220:A:LEU:HD22	1:221:A:SER:H	5	0.24	0.0	0.24
(1,256)	1:220:A:LEU:HD23	1:221:A:SER:H	5	0.24	0.0	0.24
(1,667)	1:219:A:THR:H	1:220:A:LEU:HD11	5	0.22	0.01	0.22
(1,667)	1:219:A:THR:H	1:220:A:LEU:HD12	5	0.22	0.01	0.22
(1,667)	1:219:A:THR:H	1:220:A:LEU:HD13	5	0.22	0.01	0.22
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD11	5	0.21	0.0	0.21
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD12	5	0.21	0.0	0.21
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD13	5	0.21	0.0	0.21
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD21	5	0.21	0.0	0.21
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD22	5	0.21	0.0	0.21
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD23	5	0.21	0.0	0.21
(1,242)	1:218:A:GLN:H	1:219:A:THR:HG21	5	0.13	0.01	0.13
(1,242)	1:218:A:GLN:H	1:219:A:THR:HG22	5	0.13	0.01	0.13
(1,242)	1:218:A:GLN:H	1:219:A:THR:HG23	5	0.13	0.01	0.13
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG11	5	0.11	0.01	0.1
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG12	5	0.11	0.01	0.1
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG13	5	0.11	0.01	0.1
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG21	5	0.11	0.01	0.1
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG22	5	0.11	0.01	0.1
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG23	5	0.11	0.01	0.1
(1,1096)	1:162:A:LEU:HD11	1:163:A:GLN:HG3	4	0.17	0.0	0.17
(1,1096)	1:162:A:LEU:HD12	1:163:A:GLN:HG3	4	0.17	0.0	0.17
(1,1096)	1:162:A:LEU:HD13	1:163:A:GLN:HG3	4	0.17	0.0	0.17
(1,1096)	1:162:A:LEU:HD21	1:163:A:GLN:HG3	4	0.17	0.0	0.17
(1,1096)	1:162:A:LEU:HD22	1:163:A:GLN:HG3	4	0.17	0.0	0.17
(1,1096)	1:162:A:LEU:HD23	1:163:A:GLN:HG3	4	0.17	0.0	0.17
(1,841)	1:176:A:ILE:HA	1:176:A:ILE:HD11	3	0.22	0.01	0.23
(1,841)	1:176:A:ILE:HA	1:176:A:ILE:HD12	3	0.22	0.01	0.23
(1,841)	1:176:A:ILE:HA	1:176:A:ILE:HD13	3	0.22	0.01	0.23
(1,1191)	1:209:A:VAL:HG11	1:211:A:GLU:H	3	0.19	0.02	0.2
(1,1191)	1:209:A:VAL:HG12	1:211:A:GLU:H	3	0.19	0.02	0.2
(1,1191)	1:209:A:VAL:HG13	1:211:A:GLU:H	3	0.19	0.02	0.2
(1,1191)	1:209:A:VAL:HG21	1:211:A:GLU:H	3	0.19	0.02	0.2

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1191)	1:209:A:VAL:HG22	1:211:A:GLU:H	3	0.19	0.02	0.2
(1,1191)	1:209:A:VAL:HG23	1:211:A:GLU:H	3	0.19	0.02	0.2
(1,429)	1:208:A:GLN:HA	1:210:A:LYS:H	3	0.16	0.0	0.16
(1,1190)	1:209:A:VAL:HG11	1:210:A:LYS:HE2	3	0.15	0.02	0.14
(1,1190)	1:209:A:VAL:HG11	1:210:A:LYS:HE3	3	0.15	0.02	0.14
(1,1190)	1:209:A:VAL:HG12	1:210:A:LYS:HE2	3	0.15	0.02	0.14
(1,1190)	1:209:A:VAL:HG12	1:210:A:LYS:HE3	3	0.15	0.02	0.14
(1,1190)	1:209:A:VAL:HG13	1:210:A:LYS:HE2	3	0.15	0.02	0.14
(1,1190)	1:209:A:VAL:HG13	1:210:A:LYS:HE3	3	0.15	0.02	0.14
(1,1190)	1:209:A:VAL:HG21	1:210:A:LYS:HE2	3	0.15	0.02	0.14
(1,1190)	1:209:A:VAL:HG21	1:210:A:LYS:HE3	3	0.15	0.02	0.14
(1,1190)	1:209:A:VAL:HG22	1:210:A:LYS:HE2	3	0.15	0.02	0.14
(1,1190)	1:209:A:VAL:HG22	1:210:A:LYS:HE3	3	0.15	0.02	0.14
(1,1190)	1:209:A:VAL:HG23	1:210:A:LYS:HE2	3	0.15	0.02	0.14
(1,1190)	1:209:A:VAL:HG23	1:210:A:LYS:HE3	3	0.15	0.02	0.14
(1,532)	1:215:A:ARG:HA	1:215:A:ARG:HG2	3	0.13	0.01	0.14
(1,375)	1:209:A:VAL:HG21	1:210:A:LYS:H	3	0.13	0.02	0.13
(1,375)	1:209:A:VAL:HG22	1:210:A:LYS:H	3	0.13	0.02	0.13
(1,375)	1:209:A:VAL:HG23	1:210:A:LYS:H	3	0.13	0.02	0.13
(1,816)	1:175:A:THR:HB	1:176:A:ILE:HG21	3	0.13	0.0	0.13
(1,816)	1:175:A:THR:HB	1:176:A:ILE:HG22	3	0.13	0.0	0.13
(1,816)	1:175:A:THR:HB	1:176:A:ILE:HG23	3	0.13	0.0	0.13
(1,1241)	1:215:A:ARG:HB2	1:216:A:TYR:H	3	0.12	0.0	0.12
(1,1241)	1:215:A:ARG:HB3	1:216:A:TYR:H	3	0.12	0.0	0.12
(1,240)	1:216:A:TYR:HD1	1:217:A:LEU:H	2	0.32	0.03	0.32
(1,240)	1:216:A:TYR:HD2	1:217:A:LEU:H	2	0.32	0.03	0.32
(1,1072)	1:153:A:GLN:HG2	1:154:A:ASP:H	2	0.3	0.04	0.3
(1,1072)	1:153:A:GLN:HG3	1:154:A:ASP:H	2	0.3	0.04	0.3
(1,1201)	1:210:A:LYS:HD2	1:211:A:GLU:H	2	0.2	0.0	0.2
(1,1201)	1:210:A:LYS:HD3	1:211:A:GLU:H	2	0.2	0.0	0.2
(1,339)	1:215:A:ARG:H	1:216:A:TYR:HD1	2	0.18	0.03	0.18
(1,339)	1:215:A:ARG:H	1:216:A:TYR:HD2	2	0.18	0.03	0.18
(1,1212)	1:212:A:ALA:H	1:215:A:ARG:HD2	2	0.16	0.05	0.16
(1,1212)	1:212:A:ALA:H	1:215:A:ARG:HD3	2	0.16	0.05	0.16
(1,235)	1:216:A:TYR:H	1:216:A:TYR:HD1	2	0.12	0.02	0.12
(1,235)	1:216:A:TYR:H	1:216:A:TYR:HD2	2	0.12	0.02	0.12
(1,847)	1:144:A:VAL:HA	1:176:A:ILE:HD11	2	0.12	0.01	0.12
(1,847)	1:144:A:VAL:HA	1:176:A:ILE:HD12	2	0.12	0.01	0.12
(1,847)	1:144:A:VAL:HA	1:176:A:ILE:HD13	2	0.12	0.01	0.12
(1,1256)	1:217:A:LEU:HB2	1:218:A:GLN:H	2	0.12	0.01	0.12
(1,1256)	1:217:A:LEU:HB3	1:218:A:GLN:H	2	0.12	0.01	0.12
(1,696)	1:106:A:TYR:HD1	1:107:A:LEU:HA	2	0.11	0.0	0.11

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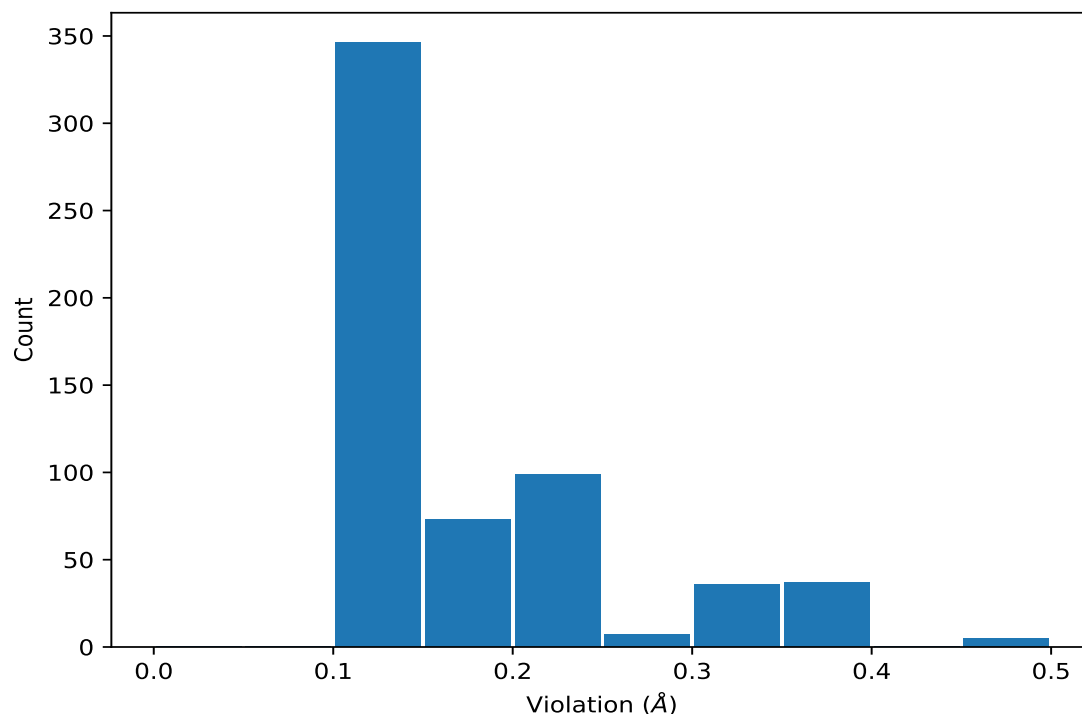
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,696)	1:106:A:TYR:HD2	1:107:A:LEU:HA	2	0.11	0.0	0.11
(1,946)	1:104:A:VAL:HG11	1:107:A:LEU:HB2	2	0.11	0.0	0.11
(1,946)	1:104:A:VAL:HG11	1:107:A:LEU:HB3	2	0.11	0.0	0.11
(1,946)	1:104:A:VAL:HG12	1:107:A:LEU:HB2	2	0.11	0.0	0.11
(1,946)	1:104:A:VAL:HG12	1:107:A:LEU:HB3	2	0.11	0.0	0.11
(1,946)	1:104:A:VAL:HG13	1:107:A:LEU:HB2	2	0.11	0.0	0.11
(1,946)	1:104:A:VAL:HG13	1:107:A:LEU:HB3	2	0.11	0.0	0.11
(1,946)	1:104:A:VAL:HG21	1:107:A:LEU:HB2	2	0.11	0.0	0.11
(1,946)	1:104:A:VAL:HG21	1:107:A:LEU:HB3	2	0.11	0.0	0.11
(1,946)	1:104:A:VAL:HG22	1:107:A:LEU:HB2	2	0.11	0.0	0.11
(1,946)	1:104:A:VAL:HG22	1:107:A:LEU:HB3	2	0.11	0.0	0.11
(1,946)	1:104:A:VAL:HG23	1:107:A:LEU:HB2	2	0.11	0.0	0.11
(1,946)	1:104:A:VAL:HG23	1:107:A:LEU:HB3	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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,814)	1:141:A:HIS:HA	1:141:A:HIS:HE1	12	0.46
(1,814)	1:141:A:HIS:HA	1:141:A:HIS:HE1	6	0.45
(1,814)	1:141:A:HIS:HA	1:141:A:HIS:HE1	9	0.45
(1,814)	1:141:A:HIS:HA	1:141:A:HIS:HE1	17	0.45
(1,814)	1:141:A:HIS:HA	1:141:A:HIS:HE1	18	0.45
(1,1267)	1:220:A:LEU:HD11	1:221:A:SER:H	7	0.38
(1,1267)	1:220:A:LEU:HD12	1:221:A:SER:H	7	0.38
(1,1267)	1:220:A:LEU:HD13	1:221:A:SER:H	7	0.38
(1,1267)	1:220:A:LEU:HD21	1:221:A:SER:H	7	0.38
(1,1267)	1:220:A:LEU:HD22	1:221:A:SER:H	7	0.38
(1,1267)	1:220:A:LEU:HD23	1:221:A:SER:H	7	0.38
(1,1267)	1:220:A:LEU:HD11	1:221:A:SER:H	10	0.38
(1,1267)	1:220:A:LEU:HD12	1:221:A:SER:H	10	0.38
(1,1267)	1:220:A:LEU:HD13	1:221:A:SER:H	10	0.38
(1,1267)	1:220:A:LEU:HD21	1:221:A:SER:H	10	0.38
(1,1267)	1:220:A:LEU:HD22	1:221:A:SER:H	10	0.38
(1,1267)	1:220:A:LEU:HD23	1:221:A:SER:H	10	0.38
(1,1267)	1:220:A:LEU:HD11	1:221:A:SER:H	13	0.38
(1,1267)	1:220:A:LEU:HD12	1:221:A:SER:H	13	0.38
(1,1267)	1:220:A:LEU:HD13	1:221:A:SER:H	13	0.38
(1,1267)	1:220:A:LEU:HD21	1:221:A:SER:H	13	0.38
(1,1267)	1:220:A:LEU:HD22	1:221:A:SER:H	13	0.38
(1,1267)	1:220:A:LEU:HD23	1:221:A:SER:H	13	0.38
(1,1267)	1:220:A:LEU:HD11	1:221:A:SER:H	14	0.38
(1,1267)	1:220:A:LEU:HD12	1:221:A:SER:H	14	0.38
(1,1267)	1:220:A:LEU:HD13	1:221:A:SER:H	14	0.38
(1,1267)	1:220:A:LEU:HD21	1:221:A:SER:H	14	0.38
(1,1267)	1:220:A:LEU:HD22	1:221:A:SER:H	14	0.38
(1,1267)	1:220:A:LEU:HD23	1:221:A:SER:H	14	0.38
(1,1267)	1:220:A:LEU:HD11	1:221:A:SER:H	15	0.38
(1,1267)	1:220:A:LEU:HD12	1:221:A:SER:H	15	0.38
(1,1267)	1:220:A:LEU:HD13	1:221:A:SER:H	15	0.38
(1,1267)	1:220:A:LEU:HD21	1:221:A:SER:H	15	0.38
(1,1267)	1:220:A:LEU:HD22	1:221:A:SER:H	15	0.38
(1,1267)	1:220:A:LEU:HD23	1:221:A:SER:H	15	0.38
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG21	19	0.38
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG22	19	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG23	19	0.38
(1,673)	1:114:A:LEU:HA	1:114:A:LEU:HG	17	0.37
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG21	1	0.36
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG22	1	0.36
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG23	1	0.36
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG21	8	0.35
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG22	8	0.35
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG23	8	0.35
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG21	20	0.35
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG22	20	0.35
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG23	20	0.35
(1,240)	1:216:A:TYR:HD1	1:217:A:LEU:H	4	0.35
(1,240)	1:216:A:TYR:HD2	1:217:A:LEU:H	4	0.35
(1,1072)	1:153:A:GLN:HG2	1:154:A:ASP:H	12	0.34
(1,1072)	1:153:A:GLN:HG3	1:154:A:ASP:H	12	0.34
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG21	13	0.34
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG22	13	0.34
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG23	13	0.34
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG21	15	0.34
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG22	15	0.34
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG23	15	0.34
(1,852)	1:141:A:HIS:H	1:141:A:HIS:HD2	17	0.33
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG21	2	0.33
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG22	2	0.33
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG23	2	0.33
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG21	5	0.33
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG22	5	0.33
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG23	5	0.33
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG21	6	0.33
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG22	6	0.33
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG23	6	0.33
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG21	10	0.33
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG22	10	0.33
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG23	10	0.33
(1,852)	1:141:A:HIS:H	1:141:A:HIS:HD2	6	0.32
(1,852)	1:141:A:HIS:H	1:141:A:HIS:HD2	9	0.32
(1,852)	1:141:A:HIS:H	1:141:A:HIS:HD2	12	0.32
(1,852)	1:141:A:HIS:H	1:141:A:HIS:HD2	18	0.32
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG21	3	0.32
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG22	3	0.32
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG23	3	0.32
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG21	11	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG22	11	0.3
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG23	11	0.3
(1,240)	1:216:A:TYR:HD1	1:217:A:LEU:H	8	0.28
(1,240)	1:216:A:TYR:HD2	1:217:A:LEU:H	8	0.28
(1,1072)	1:153:A:GLN:HG2	1:154:A:ASP:H	20	0.26
(1,1072)	1:153:A:GLN:HG3	1:154:A:ASP:H	20	0.26
(1,616)	1:162:A:LEU:HA	1:167:A:GLU:H	20	0.24
(1,256)	1:220:A:LEU:HD21	1:221:A:SER:H	7	0.24
(1,256)	1:220:A:LEU:HD22	1:221:A:SER:H	7	0.24
(1,256)	1:220:A:LEU:HD23	1:221:A:SER:H	7	0.24
(1,256)	1:220:A:LEU:HD21	1:221:A:SER:H	10	0.24
(1,256)	1:220:A:LEU:HD22	1:221:A:SER:H	10	0.24
(1,256)	1:220:A:LEU:HD23	1:221:A:SER:H	10	0.24
(1,256)	1:220:A:LEU:HD21	1:221:A:SER:H	13	0.24
(1,256)	1:220:A:LEU:HD22	1:221:A:SER:H	13	0.24
(1,256)	1:220:A:LEU:HD23	1:221:A:SER:H	13	0.24
(1,256)	1:220:A:LEU:HD21	1:221:A:SER:H	14	0.24
(1,256)	1:220:A:LEU:HD22	1:221:A:SER:H	14	0.24
(1,256)	1:220:A:LEU:HD23	1:221:A:SER:H	14	0.24
(1,841)	1:176:A:ILE:HA	1:176:A:ILE:HD11	2	0.23
(1,841)	1:176:A:ILE:HA	1:176:A:ILE:HD12	2	0.23
(1,841)	1:176:A:ILE:HA	1:176:A:ILE:HD13	2	0.23
(1,841)	1:176:A:ILE:HA	1:176:A:ILE:HD11	3	0.23
(1,841)	1:176:A:ILE:HA	1:176:A:ILE:HD12	3	0.23
(1,841)	1:176:A:ILE:HA	1:176:A:ILE:HD13	3	0.23
(1,667)	1:219:A:THR:H	1:220:A:LEU:HD11	15	0.23
(1,667)	1:219:A:THR:H	1:220:A:LEU:HD12	15	0.23
(1,667)	1:219:A:THR:H	1:220:A:LEU:HD13	15	0.23
(1,256)	1:220:A:LEU:HD21	1:221:A:SER:H	15	0.23
(1,256)	1:220:A:LEU:HD22	1:221:A:SER:H	15	0.23
(1,256)	1:220:A:LEU:HD23	1:221:A:SER:H	15	0.23
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD11	13	0.22
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD12	13	0.22
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD13	13	0.22
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD21	13	0.22
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD22	13	0.22
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD23	13	0.22
(1,667)	1:219:A:THR:H	1:220:A:LEU:HD11	7	0.22
(1,667)	1:219:A:THR:H	1:220:A:LEU:HD12	7	0.22
(1,667)	1:219:A:THR:H	1:220:A:LEU:HD13	7	0.22
(1,667)	1:219:A:THR:H	1:220:A:LEU:HD11	10	0.22
(1,667)	1:219:A:THR:H	1:220:A:LEU:HD12	10	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,667)	1:219:A:THR:H	1:220:A:LEU:HD13	10	0.22
(1,667)	1:219:A:THR:H	1:220:A:LEU:HD11	14	0.22
(1,667)	1:219:A:THR:H	1:220:A:LEU:HD12	14	0.22
(1,667)	1:219:A:THR:H	1:220:A:LEU:HD13	14	0.22
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG21	18	0.22
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG22	18	0.22
(1,418)	1:145:A:LEU:H	1:176:A:ILE:HG23	18	0.22
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD11	7	0.21
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD12	7	0.21
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD13	7	0.21
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD21	7	0.21
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD22	7	0.21
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD23	7	0.21
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD11	10	0.21
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD12	10	0.21
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD13	10	0.21
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD21	10	0.21
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD22	10	0.21
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD23	10	0.21
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD11	14	0.21
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD12	14	0.21
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD13	14	0.21
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD21	14	0.21
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD22	14	0.21
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD23	14	0.21
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD11	15	0.21
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD12	15	0.21
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD13	15	0.21
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD21	15	0.21
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD22	15	0.21
(1,1265)	1:220:A:LEU:HA	1:220:A:LEU:HD23	15	0.21
(1,1212)	1:212:A:ALA:H	1:215:A:ARG:HD2	16	0.21
(1,1212)	1:212:A:ALA:H	1:215:A:ARG:HD3	16	0.21
(1,1201)	1:210:A:LYS:HD2	1:211:A:GLU:H	16	0.21
(1,1201)	1:210:A:LYS:HD3	1:211:A:GLU:H	16	0.21
(1,841)	1:176:A:ILE:HA	1:176:A:ILE:HD11	11	0.21
(1,841)	1:176:A:ILE:HA	1:176:A:ILE:HD12	11	0.21
(1,841)	1:176:A:ILE:HA	1:176:A:ILE:HD13	11	0.21
(1,667)	1:219:A:THR:H	1:220:A:LEU:HD11	13	0.21
(1,667)	1:219:A:THR:H	1:220:A:LEU:HD12	13	0.21
(1,667)	1:219:A:THR:H	1:220:A:LEU:HD13	13	0.21
(1,1201)	1:210:A:LYS:HD2	1:211:A:GLU:H	18	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1201)	1:210:A:LYS:HD3	1:211:A:GLU:H	18	0.2
(1,1191)	1:209:A:VAL:HG11	1:211:A:GLU:H	9	0.2
(1,1191)	1:209:A:VAL:HG12	1:211:A:GLU:H	9	0.2
(1,1191)	1:209:A:VAL:HG13	1:211:A:GLU:H	9	0.2
(1,1191)	1:209:A:VAL:HG21	1:211:A:GLU:H	9	0.2
(1,1191)	1:209:A:VAL:HG22	1:211:A:GLU:H	9	0.2
(1,1191)	1:209:A:VAL:HG23	1:211:A:GLU:H	9	0.2
(1,1191)	1:209:A:VAL:HG11	1:211:A:GLU:H	14	0.2
(1,1191)	1:209:A:VAL:HG12	1:211:A:GLU:H	14	0.2
(1,1191)	1:209:A:VAL:HG13	1:211:A:GLU:H	14	0.2
(1,1191)	1:209:A:VAL:HG21	1:211:A:GLU:H	14	0.2
(1,1191)	1:209:A:VAL:HG22	1:211:A:GLU:H	14	0.2
(1,1191)	1:209:A:VAL:HG23	1:211:A:GLU:H	14	0.2
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD11	12	0.2
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD12	12	0.2
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD13	12	0.2
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD21	12	0.2
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD22	12	0.2
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD23	12	0.2
(1,339)	1:215:A:ARG:H	1:216:A:TYR:HD1	4	0.2
(1,339)	1:215:A:ARG:H	1:216:A:TYR:HD2	4	0.2
(1,1190)	1:209:A:VAL:HG11	1:210:A:LYS:HE2	11	0.18
(1,1190)	1:209:A:VAL:HG11	1:210:A:LYS:HE3	11	0.18
(1,1190)	1:209:A:VAL:HG12	1:210:A:LYS:HE2	11	0.18
(1,1190)	1:209:A:VAL:HG12	1:210:A:LYS:HE3	11	0.18
(1,1190)	1:209:A:VAL:HG13	1:210:A:LYS:HE2	11	0.18
(1,1190)	1:209:A:VAL:HG13	1:210:A:LYS:HE3	11	0.18
(1,1190)	1:209:A:VAL:HG21	1:210:A:LYS:HE2	11	0.18
(1,1190)	1:209:A:VAL:HG21	1:210:A:LYS:HE3	11	0.18
(1,1190)	1:209:A:VAL:HG22	1:210:A:LYS:HE2	11	0.18
(1,1190)	1:209:A:VAL:HG22	1:210:A:LYS:HE3	11	0.18
(1,1190)	1:209:A:VAL:HG23	1:210:A:LYS:HE2	11	0.18
(1,1190)	1:209:A:VAL:HG23	1:210:A:LYS:HE3	11	0.18
(1,1096)	1:162:A:LEU:HD11	1:163:A:GLN:HG3	5	0.18
(1,1096)	1:162:A:LEU:HD12	1:163:A:GLN:HG3	5	0.18
(1,1096)	1:162:A:LEU:HD13	1:163:A:GLN:HG3	5	0.18
(1,1096)	1:162:A:LEU:HD21	1:163:A:GLN:HG3	5	0.18
(1,1096)	1:162:A:LEU:HD22	1:163:A:GLN:HG3	5	0.18
(1,1096)	1:162:A:LEU:HD23	1:163:A:GLN:HG3	5	0.18
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD11	1	0.18
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD12	1	0.18
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD13	1	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD21	1	0.18
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD22	1	0.18
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD23	1	0.18
(1,988)	1:120:A:LEU:HA	1:120:A:LEU:HD11	13	0.18
(1,988)	1:120:A:LEU:HA	1:120:A:LEU:HD12	13	0.18
(1,988)	1:120:A:LEU:HA	1:120:A:LEU:HD13	13	0.18
(1,988)	1:120:A:LEU:HA	1:120:A:LEU:HD21	13	0.18
(1,988)	1:120:A:LEU:HA	1:120:A:LEU:HD22	13	0.18
(1,988)	1:120:A:LEU:HA	1:120:A:LEU:HD23	13	0.18
(1,616)	1:162:A:LEU:HA	1:167:A:GLU:H	4	0.18
(1,616)	1:162:A:LEU:HA	1:167:A:GLU:H	5	0.18
(1,616)	1:162:A:LEU:HA	1:167:A:GLU:H	8	0.18
(1,616)	1:162:A:LEU:HA	1:167:A:GLU:H	15	0.18
(1,1096)	1:162:A:LEU:HD11	1:163:A:GLN:HG3	4	0.17
(1,1096)	1:162:A:LEU:HD12	1:163:A:GLN:HG3	4	0.17
(1,1096)	1:162:A:LEU:HD13	1:163:A:GLN:HG3	4	0.17
(1,1096)	1:162:A:LEU:HD21	1:163:A:GLN:HG3	4	0.17
(1,1096)	1:162:A:LEU:HD22	1:163:A:GLN:HG3	4	0.17
(1,1096)	1:162:A:LEU:HD23	1:163:A:GLN:HG3	4	0.17
(1,1096)	1:162:A:LEU:HD11	1:163:A:GLN:HG3	8	0.17
(1,1096)	1:162:A:LEU:HD12	1:163:A:GLN:HG3	8	0.17
(1,1096)	1:162:A:LEU:HD13	1:163:A:GLN:HG3	8	0.17
(1,1096)	1:162:A:LEU:HD21	1:163:A:GLN:HG3	8	0.17
(1,1096)	1:162:A:LEU:HD22	1:163:A:GLN:HG3	8	0.17
(1,1096)	1:162:A:LEU:HD23	1:163:A:GLN:HG3	8	0.17
(1,1096)	1:162:A:LEU:HD11	1:163:A:GLN:HG3	15	0.17
(1,1096)	1:162:A:LEU:HD12	1:163:A:GLN:HG3	15	0.17
(1,1096)	1:162:A:LEU:HD13	1:163:A:GLN:HG3	15	0.17
(1,1096)	1:162:A:LEU:HD21	1:163:A:GLN:HG3	15	0.17
(1,1096)	1:162:A:LEU:HD22	1:163:A:GLN:HG3	15	0.17
(1,1096)	1:162:A:LEU:HD23	1:163:A:GLN:HG3	15	0.17
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD11	20	0.17
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD12	20	0.17
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD13	20	0.17
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD21	20	0.17
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD22	20	0.17
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD23	20	0.17
(1,429)	1:208:A:GLN:HA	1:210:A:LYS:H	14	0.17
(1,1191)	1:209:A:VAL:HG11	1:211:A:GLU:H	11	0.16
(1,1191)	1:209:A:VAL:HG12	1:211:A:GLU:H	11	0.16
(1,1191)	1:209:A:VAL:HG13	1:211:A:GLU:H	11	0.16
(1,1191)	1:209:A:VAL:HG21	1:211:A:GLU:H	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1191)	1:209:A:VAL:HG22	1:211:A:GLU:H	11	0.16
(1,1191)	1:209:A:VAL:HG23	1:211:A:GLU:H	11	0.16
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD11	11	0.16
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD12	11	0.16
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD13	11	0.16
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD21	11	0.16
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD22	11	0.16
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD23	11	0.16
(1,429)	1:208:A:GLN:HA	1:210:A:LYS:H	9	0.16
(1,429)	1:208:A:GLN:HA	1:210:A:LYS:H	11	0.16
(1,1125)	1:178:A:LEU:HD11	1:199:A:GLY:HA2	19	0.15
(1,1125)	1:178:A:LEU:HD11	1:199:A:GLY:HA3	19	0.15
(1,1125)	1:178:A:LEU:HD12	1:199:A:GLY:HA2	19	0.15
(1,1125)	1:178:A:LEU:HD12	1:199:A:GLY:HA3	19	0.15
(1,1125)	1:178:A:LEU:HD13	1:199:A:GLY:HA2	19	0.15
(1,1125)	1:178:A:LEU:HD13	1:199:A:GLY:HA3	19	0.15
(1,1125)	1:178:A:LEU:HD21	1:199:A:GLY:HA2	19	0.15
(1,1125)	1:178:A:LEU:HD21	1:199:A:GLY:HA3	19	0.15
(1,1125)	1:178:A:LEU:HD22	1:199:A:GLY:HA2	19	0.15
(1,1125)	1:178:A:LEU:HD22	1:199:A:GLY:HA3	19	0.15
(1,1125)	1:178:A:LEU:HD23	1:199:A:GLY:HA2	19	0.15
(1,1125)	1:178:A:LEU:HD23	1:199:A:GLY:HA3	19	0.15
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD11	8	0.15
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD12	8	0.15
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD13	8	0.15
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD21	8	0.15
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD22	8	0.15
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD23	8	0.15
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD11	16	0.15
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD12	16	0.15
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD13	16	0.15
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD21	16	0.15
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD22	16	0.15
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD23	16	0.15
(1,375)	1:209:A:VAL:HG21	1:210:A:LYS:H	11	0.15
(1,375)	1:209:A:VAL:HG22	1:210:A:LYS:H	11	0.15
(1,375)	1:209:A:VAL:HG23	1:210:A:LYS:H	11	0.15
(1,339)	1:215:A:ARG:H	1:216:A:TYR:HD1	8	0.15
(1,339)	1:215:A:ARG:H	1:216:A:TYR:HD2	8	0.15
(1,1238)	1:215:A:ARG:HA	1:215:A:ARG:HD2	11	0.14
(1,1238)	1:215:A:ARG:HA	1:215:A:ARG:HD3	11	0.14
(1,1190)	1:209:A:VAL:HG11	1:210:A:LYS:HE2	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1190)	1:209:A:VAL:HG11	1:210:A:LYS:HE3	9	0.14
(1,1190)	1:209:A:VAL:HG12	1:210:A:LYS:HE2	9	0.14
(1,1190)	1:209:A:VAL:HG12	1:210:A:LYS:HE3	9	0.14
(1,1190)	1:209:A:VAL:HG13	1:210:A:LYS:HE2	9	0.14
(1,1190)	1:209:A:VAL:HG13	1:210:A:LYS:HE3	9	0.14
(1,1190)	1:209:A:VAL:HG21	1:210:A:LYS:HE2	9	0.14
(1,1190)	1:209:A:VAL:HG21	1:210:A:LYS:HE3	9	0.14
(1,1190)	1:209:A:VAL:HG22	1:210:A:LYS:HE2	9	0.14
(1,1190)	1:209:A:VAL:HG22	1:210:A:LYS:HE3	9	0.14
(1,1190)	1:209:A:VAL:HG23	1:210:A:LYS:HE2	9	0.14
(1,1190)	1:209:A:VAL:HG23	1:210:A:LYS:HE3	9	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD11	2	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD12	2	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD13	2	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD21	2	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD22	2	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD23	2	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD11	3	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD12	3	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD13	3	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD21	3	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD22	3	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD23	3	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD11	6	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD12	6	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD13	6	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD21	6	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD22	6	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD23	6	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD11	9	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD12	9	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD13	9	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD21	9	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD22	9	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD23	9	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD11	10	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD12	10	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD13	10	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD21	10	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD22	10	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD23	10	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD11	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD12	11	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD13	11	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD21	11	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD22	11	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD23	11	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD11	13	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD12	13	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD13	13	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD21	13	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD22	13	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD23	13	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD11	14	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD12	14	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD13	14	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD21	14	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD22	14	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD23	14	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD11	17	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD12	17	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD13	17	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD21	17	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD22	17	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD23	17	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD11	18	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD12	18	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD13	18	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD21	18	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD22	18	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD23	18	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD11	19	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD12	19	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD13	19	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD21	19	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD22	19	0.14
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD23	19	0.14
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD11	5	0.14
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD12	5	0.14
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD13	5	0.14
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD21	5	0.14
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD22	5	0.14
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD23	5	0.14
(1,858)	1:186:A:ALA:HB1	1:187:A:TYR:HE1	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,858)	1:186:A:ALA:HB1	1:187:A:TYR:HE2	19	0.14
(1,858)	1:186:A:ALA:HB2	1:187:A:TYR:HE1	19	0.14
(1,858)	1:186:A:ALA:HB2	1:187:A:TYR:HE2	19	0.14
(1,858)	1:186:A:ALA:HB3	1:187:A:TYR:HE1	19	0.14
(1,858)	1:186:A:ALA:HB3	1:187:A:TYR:HE2	19	0.14
(1,532)	1:215:A:ARG:HA	1:215:A:ARG:HG2	10	0.14
(1,532)	1:215:A:ARG:HA	1:215:A:ARG:HG2	15	0.14
(1,242)	1:218:A:GLN:H	1:219:A:THR:HG21	7	0.14
(1,242)	1:218:A:GLN:H	1:219:A:THR:HG22	7	0.14
(1,242)	1:218:A:GLN:H	1:219:A:THR:HG23	7	0.14
(1,235)	1:216:A:TYR:H	1:216:A:TYR:HD1	8	0.14
(1,235)	1:216:A:TYR:H	1:216:A:TYR:HD2	8	0.14
(1,224)	1:210:A:LYS:HG2	1:213:A:VAL:H	18	0.14
(1,216)	1:207:A:ARG:HA	1:211:A:GLU:H	18	0.14
(1,1256)	1:217:A:LEU:HB2	1:218:A:GLN:H	13	0.13
(1,1256)	1:217:A:LEU:HB3	1:218:A:GLN:H	13	0.13
(1,1190)	1:209:A:VAL:HG11	1:210:A:LYS:HE2	14	0.13
(1,1190)	1:209:A:VAL:HG11	1:210:A:LYS:HE3	14	0.13
(1,1190)	1:209:A:VAL:HG12	1:210:A:LYS:HE2	14	0.13
(1,1190)	1:209:A:VAL:HG12	1:210:A:LYS:HE3	14	0.13
(1,1190)	1:209:A:VAL:HG13	1:210:A:LYS:HE2	14	0.13
(1,1190)	1:209:A:VAL:HG13	1:210:A:LYS:HE3	14	0.13
(1,1190)	1:209:A:VAL:HG21	1:210:A:LYS:HE2	14	0.13
(1,1190)	1:209:A:VAL:HG21	1:210:A:LYS:HE3	14	0.13
(1,1190)	1:209:A:VAL:HG22	1:210:A:LYS:HE2	14	0.13
(1,1190)	1:209:A:VAL:HG22	1:210:A:LYS:HE3	14	0.13
(1,1190)	1:209:A:VAL:HG23	1:210:A:LYS:HE2	14	0.13
(1,1190)	1:209:A:VAL:HG23	1:210:A:LYS:HE3	14	0.13
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD11	1	0.13
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD12	1	0.13
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD13	1	0.13
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD21	1	0.13
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD22	1	0.13
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD23	1	0.13
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD11	7	0.13
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD12	7	0.13
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD13	7	0.13
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD21	7	0.13
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD22	7	0.13
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD23	7	0.13
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD11	12	0.13
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD12	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD13	12	0.13
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD21	12	0.13
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD22	12	0.13
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD23	12	0.13
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD11	16	0.13
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD12	16	0.13
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD13	16	0.13
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD21	16	0.13
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD22	16	0.13
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD23	16	0.13
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG11	9	0.13
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG12	9	0.13
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG13	9	0.13
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG21	9	0.13
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG22	9	0.13
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG23	9	0.13
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG11	10	0.13
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG12	10	0.13
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG13	10	0.13
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG21	10	0.13
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG22	10	0.13
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG23	10	0.13
(1,847)	1:144:A:VAL:HA	1:176:A:ILE:HD11	4	0.13
(1,847)	1:144:A:VAL:HA	1:176:A:ILE:HD12	4	0.13
(1,847)	1:144:A:VAL:HA	1:176:A:ILE:HD13	4	0.13
(1,816)	1:175:A:THR:HB	1:176:A:ILE:HG21	2	0.13
(1,816)	1:175:A:THR:HB	1:176:A:ILE:HG22	2	0.13
(1,816)	1:175:A:THR:HB	1:176:A:ILE:HG23	2	0.13
(1,816)	1:175:A:THR:HB	1:176:A:ILE:HG21	3	0.13
(1,816)	1:175:A:THR:HB	1:176:A:ILE:HG22	3	0.13
(1,816)	1:175:A:THR:HB	1:176:A:ILE:HG23	3	0.13
(1,651)	1:210:A:LYS:HG2	1:214:A:MET:HG3	16	0.13
(1,375)	1:209:A:VAL:HG21	1:210:A:LYS:H	9	0.13
(1,375)	1:209:A:VAL:HG22	1:210:A:LYS:H	9	0.13
(1,375)	1:209:A:VAL:HG23	1:210:A:LYS:H	9	0.13
(1,242)	1:218:A:GLN:H	1:219:A:THR:HG21	10	0.13
(1,242)	1:218:A:GLN:H	1:219:A:THR:HG22	10	0.13
(1,242)	1:218:A:GLN:H	1:219:A:THR:HG23	10	0.13
(1,242)	1:218:A:GLN:H	1:219:A:THR:HG21	15	0.13
(1,242)	1:218:A:GLN:H	1:219:A:THR:HG22	15	0.13
(1,242)	1:218:A:GLN:H	1:219:A:THR:HG23	15	0.13
(1,1241)	1:215:A:ARG:HB2	1:216:A:TYR:H	11	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1241)	1:215:A:ARG:HB3	1:216:A:TYR:H	11	0.12
(1,1241)	1:215:A:ARG:HB2	1:216:A:TYR:H	15	0.12
(1,1241)	1:215:A:ARG:HB3	1:216:A:TYR:H	15	0.12
(1,1193)	1:210:A:LYS:H	1:210:A:LYS:HE2	18	0.12
(1,1193)	1:210:A:LYS:H	1:210:A:LYS:HE3	18	0.12
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD11	17	0.12
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD12	17	0.12
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD13	17	0.12
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD21	17	0.12
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD22	17	0.12
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD23	17	0.12
(1,816)	1:175:A:THR:HB	1:176:A:ILE:HG21	11	0.12
(1,816)	1:175:A:THR:HB	1:176:A:ILE:HG22	11	0.12
(1,816)	1:175:A:THR:HB	1:176:A:ILE:HG23	11	0.12
(1,768)	1:124:A:THR:H	1:124:A:THR:HG21	18	0.12
(1,768)	1:124:A:THR:H	1:124:A:THR:HG22	18	0.12
(1,768)	1:124:A:THR:H	1:124:A:THR:HG23	18	0.12
(1,616)	1:162:A:LEU:HA	1:167:A:GLU:H	2	0.12
(1,532)	1:215:A:ARG:HA	1:215:A:ARG:HG2	16	0.12
(1,242)	1:218:A:GLN:H	1:219:A:THR:HG21	13	0.12
(1,242)	1:218:A:GLN:H	1:219:A:THR:HG22	13	0.12
(1,242)	1:218:A:GLN:H	1:219:A:THR:HG23	13	0.12
(1,242)	1:218:A:GLN:H	1:219:A:THR:HG21	14	0.12
(1,242)	1:218:A:GLN:H	1:219:A:THR:HG22	14	0.12
(1,242)	1:218:A:GLN:H	1:219:A:THR:HG23	14	0.12
(1,146)	1:152:A:LEU:HB3	1:153:A:GLN:H	8	0.12
(1,1256)	1:217:A:LEU:HB2	1:218:A:GLN:H	7	0.11
(1,1256)	1:217:A:LEU:HB3	1:218:A:GLN:H	7	0.11
(1,1241)	1:215:A:ARG:HB2	1:216:A:TYR:H	10	0.11
(1,1241)	1:215:A:ARG:HB3	1:216:A:TYR:H	10	0.11
(1,1212)	1:212:A:ALA:H	1:215:A:ARG:HD2	15	0.11
(1,1212)	1:212:A:ALA:H	1:215:A:ARG:HD3	15	0.11
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD11	4	0.11
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD12	4	0.11
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD13	4	0.11
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD21	4	0.11
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD22	4	0.11
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD23	4	0.11
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD11	5	0.11
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD12	5	0.11
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD13	5	0.11
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD21	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD22	5	0.11
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD23	5	0.11
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD11	8	0.11
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD12	8	0.11
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD13	8	0.11
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD21	8	0.11
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD22	8	0.11
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD23	8	0.11
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD11	15	0.11
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD12	15	0.11
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD13	15	0.11
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD21	15	0.11
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD22	15	0.11
(1,1093)	1:162:A:LEU:HA	1:162:A:LEU:HD23	15	0.11
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD11	2	0.11
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD12	2	0.11
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD13	2	0.11
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD21	2	0.11
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD22	2	0.11
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD23	2	0.11
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD11	10	0.11
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD12	10	0.11
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD13	10	0.11
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD21	10	0.11
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD22	10	0.11
(1,1057)	1:151:A:PHE:H	1:152:A:LEU:HD23	10	0.11
(1,946)	1:104:A:VAL:HG11	1:107:A:LEU:HB2	17	0.11
(1,946)	1:104:A:VAL:HG11	1:107:A:LEU:HB3	17	0.11
(1,946)	1:104:A:VAL:HG12	1:107:A:LEU:HB2	17	0.11
(1,946)	1:104:A:VAL:HG12	1:107:A:LEU:HB3	17	0.11
(1,946)	1:104:A:VAL:HG13	1:107:A:LEU:HB2	17	0.11
(1,946)	1:104:A:VAL:HG13	1:107:A:LEU:HB3	17	0.11
(1,946)	1:104:A:VAL:HG21	1:107:A:LEU:HB2	17	0.11
(1,946)	1:104:A:VAL:HG21	1:107:A:LEU:HB3	17	0.11
(1,946)	1:104:A:VAL:HG22	1:107:A:LEU:HB2	17	0.11
(1,946)	1:104:A:VAL:HG22	1:107:A:LEU:HB3	17	0.11
(1,946)	1:104:A:VAL:HG23	1:107:A:LEU:HB2	17	0.11
(1,946)	1:104:A:VAL:HG23	1:107:A:LEU:HB3	17	0.11
(1,847)	1:144:A:VAL:HA	1:176:A:ILE:HD11	12	0.11
(1,847)	1:144:A:VAL:HA	1:176:A:ILE:HD12	12	0.11
(1,847)	1:144:A:VAL:HA	1:176:A:ILE:HD13	12	0.11
(1,696)	1:106:A:TYR:HD1	1:107:A:LEU:HA	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,696)	1:106:A:TYR:HD2	1:107:A:LEU:HA	9	0.11
(1,644)	1:176:A:ILE:HG21	1:212:A:ALA:HA	16	0.11
(1,644)	1:176:A:ILE:HG22	1:212:A:ALA:HA	16	0.11
(1,644)	1:176:A:ILE:HG23	1:212:A:ALA:HA	16	0.11
(1,616)	1:162:A:LEU:HA	1:167:A:GLU:H	1	0.11
(1,616)	1:162:A:LEU:HA	1:167:A:GLU:H	3	0.11
(1,616)	1:162:A:LEU:HA	1:167:A:GLU:H	7	0.11
(1,616)	1:162:A:LEU:HA	1:167:A:GLU:H	9	0.11
(1,616)	1:162:A:LEU:HA	1:167:A:GLU:H	10	0.11
(1,616)	1:162:A:LEU:HA	1:167:A:GLU:H	11	0.11
(1,616)	1:162:A:LEU:HA	1:167:A:GLU:H	13	0.11
(1,616)	1:162:A:LEU:HA	1:167:A:GLU:H	14	0.11
(1,616)	1:162:A:LEU:HA	1:167:A:GLU:H	16	0.11
(1,616)	1:162:A:LEU:HA	1:167:A:GLU:H	17	0.11
(1,616)	1:162:A:LEU:HA	1:167:A:GLU:H	18	0.11
(1,616)	1:162:A:LEU:HA	1:167:A:GLU:H	19	0.11
(1,375)	1:209:A:VAL:HG21	1:210:A:LYS:H	14	0.11
(1,375)	1:209:A:VAL:HG22	1:210:A:LYS:H	14	0.11
(1,375)	1:209:A:VAL:HG23	1:210:A:LYS:H	14	0.11
(1,1164)	1:191:A:LEU:HA	1:191:A:LEU:HD11	12	0.1
(1,1164)	1:191:A:LEU:HA	1:191:A:LEU:HD12	12	0.1
(1,1164)	1:191:A:LEU:HA	1:191:A:LEU:HD13	12	0.1
(1,1164)	1:191:A:LEU:HA	1:191:A:LEU:HD21	12	0.1
(1,1164)	1:191:A:LEU:HA	1:191:A:LEU:HD22	12	0.1
(1,1164)	1:191:A:LEU:HA	1:191:A:LEU:HD23	12	0.1
(1,946)	1:104:A:VAL:HG11	1:107:A:LEU:HB2	9	0.1
(1,946)	1:104:A:VAL:HG11	1:107:A:LEU:HB3	9	0.1
(1,946)	1:104:A:VAL:HG12	1:107:A:LEU:HB2	9	0.1
(1,946)	1:104:A:VAL:HG12	1:107:A:LEU:HB3	9	0.1
(1,946)	1:104:A:VAL:HG13	1:107:A:LEU:HB2	9	0.1
(1,946)	1:104:A:VAL:HG13	1:107:A:LEU:HB3	9	0.1
(1,946)	1:104:A:VAL:HG21	1:107:A:LEU:HB2	9	0.1
(1,946)	1:104:A:VAL:HG21	1:107:A:LEU:HB3	9	0.1
(1,946)	1:104:A:VAL:HG22	1:107:A:LEU:HB2	9	0.1
(1,946)	1:104:A:VAL:HG22	1:107:A:LEU:HB3	9	0.1
(1,946)	1:104:A:VAL:HG23	1:107:A:LEU:HB2	9	0.1
(1,946)	1:104:A:VAL:HG23	1:107:A:LEU:HB3	9	0.1
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG11	6	0.1
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG12	6	0.1
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG13	6	0.1
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG21	6	0.1
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG22	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG23	6	0.1
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG11	7	0.1
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG12	7	0.1
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG13	7	0.1
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG21	7	0.1
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG22	7	0.1
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG23	7	0.1
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG11	20	0.1
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG12	20	0.1
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG13	20	0.1
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG21	20	0.1
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG22	20	0.1
(1,929)	1:101:A:GLN:HG3	1:104:A:VAL:HG23	20	0.1
(1,696)	1:106:A:TYR:HD1	1:107:A:LEU:HA	10	0.1
(1,696)	1:106:A:TYR:HD2	1:107:A:LEU:HA	10	0.1
(1,616)	1:162:A:LEU:HA	1:167:A:GLU:H	6	0.1
(1,616)	1:162:A:LEU:HA	1:167:A:GLU:H	12	0.1
(1,300)	1:96:A:ASP:H	1:100:A:ALA:H	19	0.1
(1,235)	1:216:A:TYR:H	1:216:A:TYR:HD1	4	0.1
(1,235)	1:216:A:TYR:H	1:216:A:TYR:HD2	4	0.1

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

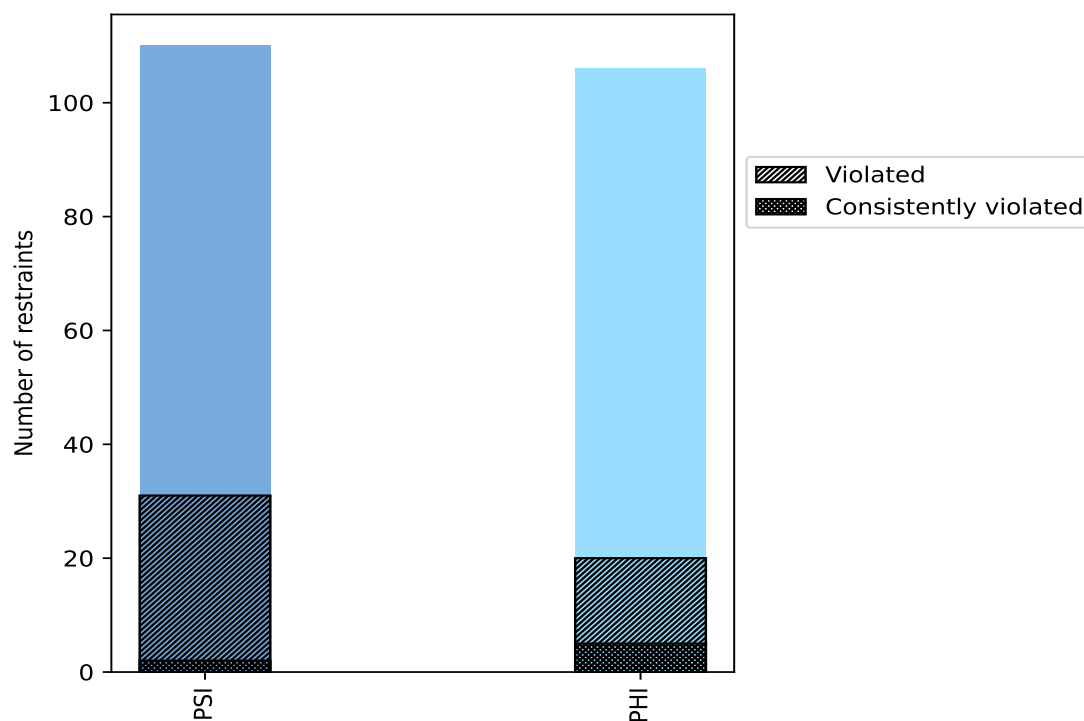
10.1 Summary of dihedral-angle violations [i](#)

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	110	50.9	31	28.2	14.4	2	1.8	0.9
PHI	106	49.1	20	18.9	9.3	5	4.7	2.3
Total	216	100.0	51	23.6	23.6	7	3.2	3.2

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](#)



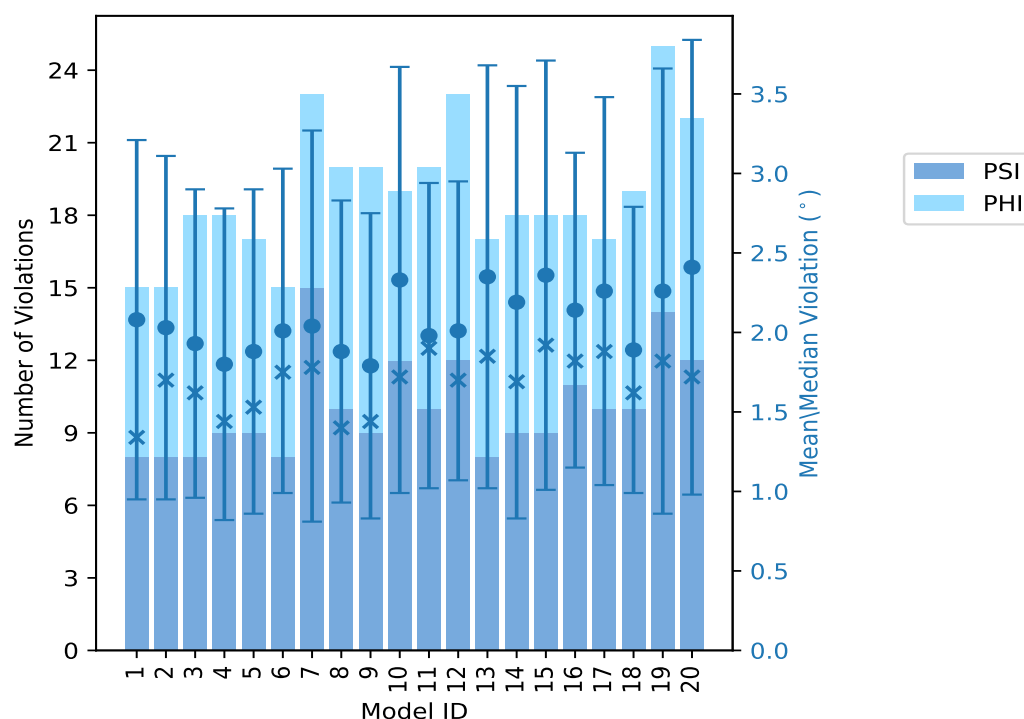
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	8	7	15	2.08	4.89	1.13	1.34
2	8	7	15	2.03	5.02	1.08	1.7
3	8	10	18	1.93	4.99	0.97	1.62
4	9	9	18	1.8	4.17	0.98	1.44
5	9	8	17	1.88	4.37	1.02	1.53
6	8	7	15	2.01	5.06	1.02	1.75
7	15	8	23	2.04	6.09	1.23	1.78
8	10	10	20	1.88	4.1	0.95	1.4
9	9	11	20	1.79	5.1	0.96	1.44
10	12	7	19	2.33	6.01	1.34	1.72
11	10	10	20	1.98	5.01	0.96	1.9
12	12	11	23	2.01	4.62	0.94	1.7
13	8	9	17	2.35	6.01	1.33	1.85
14	9	9	18	2.19	5.89	1.36	1.69
15	9	9	18	2.36	6.06	1.35	1.92
16	11	7	18	2.14	4.8	0.99	1.82
17	10	7	17	2.26	5.06	1.22	1.88
18	10	9	19	1.89	4.9	0.9	1.62
19	14	11	25	2.26	7.25	1.4	1.82
20	12	10	22	2.41	7.08	1.43	1.72

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	%
8	5	13	1	5.0
3	1	4	2	10.0
1	1	2	3	15.0
4	0	4	4	20.0
2	2	4	5	25.0
3	0	3	6	30.0
0	2	2	7	35.0
1	1	2	8	40.0
1	2	3	9	45.0
2	0	2	10	50.0
0	0	0	11	55.0

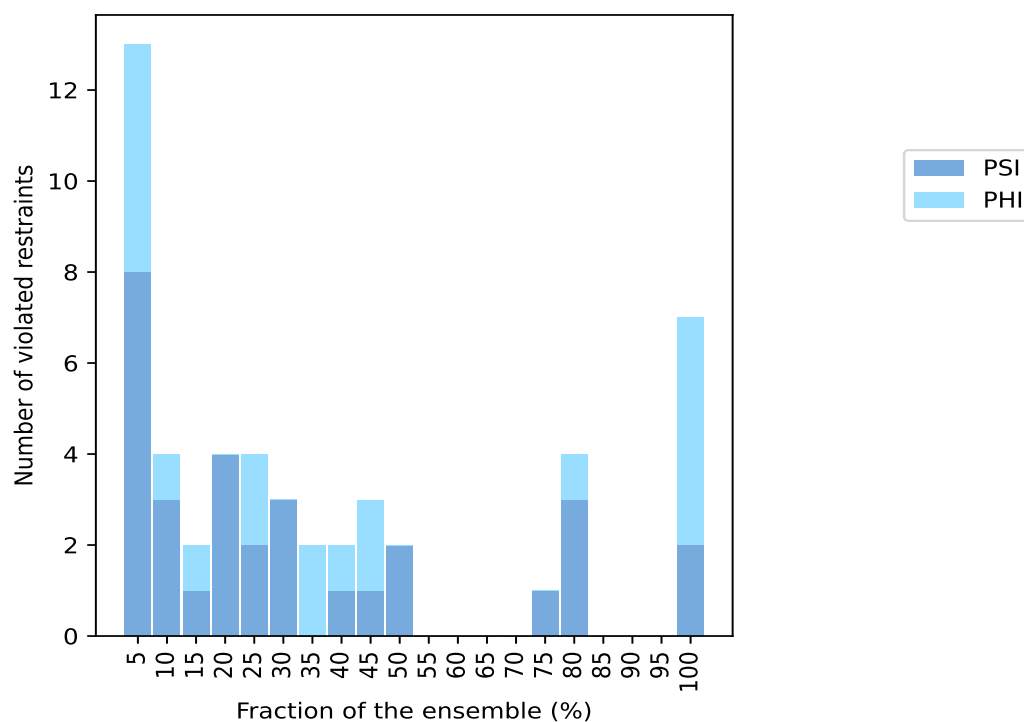
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
1	0	1	15	75.0
3	1	4	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
2	5	7	20	100.0

¹ Number of models with violations

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

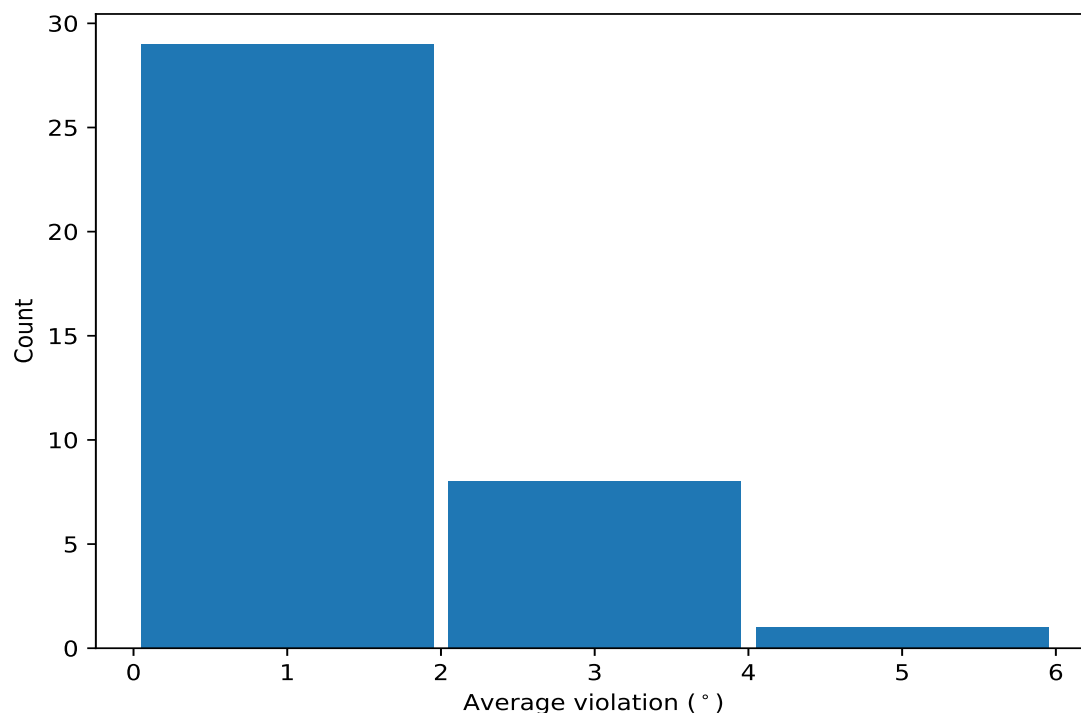


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

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
(1,136)	1:163:A:GLN:C	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	20	4.66	0.55	4.94
(1,139)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:THR:N	20	3.61	0.13	3.56
(1,112)	1:150:A:GLY:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	20	2.41	0.75	2.61
(1,216)	1:220:A:LEU:N	1:220:A:LEU:CA	1:220:A:LEU:C	1:221:A:SER:N	20	2.4	2.09	1.21
(1,131)	1:160:A:GLN:C	1:161:A:MET:N	1:161:A:MET:CA	1:161:A:MET:C	20	2.39	1.04	1.87
(1,140)	1:165:A:LEU:C	1:166:A:THR:N	1:166:A:THR:CA	1:166:A:THR:C	20	2.03	0.13	2.04
(1,110)	1:149:A:PRO:C	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	20	1.79	0.35	1.67
(1,128)	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	1:160:A:GLN:N	16	2.49	0.42	2.3
(1,190)	1:207:A:ARG:N	1:207:A:ARG:CA	1:207:A:ARG:C	1:208:A:GLN:N	16	2.15	0.61	1.96
(1,210)	1:217:A:LEU:N	1:217:A:LEU:CA	1:217:A:LEU:C	1:218:A:GLN:N	16	1.96	0.64	1.6
(1,165)	1:184:A:ARG:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	16	1.55	0.1	1.55
(1,166)	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	1:186:A:ALA:N	15	1.35	0.56	1.2
(1,133)	1:162:A:LEU:N	1:162:A:LEU:CA	1:162:A:LEU:C	1:163:A:GLN:N	10	1.95	1.75	1.25
(1,44)	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	1:105:A:SER:N	10	1.72	0.43	1.87
(1,48)	1:106:A:TYR:N	1:106:A:TYR:CA	1:106:A:TYR:C	1:107:A:LEU:N	9	1.65	0.2	1.64
(1,191)	1:207:A:ARG:C	1:208:A:GLN:N	1:208:A:GLN:CA	1:208:A:GLN:C	9	1.32	0.15	1.34
(1,213)	1:218:A:GLN:C	1:219:A:THR:N	1:219:A:THR:CA	1:219:A:THR:C	9	1.08	0.08	1.05
(1,198)	1:211:A:GLU:N	1:211:A:GLU:CA	1:211:A:GLU:C	1:212:A:ALA:N	8	1.75	0.76	1.4
(1,116)	1:152:A:LEU:C	1:153:A:GLN:N	1:153:A:GLN:CA	1:153:A:GLN:C	8	1.18	0.12	1.16
(1,193)	1:208:A:GLN:C	1:209:A:VAL:N	1:209:A:VAL:CA	1:209:A:VAL:C	7	1.84	0.26	1.91

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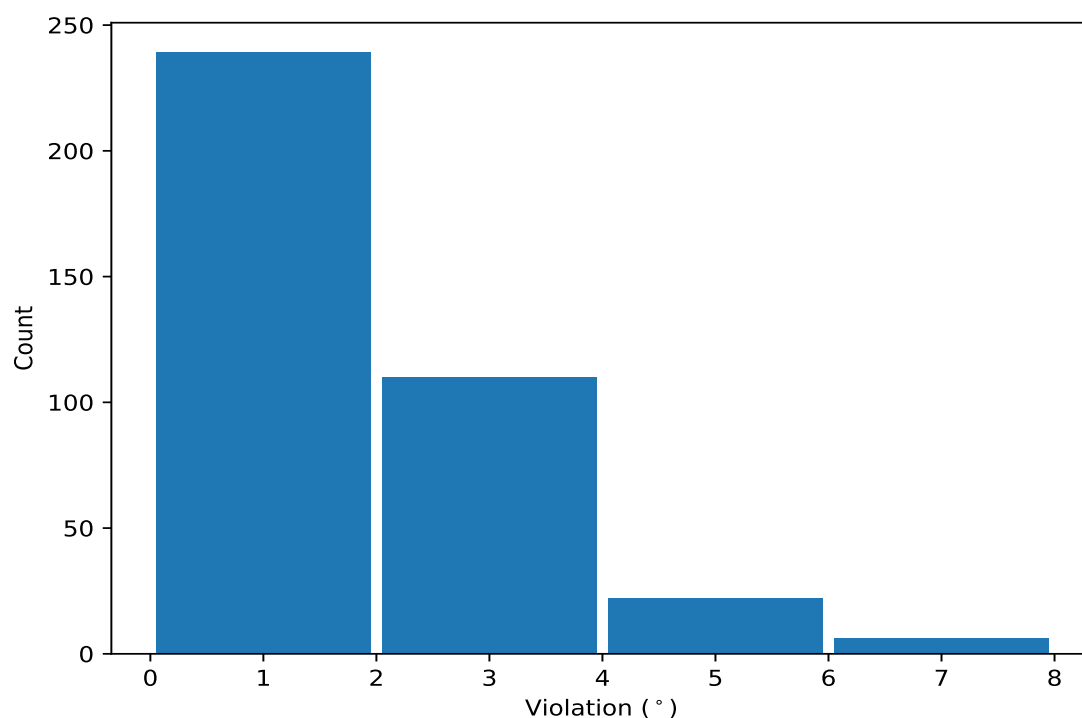
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,47)	1:105:A:SER:C	1:106:A:TYR:N	1:106:A:TYR:CA	1:106:A:TYR:C	7	1.2	0.13	1.14
(1,124)	1:157:A:CYS:N	1:157:A:CYS:CA	1:157:A:CYS:C	1:158:A:LYS:N	6	1.46	0.6	1.21
(1,137)	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	1:165:A:LEU:N	6	1.32	0.15	1.29
(1,20)	1:92:A:HIS:N	1:92:A:HIS:CA	1:92:A:HIS:C	1:93:A:SER:N	6	1.15	0.08	1.14
(1,38)	1:101:A:GLN:N	1:101:A:GLN:CA	1:101:A:GLN:C	1:102:A:ASP:N	5	1.7	0.24	1.72
(1,171)	1:188:A:PRO:N	1:188:A:PRO:CA	1:188:A:PRO:C	1:189:A:PRO:N	5	1.59	0.96	1.16
(1,195)	1:209:A:VAL:C	1:210:A:LYS:N	1:210:A:LYS:CA	1:210:A:LYS:C	5	1.33	0.29	1.35
(1,31)	1:97:A:LEU:C	1:98:A:VAL:N	1:98:A:VAL:CA	1:98:A:VAL:C	5	1.19	0.07	1.21
(1,196)	1:210:A:LYS:N	1:210:A:LYS:CA	1:210:A:LYS:C	1:211:A:GLU:N	4	1.65	0.37	1.52
(1,192)	1:208:A:GLN:N	1:208:A:GLN:CA	1:208:A:GLN:C	1:209:A:VAL:N	4	1.39	0.31	1.37
(1,204)	1:214:A:MET:N	1:214:A:MET:CA	1:214:A:MET:C	1:215:A:ARG:N	4	1.28	0.19	1.24
(1,141)	1:166:A:THR:N	1:166:A:THR:CA	1:166:A:THR:C	1:167:A:GLU:N	4	1.04	0.03	1.04
(1,80)	1:124:A:THR:N	1:124:A:THR:CA	1:124:A:THR:C	1:125:A:PRO:N	3	2.24	0.03	2.24
(1,127)	1:158:A:LYS:C	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	3	1.09	0.04	1.11
(1,197)	1:210:A:LYS:C	1:211:A:GLU:N	1:211:A:GLU:CA	1:211:A:GLU:C	2	1.88	0.62	1.88
(1,122)	1:156:A:TRP:N	1:156:A:TRP:CA	1:156:A:TRP:C	1:157:A:CYS:N	2	1.67	0.35	1.67
(1,206)	1:215:A:ARG:N	1:215:A:ARG:CA	1:215:A:ARG:C	1:216:A:TYR:N	2	1.23	0.23	1.23
(1,208)	1:216:A:TYR:N	1:216:A:TYR:CA	1:216:A:TYR:C	1:217:A:LEU:N	2	1.2	0.01	1.2

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 (°)
(1,180)	1:199:A:GLY:N	1:199:A:GLY:CA	1:199:A:GLY:C	1:200:A:ARG:N	19	7.25
(1,133)	1:162:A:LEU:N	1:162:A:LEU:CA	1:162:A:LEU:C	1:163:A:GLN:N	20	7.08
(1,216)	1:220:A:LEU:N	1:220:A:LEU:CA	1:220:A:LEU:C	1:221:A:SER:N	7	6.09
(1,216)	1:220:A:LEU:N	1:220:A:LEU:CA	1:220:A:LEU:C	1:221:A:SER:N	15	6.06
(1,216)	1:220:A:LEU:N	1:220:A:LEU:CA	1:220:A:LEU:C	1:221:A:SER:N	10	6.01
(1,216)	1:220:A:LEU:N	1:220:A:LEU:CA	1:220:A:LEU:C	1:221:A:SER:N	13	6.01
(1,216)	1:220:A:LEU:N	1:220:A:LEU:CA	1:220:A:LEU:C	1:221:A:SER:N	14	5.89
(1,136)	1:163:A:GLN:C	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	9	5.1
(1,136)	1:163:A:GLN:C	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	10	5.1
(1,136)	1:163:A:GLN:C	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	6	5.06
(1,86)	1:137:A:LEU:N	1:137:A:LEU:CA	1:137:A:LEU:C	1:138:A:SER:N	17	5.06
(1,136)	1:163:A:GLN:C	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	14	5.05
(1,136)	1:163:A:GLN:C	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	17	5.05
(1,136)	1:163:A:GLN:C	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	2	5.02
(1,136)	1:163:A:GLN:C	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	13	5.02
(1,136)	1:163:A:GLN:C	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	11	5.01
(1,136)	1:163:A:GLN:C	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	3	4.99
(1,136)	1:163:A:GLN:C	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	19	4.99
(1,136)	1:163:A:GLN:C	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	18	4.9
(1,136)	1:163:A:GLN:C	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	1	4.89
(1,136)	1:163:A:GLN:C	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	16	4.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,136)	1:163:A:GLN:C	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	7	4.73
(1,136)	1:163:A:GLN:C	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	12	4.62
(1,131)	1:160:A:GLN:C	1:161:A:MET:N	1:161:A:MET:CA	1:161:A:MET:C	15	4.5
(1,136)	1:163:A:GLN:C	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	20	4.43
(1,131)	1:160:A:GLN:C	1:161:A:MET:N	1:161:A:MET:CA	1:161:A:MET:C	5	4.37
(1,131)	1:160:A:GLN:C	1:161:A:MET:N	1:161:A:MET:CA	1:161:A:MET:C	4	4.17
(1,131)	1:160:A:GLN:C	1:161:A:MET:N	1:161:A:MET:CA	1:161:A:MET:C	8	4.1
(1,139)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:THR:N	20	3.98
(1,136)	1:163:A:GLN:C	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	4	3.8
(1,139)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:THR:N	8	3.76
(1,139)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:THR:N	1	3.75
(1,139)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:THR:N	15	3.73
(1,139)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:THR:N	4	3.72
(1,139)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:THR:N	14	3.72
(1,139)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:THR:N	17	3.64
(1,136)	1:163:A:GLN:C	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	15	3.63
(1,139)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:THR:N	5	3.62
(1,139)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:THR:N	18	3.62
(1,131)	1:160:A:GLN:C	1:161:A:MET:N	1:161:A:MET:CA	1:161:A:MET:C	20	3.62
(1,136)	1:163:A:GLN:C	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	5	3.6
(1,139)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:THR:N	9	3.57
(1,139)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:THR:N	6	3.56
(1,181)	1:199:A:GLY:C	1:200:A:ARG:N	1:200:A:ARG:CA	1:200:A:ARG:C	19	3.55
(1,139)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:THR:N	11	3.55
(1,139)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:THR:N	10	3.53
(1,139)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:THR:N	3	3.52
(1,171)	1:188:A:PRO:N	1:188:A:PRO:CA	1:188:A:PRO:C	1:189:A:PRO:N	10	3.51
(1,139)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:THR:N	12	3.51
(1,139)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:THR:N	13	3.5
(1,139)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:THR:N	16	3.5
(1,139)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:THR:N	2	3.49
(1,136)	1:163:A:GLN:C	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	8	3.48
(1,139)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:THR:N	7	3.46
(1,166)	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	1:186:A:ALA:N	19	3.4
(1,139)	1:165:A:LEU:N	1:165:A:LEU:CA	1:165:A:LEU:C	1:166:A:THR:N	19	3.4
(1,112)	1:150:A:GLY:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	12	3.4
(1,112)	1:150:A:GLY:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	1	3.39
(1,128)	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	1:160:A:GLN:N	20	3.36
(1,112)	1:150:A:GLY:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	20	3.36
(1,128)	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	1:160:A:GLN:N	12	3.29
(1,112)	1:150:A:GLY:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	16	3.28
(1,210)	1:217:A:LEU:N	1:217:A:LEU:CA	1:217:A:LEU:C	1:218:A:GLN:N	15	3.13
(1,112)	1:150:A:GLY:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	11	3.13
(1,128)	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	1:160:A:GLN:N	7	3.12
(1,198)	1:211:A:GLU:N	1:211:A:GLU:CA	1:211:A:GLU:C	1:212:A:ALA:N	16	3.1
(1,210)	1:217:A:LEU:N	1:217:A:LEU:CA	1:217:A:LEU:C	1:218:A:GLN:N	14	3.09
(1,112)	1:150:A:GLY:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	8	3.09
(1,178)	1:198:A:ASP:N	1:198:A:ASP:CA	1:198:A:ASP:C	1:199:A:GLY:N	19	3.06
(1,190)	1:207:A:ARG:N	1:207:A:ARG:CA	1:207:A:ARG:C	1:208:A:GLN:N	17	2.99
(1,210)	1:217:A:LEU:N	1:217:A:LEU:CA	1:217:A:LEU:C	1:218:A:GLN:N	10	2.98
(1,134)	1:162:A:LEU:C	1:163:A:GLN:N	1:163:A:GLN:CA	1:163:A:GLN:C	20	2.98

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,190)	1:207:A:ARG:N	1:207:A:ARG:CA	1:207:A:ARG:C	1:208:A:GLN:N	2	2.93
(1,112)	1:150:A:GLY:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	5	2.9
(1,210)	1:217:A:LEU:N	1:217:A:LEU:CA	1:217:A:LEU:C	1:218:A:GLN:N	13	2.87
(1,190)	1:207:A:ARG:N	1:207:A:ARG:CA	1:207:A:ARG:C	1:208:A:GLN:N	20	2.86
(1,112)	1:150:A:GLY:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	2	2.86
(1,209)	1:216:A:TYR:C	1:217:A:LEU:N	1:217:A:LEU:CA	1:217:A:LEU:C	13	2.83
(1,124)	1:157:A:CYS:N	1:157:A:CYS:CA	1:157:A:CYS:C	1:158:A:LYS:N	16	2.77
(1,112)	1:150:A:GLY:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	10	2.77
(1,190)	1:207:A:ARG:N	1:207:A:ARG:CA	1:207:A:ARG:C	1:208:A:GLN:N	8	2.74
(1,128)	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	1:160:A:GLN:N	19	2.74
(1,190)	1:207:A:ARG:N	1:207:A:ARG:CA	1:207:A:ARG:C	1:208:A:GLN:N	3	2.73
(1,112)	1:150:A:GLY:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	15	2.72
(1,190)	1:207:A:ARG:N	1:207:A:ARG:CA	1:207:A:ARG:C	1:208:A:GLN:N	12	2.7
(1,190)	1:207:A:ARG:N	1:207:A:ARG:CA	1:207:A:ARG:C	1:208:A:GLN:N	1	2.69
(1,198)	1:211:A:GLU:N	1:211:A:GLU:CA	1:211:A:GLU:C	1:212:A:ALA:N	12	2.61
(1,128)	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	1:160:A:GLN:N	16	2.61
(1,128)	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	1:160:A:GLN:N	1	2.59
(1,112)	1:150:A:GLY:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	17	2.5
(1,197)	1:210:A:LYS:C	1:211:A:GLU:N	1:211:A:GLU:CA	1:211:A:GLU:C	15	2.49
(1,110)	1:149:A:PRO:C	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	12	2.47
(1,128)	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	1:160:A:GLN:N	10	2.41
(1,140)	1:165:A:LEU:C	1:166:A:THR:N	1:166:A:THR:CA	1:166:A:THR:C	19	2.36
(1,128)	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	1:160:A:GLN:N	3	2.35
(1,198)	1:211:A:GLU:N	1:211:A:GLU:CA	1:211:A:GLU:C	1:212:A:ALA:N	15	2.34
(1,80)	1:124:A:THR:N	1:124:A:THR:CA	1:124:A:THR:C	1:125:A:PRO:N	20	2.28
(1,210)	1:217:A:LEU:N	1:217:A:LEU:CA	1:217:A:LEU:C	1:218:A:GLN:N	7	2.27
(1,110)	1:149:A:PRO:C	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	13	2.27
(1,196)	1:210:A:LYS:N	1:210:A:LYS:CA	1:210:A:LYS:C	1:211:A:GLU:N	11	2.26
(1,128)	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	1:160:A:GLN:N	9	2.26
(1,110)	1:149:A:PRO:C	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	9	2.26
(1,128)	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	1:160:A:GLN:N	14	2.24
(1,80)	1:124:A:THR:N	1:124:A:THR:CA	1:124:A:THR:C	1:125:A:PRO:N	18	2.24
(1,44)	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	1:105:A:SER:N	7	2.24
(1,128)	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	1:160:A:GLN:N	6	2.23
(1,128)	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	1:160:A:GLN:N	17	2.2
(1,80)	1:124:A:THR:N	1:124:A:THR:CA	1:124:A:THR:C	1:125:A:PRO:N	6	2.2
(1,193)	1:208:A:GLN:C	1:209:A:VAL:N	1:209:A:VAL:CA	1:209:A:VAL:C	19	2.18
(1,140)	1:165:A:LEU:C	1:166:A:THR:N	1:166:A:THR:CA	1:166:A:THR:C	16	2.18
(1,131)	1:160:A:GLN:C	1:161:A:MET:N	1:161:A:MET:CA	1:161:A:MET:C	1	2.18
(1,110)	1:149:A:PRO:C	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	3	2.18
(1,140)	1:165:A:LEU:C	1:166:A:THR:N	1:166:A:THR:CA	1:166:A:THR:C	10	2.17
(1,140)	1:165:A:LEU:C	1:166:A:THR:N	1:166:A:THR:CA	1:166:A:THR:C	20	2.17
(1,131)	1:160:A:GLN:C	1:161:A:MET:N	1:161:A:MET:CA	1:161:A:MET:C	11	2.17
(1,128)	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	1:160:A:GLN:N	13	2.16
(1,193)	1:208:A:GLN:C	1:209:A:VAL:N	1:209:A:VAL:CA	1:209:A:VAL:C	11	2.15
(1,140)	1:165:A:LEU:C	1:166:A:THR:N	1:166:A:THR:CA	1:166:A:THR:C	17	2.15
(1,128)	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	1:160:A:GLN:N	18	2.13
(1,110)	1:149:A:PRO:C	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	6	2.13
(1,44)	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	1:105:A:SER:N	11	2.13
(1,140)	1:165:A:LEU:C	1:166:A:THR:N	1:166:A:THR:CA	1:166:A:THR:C	13	2.11
(1,110)	1:149:A:PRO:C	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	7	2.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,140)	1:165:A:LEU:C	1:166:A:THR:N	1:166:A:THR:CA	1:166:A:THR:C	2	2.09
(1,140)	1:165:A:LEU:C	1:166:A:THR:N	1:166:A:THR:CA	1:166:A:THR:C	3	2.09
(1,133)	1:162:A:LEU:N	1:162:A:LEU:CA	1:162:A:LEU:C	1:163:A:GLN:N	7	2.09
(1,140)	1:165:A:LEU:C	1:166:A:THR:N	1:166:A:THR:CA	1:166:A:THR:C	18	2.08
(1,128)	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	1:160:A:GLN:N	11	2.08
(1,140)	1:165:A:LEU:C	1:166:A:THR:N	1:166:A:THR:CA	1:166:A:THR:C	14	2.06
(1,44)	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	1:105:A:SER:N	17	2.06
(1,112)	1:150:A:GLY:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	19	2.04
(1,133)	1:162:A:LEU:N	1:162:A:LEU:CA	1:162:A:LEU:C	1:163:A:GLN:N	12	2.03
(1,48)	1:106:A:TYR:N	1:106:A:TYR:CA	1:106:A:TYR:C	1:107:A:LEU:N	11	2.03
(1,190)	1:207:A:ARG:N	1:207:A:ARG:CA	1:207:A:ARG:C	1:208:A:GLN:N	15	2.02
(1,122)	1:156:A:TRP:N	1:156:A:TRP:CA	1:156:A:TRP:C	1:157:A:CYS:N	16	2.02
(1,140)	1:165:A:LEU:C	1:166:A:THR:N	1:166:A:THR:CA	1:166:A:THR:C	6	2.01
(1,110)	1:149:A:PRO:C	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	18	2.01
(1,128)	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	1:160:A:GLN:N	2	2.0
(1,140)	1:165:A:LEU:C	1:166:A:THR:N	1:166:A:THR:CA	1:166:A:THR:C	12	1.98
(1,110)	1:149:A:PRO:C	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	19	1.98
(1,44)	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	1:105:A:SER:N	3	1.97
(1,140)	1:165:A:LEU:C	1:166:A:THR:N	1:166:A:THR:CA	1:166:A:THR:C	1	1.96
(1,38)	1:101:A:GLN:N	1:101:A:GLN:CA	1:101:A:GLN:C	1:102:A:ASP:N	14	1.96
(1,140)	1:165:A:LEU:C	1:166:A:THR:N	1:166:A:THR:CA	1:166:A:THR:C	8	1.95
(1,140)	1:165:A:LEU:C	1:166:A:THR:N	1:166:A:THR:CA	1:166:A:THR:C	11	1.95
(1,193)	1:208:A:GLN:C	1:209:A:VAL:N	1:209:A:VAL:CA	1:209:A:VAL:C	9	1.93
(1,140)	1:165:A:LEU:C	1:166:A:THR:N	1:166:A:THR:CA	1:166:A:THR:C	9	1.93
(1,44)	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	1:105:A:SER:N	19	1.93
(1,199)	1:211:A:GLU:C	1:212:A:ALA:N	1:212:A:ALA:CA	1:212:A:ALA:C	12	1.92
(1,131)	1:160:A:GLN:C	1:161:A:MET:N	1:161:A:MET:CA	1:161:A:MET:C	6	1.92
(1,193)	1:208:A:GLN:C	1:209:A:VAL:N	1:209:A:VAL:CA	1:209:A:VAL:C	14	1.91
(1,140)	1:165:A:LEU:C	1:166:A:THR:N	1:166:A:THR:CA	1:166:A:THR:C	4	1.9
(1,140)	1:165:A:LEU:C	1:166:A:THR:N	1:166:A:THR:CA	1:166:A:THR:C	7	1.9
(1,131)	1:160:A:GLN:C	1:161:A:MET:N	1:161:A:MET:CA	1:161:A:MET:C	12	1.9
(1,190)	1:207:A:ARG:N	1:207:A:ARG:CA	1:207:A:ARG:C	1:208:A:GLN:N	10	1.89
(1,131)	1:160:A:GLN:C	1:161:A:MET:N	1:161:A:MET:CA	1:161:A:MET:C	9	1.89
(1,38)	1:101:A:GLN:N	1:101:A:GLN:CA	1:101:A:GLN:C	1:102:A:ASP:N	17	1.88
(1,151)	1:175:A:THR:N	1:175:A:THR:CA	1:175:A:THR:C	1:176:A:ILE:N	11	1.85
(1,131)	1:160:A:GLN:C	1:161:A:MET:N	1:161:A:MET:CA	1:161:A:MET:C	13	1.85
(1,195)	1:209:A:VAL:C	1:210:A:LYS:N	1:210:A:LYS:CA	1:210:A:LYS:C	19	1.82
(1,140)	1:165:A:LEU:C	1:166:A:THR:N	1:166:A:THR:CA	1:166:A:THR:C	15	1.82
(1,110)	1:149:A:PRO:C	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	16	1.82
(1,48)	1:106:A:TYR:N	1:106:A:TYR:CA	1:106:A:TYR:C	1:107:A:LEU:N	7	1.82
(1,192)	1:208:A:GLN:N	1:208:A:GLN:CA	1:208:A:GLN:C	1:209:A:VAL:N	18	1.81
(1,131)	1:160:A:GLN:C	1:161:A:MET:N	1:161:A:MET:CA	1:161:A:MET:C	16	1.81
(1,112)	1:150:A:GLY:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	4	1.81
(1,112)	1:150:A:GLY:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	7	1.81
(1,44)	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	1:105:A:SER:N	20	1.81
(1,140)	1:165:A:LEU:C	1:166:A:THR:N	1:166:A:THR:CA	1:166:A:THR:C	5	1.8
(1,131)	1:160:A:GLN:C	1:161:A:MET:N	1:161:A:MET:CA	1:161:A:MET:C	2	1.79
(1,190)	1:207:A:ARG:N	1:207:A:ARG:CA	1:207:A:ARG:C	1:208:A:GLN:N	7	1.78
(1,112)	1:150:A:GLY:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	18	1.78
(1,131)	1:160:A:GLN:C	1:161:A:MET:N	1:161:A:MET:CA	1:161:A:MET:C	17	1.77
(1,190)	1:207:A:ARG:N	1:207:A:ARG:CA	1:207:A:ARG:C	1:208:A:GLN:N	4	1.76

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,44)	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	1:105:A:SER:N	13	1.76
(1,112)	1:150:A:GLY:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	6	1.75
(1,48)	1:106:A:TYR:N	1:106:A:TYR:CA	1:106:A:TYR:C	1:107:A:LEU:N	3	1.73
(1,38)	1:101:A:GLN:N	1:101:A:GLN:CA	1:101:A:GLN:C	1:102:A:ASP:N	10	1.72
(1,193)	1:208:A:GLN:C	1:209:A:VAL:N	1:209:A:VAL:CA	1:209:A:VAL:C	12	1.7
(1,165)	1:184:A:ARG:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	2	1.7
(1,110)	1:149:A:PRO:C	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	14	1.7
(1,165)	1:184:A:ARG:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	7	1.69
(1,112)	1:150:A:GLY:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	14	1.69
(1,131)	1:160:A:GLN:C	1:161:A:MET:N	1:161:A:MET:CA	1:161:A:MET:C	18	1.68
(1,131)	1:160:A:GLN:C	1:161:A:MET:N	1:161:A:MET:CA	1:161:A:MET:C	19	1.66
(1,38)	1:101:A:GLN:N	1:101:A:GLN:CA	1:101:A:GLN:C	1:102:A:ASP:N	8	1.66
(1,165)	1:184:A:ARG:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	6	1.65
(1,190)	1:207:A:ARG:N	1:207:A:ARG:CA	1:207:A:ARG:C	1:208:A:GLN:N	6	1.64
(1,131)	1:160:A:GLN:C	1:161:A:MET:N	1:161:A:MET:CA	1:161:A:MET:C	10	1.64
(1,110)	1:149:A:PRO:C	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	4	1.64
(1,48)	1:106:A:TYR:N	1:106:A:TYR:CA	1:106:A:TYR:C	1:107:A:LEU:N	10	1.64
(1,48)	1:106:A:TYR:N	1:106:A:TYR:CA	1:106:A:TYR:C	1:107:A:LEU:N	13	1.64
(1,48)	1:106:A:TYR:N	1:106:A:TYR:CA	1:106:A:TYR:C	1:107:A:LEU:N	20	1.64
(1,24)	1:94:A:GLU:N	1:94:A:GLU:CA	1:94:A:GLU:C	1:95:A:GLU:N	12	1.64
(1,210)	1:217:A:LEU:N	1:217:A:LEU:CA	1:217:A:LEU:C	1:218:A:GLN:N	17	1.63
(1,190)	1:207:A:ARG:N	1:207:A:ARG:CA	1:207:A:ARG:C	1:208:A:GLN:N	13	1.63
(1,131)	1:160:A:GLN:C	1:161:A:MET:N	1:161:A:MET:CA	1:161:A:MET:C	3	1.63
(1,48)	1:106:A:TYR:N	1:106:A:TYR:CA	1:106:A:TYR:C	1:107:A:LEU:N	19	1.63
(1,196)	1:210:A:LYS:N	1:210:A:LYS:CA	1:210:A:LYS:C	1:211:A:GLU:N	18	1.62
(1,210)	1:217:A:LEU:N	1:217:A:LEU:CA	1:217:A:LEU:C	1:218:A:GLN:N	11	1.61
(1,191)	1:207:A:ARG:C	1:208:A:GLN:N	1:208:A:GLN:CA	1:208:A:GLN:C	3	1.61
(1,210)	1:217:A:LEU:N	1:217:A:LEU:CA	1:217:A:LEU:C	1:218:A:GLN:N	9	1.6
(1,137)	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	1:165:A:LEU:N	5	1.6
(1,110)	1:149:A:PRO:C	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	15	1.6
(1,110)	1:149:A:PRO:C	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	20	1.6
(1,210)	1:217:A:LEU:N	1:217:A:LEU:CA	1:217:A:LEU:C	1:218:A:GLN:N	5	1.59
(1,131)	1:160:A:GLN:C	1:161:A:MET:N	1:161:A:MET:CA	1:161:A:MET:C	14	1.59
(1,110)	1:149:A:PRO:C	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	17	1.59
(1,165)	1:184:A:ARG:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	4	1.58
(1,110)	1:149:A:PRO:C	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	8	1.58
(1,165)	1:184:A:ARG:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	14	1.57
(1,110)	1:149:A:PRO:C	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	11	1.57
(1,210)	1:217:A:LEU:N	1:217:A:LEU:CA	1:217:A:LEU:C	1:218:A:GLN:N	18	1.56
(1,198)	1:211:A:GLU:N	1:211:A:GLU:CA	1:211:A:GLU:C	1:212:A:ALA:N	5	1.56
(1,165)	1:184:A:ARG:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	12	1.56
(1,204)	1:214:A:MET:N	1:214:A:MET:CA	1:214:A:MET:C	1:215:A:ARG:N	4	1.55
(1,192)	1:208:A:GLN:N	1:208:A:GLN:CA	1:208:A:GLN:C	1:209:A:VAL:N	19	1.55
(1,165)	1:184:A:ARG:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	3	1.55
(1,165)	1:184:A:ARG:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	15	1.55
(1,165)	1:184:A:ARG:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	20	1.55
(1,131)	1:160:A:GLN:C	1:161:A:MET:N	1:161:A:MET:CA	1:161:A:MET:C	7	1.55
(1,210)	1:217:A:LEU:N	1:217:A:LEU:CA	1:217:A:LEU:C	1:218:A:GLN:N	12	1.54
(1,210)	1:217:A:LEU:N	1:217:A:LEU:CA	1:217:A:LEU:C	1:218:A:GLN:N	20	1.54
(1,165)	1:184:A:ARG:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	13	1.54
(1,165)	1:184:A:ARG:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	5	1.53

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,165)	1:184:A:ARG:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	9	1.53
(1,210)	1:217:A:LEU:N	1:217:A:LEU:CA	1:217:A:LEU:C	1:218:A:GLN:N	2	1.52
(1,165)	1:184:A:ARG:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	16	1.52
(1,165)	1:184:A:ARG:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	18	1.52
(1,133)	1:162:A:LEU:N	1:162:A:LEU:CA	1:162:A:LEU:C	1:163:A:GLN:N	16	1.52
(1,190)	1:207:A:ARG:N	1:207:A:ARG:CA	1:207:A:ARG:C	1:208:A:GLN:N	19	1.51
(1,193)	1:208:A:GLN:C	1:209:A:VAL:N	1:209:A:VAL:CA	1:209:A:VAL:C	8	1.5
(1,193)	1:208:A:GLN:C	1:209:A:VAL:N	1:209:A:VAL:CA	1:209:A:VAL:C	18	1.5
(1,165)	1:184:A:ARG:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	10	1.5
(1,210)	1:217:A:LEU:N	1:217:A:LEU:CA	1:217:A:LEU:C	1:218:A:GLN:N	3	1.48
(1,48)	1:106:A:TYR:N	1:106:A:TYR:CA	1:106:A:TYR:C	1:107:A:LEU:N	9	1.47
(1,206)	1:215:A:ARG:N	1:215:A:ARG:CA	1:215:A:ARG:C	1:216:A:TYR:N	8	1.46
(1,166)	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	1:186:A:ALA:N	5	1.46
(1,110)	1:149:A:PRO:C	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	10	1.46
(1,210)	1:217:A:LEU:N	1:217:A:LEU:CA	1:217:A:LEU:C	1:218:A:GLN:N	16	1.45
(1,210)	1:217:A:LEU:N	1:217:A:LEU:CA	1:217:A:LEU:C	1:218:A:GLN:N	6	1.42
(1,196)	1:210:A:LYS:N	1:210:A:LYS:CA	1:210:A:LYS:C	1:211:A:GLU:N	14	1.42
(1,191)	1:207:A:ARG:C	1:208:A:GLN:N	1:208:A:GLN:CA	1:208:A:GLN:C	20	1.41
(1,124)	1:157:A:CYS:N	1:157:A:CYS:CA	1:157:A:CYS:C	1:158:A:LYS:N	7	1.41
(1,47)	1:105:A:SER:C	1:106:A:TYR:N	1:106:A:TYR:CA	1:106:A:TYR:C	9	1.41
(1,47)	1:105:A:SER:C	1:106:A:TYR:N	1:106:A:TYR:CA	1:106:A:TYR:C	10	1.4
(1,195)	1:209:A:VAL:C	1:210:A:LYS:N	1:210:A:LYS:CA	1:210:A:LYS:C	18	1.39
(1,191)	1:207:A:ARG:C	1:208:A:GLN:N	1:208:A:GLN:CA	1:208:A:GLN:C	2	1.39
(1,191)	1:207:A:ARG:C	1:208:A:GLN:N	1:208:A:GLN:CA	1:208:A:GLN:C	17	1.39
(1,116)	1:152:A:LEU:C	1:153:A:GLN:N	1:153:A:GLN:CA	1:153:A:GLN:C	9	1.39
(1,137)	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	1:165:A:LEU:N	15	1.38
(1,110)	1:149:A:PRO:C	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	2	1.36
(1,204)	1:214:A:MET:N	1:214:A:MET:CA	1:214:A:MET:C	1:215:A:ARG:N	7	1.35
(1,195)	1:209:A:VAL:C	1:210:A:LYS:N	1:210:A:LYS:CA	1:210:A:LYS:C	8	1.35
(1,166)	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	1:186:A:ALA:N	16	1.35
(1,202)	1:213:A:VAL:N	1:213:A:VAL:CA	1:213:A:VAL:C	1:214:A:MET:N	20	1.34
(1,191)	1:207:A:ARG:C	1:208:A:GLN:N	1:208:A:GLN:CA	1:208:A:GLN:C	1	1.34
(1,216)	1:220:A:LEU:N	1:220:A:LEU:CA	1:220:A:LEU:C	1:221:A:SER:N	4	1.33
(1,216)	1:220:A:LEU:N	1:220:A:LEU:CA	1:220:A:LEU:C	1:221:A:SER:N	8	1.33
(1,190)	1:207:A:ARG:N	1:207:A:ARG:CA	1:207:A:ARG:C	1:208:A:GLN:N	5	1.33
(1,122)	1:156:A:TRP:N	1:156:A:TRP:CA	1:156:A:TRP:C	1:157:A:CYS:N	7	1.32
(1,116)	1:152:A:LEU:C	1:153:A:GLN:N	1:153:A:GLN:CA	1:153:A:GLN:C	8	1.32
(1,112)	1:150:A:GLY:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	3	1.32
(1,112)	1:150:A:GLY:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	9	1.32
(1,100)	1:144:A:VAL:N	1:144:A:VAL:CA	1:144:A:VAL:C	1:145:A:LEU:N	1	1.31
(1,196)	1:210:A:LYS:N	1:210:A:LYS:CA	1:210:A:LYS:C	1:211:A:GLU:N	9	1.3
(1,137)	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	1:165:A:LEU:N	8	1.3
(1,191)	1:207:A:ARG:C	1:208:A:GLN:N	1:208:A:GLN:CA	1:208:A:GLN:C	12	1.28
(1,137)	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	1:165:A:LEU:N	4	1.28
(1,133)	1:162:A:LEU:N	1:162:A:LEU:CA	1:162:A:LEU:C	1:163:A:GLN:N	19	1.28
(1,112)	1:150:A:GLY:C	1:151:A:PHE:N	1:151:A:PHE:CA	1:151:A:PHE:C	13	1.28
(1,31)	1:97:A:LEU:C	1:98:A:VAL:N	1:98:A:VAL:CA	1:98:A:VAL:C	18	1.28
(1,20)	1:92:A:HIS:N	1:92:A:HIS:CA	1:92:A:HIS:C	1:93:A:SER:N	12	1.28
(1,191)	1:207:A:ARG:C	1:208:A:GLN:N	1:208:A:GLN:CA	1:208:A:GLN:C	8	1.27
(1,124)	1:157:A:CYS:N	1:157:A:CYS:CA	1:157:A:CYS:C	1:158:A:LYS:N	6	1.27
(1,197)	1:210:A:LYS:C	1:211:A:GLU:N	1:211:A:GLU:CA	1:211:A:GLU:C	20	1.26

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,166)	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	1:186:A:ALA:N	11	1.26
(1,38)	1:101:A:GLN:N	1:101:A:GLN:CA	1:101:A:GLN:C	1:102:A:ASP:N	1	1.26
(1,216)	1:220:A:LEU:N	1:220:A:LEU:CA	1:220:A:LEU:C	1:221:A:SER:N	1	1.25
(1,171)	1:188:A:PRO:N	1:188:A:PRO:CA	1:188:A:PRO:C	1:189:A:PRO:N	19	1.25
(1,166)	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	1:186:A:ALA:N	18	1.25
(1,137)	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	1:165:A:LEU:N	12	1.25
(1,116)	1:152:A:LEU:C	1:153:A:GLN:N	1:153:A:GLN:CA	1:153:A:GLN:C	3	1.25
(1,110)	1:149:A:PRO:C	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	1	1.25
(1,110)	1:149:A:PRO:C	1:150:A:GLY:N	1:150:A:GLY:CA	1:150:A:GLY:C	5	1.25
(1,48)	1:106:A:TYR:N	1:106:A:TYR:CA	1:106:A:TYR:C	1:107:A:LEU:N	17	1.25
(1,198)	1:211:A:GLU:N	1:211:A:GLU:CA	1:211:A:GLU:C	1:212:A:ALA:N	20	1.24
(1,165)	1:184:A:ARG:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	11	1.24
(1,216)	1:220:A:LEU:N	1:220:A:LEU:CA	1:220:A:LEU:C	1:221:A:SER:N	11	1.23
(1,190)	1:207:A:ARG:N	1:207:A:ARG:CA	1:207:A:ARG:C	1:208:A:GLN:N	16	1.23
(1,166)	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	1:186:A:ALA:N	9	1.23
(1,216)	1:220:A:LEU:N	1:220:A:LEU:CA	1:220:A:LEU:C	1:221:A:SER:N	19	1.22
(1,213)	1:218:A:GLN:C	1:219:A:THR:N	1:219:A:THR:CA	1:219:A:THR:C	8	1.22
(1,166)	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	1:186:A:ALA:N	14	1.22
(1,31)	1:97:A:LEU:C	1:98:A:VAL:N	1:98:A:VAL:CA	1:98:A:VAL:C	19	1.22
(1,213)	1:218:A:GLN:C	1:219:A:THR:N	1:219:A:THR:CA	1:219:A:THR:C	4	1.21
(1,208)	1:216:A:TYR:N	1:216:A:TYR:CA	1:216:A:TYR:C	1:217:A:LEU:N	8	1.21
(1,133)	1:162:A:LEU:N	1:162:A:LEU:CA	1:162:A:LEU:C	1:163:A:GLN:N	18	1.21
(1,44)	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	1:105:A:SER:N	10	1.21
(1,31)	1:97:A:LEU:C	1:98:A:VAL:N	1:98:A:VAL:CA	1:98:A:VAL:C	11	1.21
(1,20)	1:92:A:HIS:N	1:92:A:HIS:CA	1:92:A:HIS:C	1:93:A:SER:N	19	1.21
(1,216)	1:220:A:LEU:N	1:220:A:LEU:CA	1:220:A:LEU:C	1:221:A:SER:N	16	1.2
(1,166)	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	1:186:A:ALA:N	15	1.2
(1,208)	1:216:A:TYR:N	1:216:A:TYR:CA	1:216:A:TYR:C	1:217:A:LEU:N	4	1.19
(1,192)	1:208:A:GLN:N	1:208:A:GLN:CA	1:208:A:GLN:C	1:209:A:VAL:N	14	1.19
(1,166)	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	1:186:A:ALA:N	20	1.19
(1,116)	1:152:A:LEU:C	1:153:A:GLN:N	1:153:A:GLN:CA	1:153:A:GLN:C	13	1.19
(1,216)	1:220:A:LEU:N	1:220:A:LEU:CA	1:220:A:LEU:C	1:221:A:SER:N	17	1.18
(1,216)	1:220:A:LEU:N	1:220:A:LEU:CA	1:220:A:LEU:C	1:221:A:SER:N	18	1.18
(1,166)	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	1:186:A:ALA:N	13	1.18
(1,47)	1:105:A:SER:C	1:106:A:TYR:N	1:106:A:TYR:CA	1:106:A:TYR:C	20	1.17
(1,216)	1:220:A:LEU:N	1:220:A:LEU:CA	1:220:A:LEU:C	1:221:A:SER:N	3	1.16
(1,216)	1:220:A:LEU:N	1:220:A:LEU:CA	1:220:A:LEU:C	1:221:A:SER:N	5	1.16
(1,216)	1:220:A:LEU:N	1:220:A:LEU:CA	1:220:A:LEU:C	1:221:A:SER:N	9	1.16
(1,216)	1:220:A:LEU:N	1:220:A:LEU:CA	1:220:A:LEU:C	1:221:A:SER:N	12	1.16
(1,171)	1:188:A:PRO:N	1:188:A:PRO:CA	1:188:A:PRO:C	1:189:A:PRO:N	1	1.16
(1,166)	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	1:186:A:ALA:N	4	1.16
(1,166)	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	1:186:A:ALA:N	10	1.16
(1,124)	1:157:A:CYS:N	1:157:A:CYS:CA	1:157:A:CYS:C	1:158:A:LYS:N	9	1.16
(1,31)	1:97:A:LEU:C	1:98:A:VAL:N	1:98:A:VAL:CA	1:98:A:VAL:C	16	1.16
(1,191)	1:207:A:ARG:C	1:208:A:GLN:N	1:208:A:GLN:CA	1:208:A:GLN:C	15	1.15
(1,166)	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	1:186:A:ALA:N	12	1.15
(1,20)	1:92:A:HIS:N	1:92:A:HIS:CA	1:92:A:HIS:C	1:93:A:SER:N	16	1.15
(1,216)	1:220:A:LEU:N	1:220:A:LEU:CA	1:220:A:LEU:C	1:221:A:SER:N	20	1.14
(1,116)	1:152:A:LEU:C	1:153:A:GLN:N	1:153:A:GLN:CA	1:153:A:GLN:C	4	1.14
(1,47)	1:105:A:SER:C	1:106:A:TYR:N	1:106:A:TYR:CA	1:106:A:TYR:C	7	1.14
(1,216)	1:220:A:LEU:N	1:220:A:LEU:CA	1:220:A:LEU:C	1:221:A:SER:N	2	1.13

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,216)	1:220:A:LEU:N	1:220:A:LEU:CA	1:220:A:LEU:C	1:221:A:SER:N	6	1.13
(1,204)	1:214:A:MET:N	1:214:A:MET:CA	1:214:A:MET:C	1:215:A:ARG:N	8	1.13
(1,127)	1:158:A:LYS:C	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	5	1.12
(1,116)	1:152:A:LEU:C	1:153:A:GLN:N	1:153:A:GLN:CA	1:153:A:GLN:C	6	1.12
(1,47)	1:105:A:SER:C	1:106:A:TYR:N	1:106:A:TYR:CA	1:106:A:TYR:C	3	1.12
(1,44)	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	1:105:A:SER:N	9	1.12
(1,20)	1:92:A:HIS:N	1:92:A:HIS:CA	1:92:A:HIS:C	1:93:A:SER:N	15	1.12
(1,133)	1:162:A:LEU:N	1:162:A:LEU:CA	1:162:A:LEU:C	1:163:A:GLN:N	1	1.11
(1,127)	1:158:A:LYS:C	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	4	1.11
(1,124)	1:157:A:CYS:N	1:157:A:CYS:CA	1:157:A:CYS:C	1:158:A:LYS:N	2	1.11
(1,213)	1:218:A:GLN:C	1:219:A:THR:N	1:219:A:THR:CA	1:219:A:THR:C	1	1.1
(1,213)	1:218:A:GLN:C	1:219:A:THR:N	1:219:A:THR:CA	1:219:A:THR:C	19	1.1
(1,133)	1:162:A:LEU:N	1:162:A:LEU:CA	1:162:A:LEU:C	1:163:A:GLN:N	3	1.1
(1,47)	1:105:A:SER:C	1:106:A:TYR:N	1:106:A:TYR:CA	1:106:A:TYR:C	13	1.1
(1,137)	1:164:A:ALA:N	1:164:A:ALA:CA	1:164:A:ALA:C	1:165:A:LEU:N	7	1.09
(1,47)	1:105:A:SER:C	1:106:A:TYR:N	1:106:A:TYR:CA	1:106:A:TYR:C	19	1.09
(1,20)	1:92:A:HIS:N	1:92:A:HIS:CA	1:92:A:HIS:C	1:93:A:SER:N	10	1.09
(1,198)	1:211:A:GLU:N	1:211:A:GLU:CA	1:211:A:GLU:C	1:212:A:ALA:N	10	1.08
(1,141)	1:166:A:THR:N	1:166:A:THR:CA	1:166:A:THR:C	1:167:A:GLU:N	5	1.08
(1,204)	1:214:A:MET:N	1:214:A:MET:CA	1:214:A:MET:C	1:215:A:ARG:N	12	1.07
(1,31)	1:97:A:LEU:C	1:98:A:VAL:N	1:98:A:VAL:CA	1:98:A:VAL:C	9	1.07
(1,124)	1:157:A:CYS:N	1:157:A:CYS:CA	1:157:A:CYS:C	1:158:A:LYS:N	19	1.06
(1,98)	1:143:A:ARG:N	1:143:A:ARG:CA	1:143:A:ARG:C	1:144:A:VAL:N	18	1.06
(1,213)	1:218:A:GLN:C	1:219:A:THR:N	1:219:A:THR:CA	1:219:A:THR:C	11	1.05
(1,198)	1:211:A:GLU:N	1:211:A:GLU:CA	1:211:A:GLU:C	1:212:A:ALA:N	8	1.05
(1,195)	1:209:A:VAL:C	1:210:A:LYS:N	1:210:A:LYS:CA	1:210:A:LYS:C	12	1.05
(1,141)	1:166:A:THR:N	1:166:A:THR:CA	1:166:A:THR:C	1:167:A:GLU:N	4	1.05
(1,116)	1:152:A:LEU:C	1:153:A:GLN:N	1:153:A:GLN:CA	1:153:A:GLN:C	11	1.05
(1,213)	1:218:A:GLN:C	1:219:A:THR:N	1:219:A:THR:CA	1:219:A:THR:C	12	1.04
(1,191)	1:207:A:ARG:C	1:208:A:GLN:N	1:208:A:GLN:CA	1:208:A:GLN:C	7	1.04
(1,133)	1:162:A:LEU:N	1:162:A:LEU:CA	1:162:A:LEU:C	1:163:A:GLN:N	17	1.04
(1,141)	1:166:A:THR:N	1:166:A:THR:CA	1:166:A:THR:C	1:167:A:GLU:N	7	1.03
(1,127)	1:158:A:LYS:C	1:159:A:TYR:N	1:159:A:TYR:CA	1:159:A:TYR:C	15	1.03
(1,20)	1:92:A:HIS:N	1:92:A:HIS:CA	1:92:A:HIS:C	1:93:A:SER:N	2	1.03
(1,213)	1:218:A:GLN:C	1:219:A:THR:N	1:219:A:THR:CA	1:219:A:THR:C	9	1.02
(1,198)	1:211:A:GLU:N	1:211:A:GLU:CA	1:211:A:GLU:C	1:212:A:ALA:N	14	1.02
(1,195)	1:209:A:VAL:C	1:210:A:LYS:N	1:210:A:LYS:CA	1:210:A:LYS:C	14	1.02
(1,171)	1:188:A:PRO:N	1:188:A:PRO:CA	1:188:A:PRO:C	1:189:A:PRO:N	5	1.02
(1,133)	1:162:A:LEU:N	1:162:A:LEU:CA	1:162:A:LEU:C	1:163:A:GLN:N	2	1.02
(1,116)	1:152:A:LEU:C	1:153:A:GLN:N	1:153:A:GLN:CA	1:153:A:GLN:C	17	1.02
(1,213)	1:218:A:GLN:C	1:219:A:THR:N	1:219:A:THR:CA	1:219:A:THR:C	5	1.01
(1,192)	1:208:A:GLN:N	1:208:A:GLN:CA	1:208:A:GLN:C	1:209:A:VAL:N	11	1.01
(1,171)	1:188:A:PRO:N	1:188:A:PRO:CA	1:188:A:PRO:C	1:189:A:PRO:N	4	1.01
(1,166)	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	1:186:A:ALA:N	6	1.01
(1,141)	1:166:A:THR:N	1:166:A:THR:CA	1:166:A:THR:C	1:167:A:GLU:N	15	1.01
(1,39)	1:101:A:GLN:C	1:102:A:ASP:N	1:102:A:ASP:CA	1:102:A:ASP:C	14	1.01
(1,213)	1:218:A:GLN:C	1:219:A:THR:N	1:219:A:THR:CA	1:219:A:THR:C	3	1.0
(1,206)	1:215:A:ARG:N	1:215:A:ARG:CA	1:215:A:ARG:C	1:216:A:TYR:N	7	1.0
(1,166)	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	1:186:A:ALA:N	7	1.0
(1,44)	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	1:105:A:SER:N	8	1.0