



Full wwPDB NMR Structure Validation Report ⓘ

Dec 24, 2024 – 01:56 PM EST

PDB ID : 2KUE
BMRB ID : 16733
Title : NMR structure of the PASTA domain 2 and 3 of Mycobacterium tuberculosis of PknB
Authors : Barthe, P.; Mukamolova, G.; Roumestand, C.; Cohen-Gonsaud, M.
Deposited on : 2010-02-17

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 : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.40

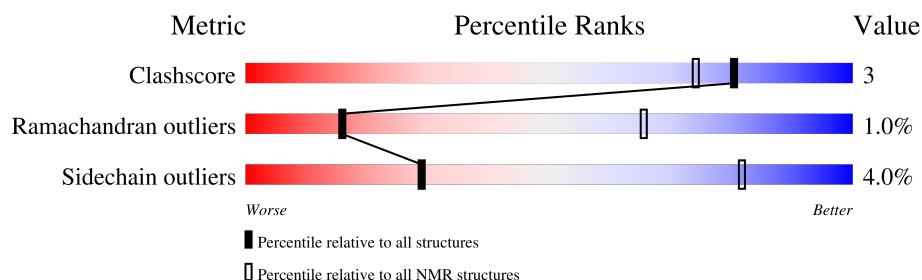
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 84%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	138	 90% 6% ..

2 Ensemble composition and analysis

This entry contains 30 models. Model 2 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:425-A:491 (67)	0.62	2
2	A:493-A:557 (65)	0.76	3

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

Cluster number	Models
1	2, 3, 5, 6, 7, 9, 10, 11, 15, 18, 19, 21, 22, 23, 25, 26, 27, 28, 30
2	8, 12, 14, 17, 20, 24, 29
3	1, 13
Single-model clusters	4; 16

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1971 atoms, of which 991 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Serine/threonine-protein kinase pknB.

Mol	Chain	Residues	Atoms					Trace
1	A	135	Total	C	H	N	O	0
			1971	614	991	166	200	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	GLY	-	expression tag	UNP P0A5S4
A	421	HIS	-	expression tag	UNP P0A5S4
A	422	MET	-	expression tag	UNP P0A5S4

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Serine/threonine-protein kinase pknB

Chain A:  90% 6% ..




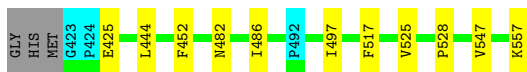
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1


- Molecule 1: Serine/threonine-protein kinase pknB

Chain A:  88% 8% ..



4.2.2 Score per residue for model 2 (medoid)

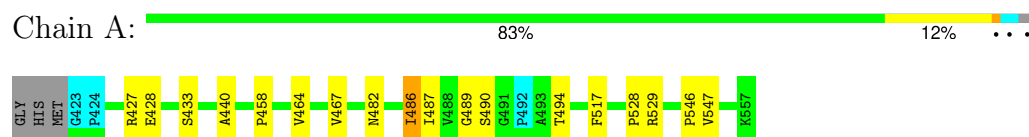
- Molecule 1: Serine/threonine-protein kinase pknB

Chain A:  86% 9% ...



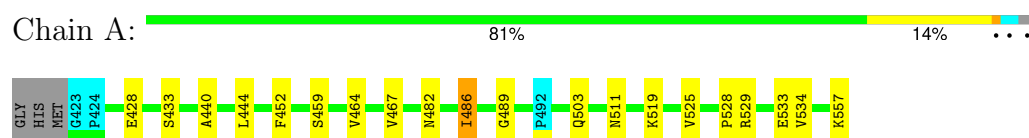
4.2.3 Score per residue for model 3

- Molecule 1: Serine/threonine-protein kinase pknB



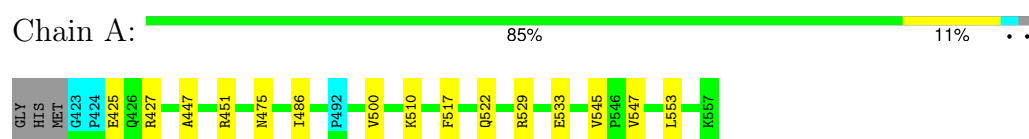
4.2.4 Score per residue for model 4

- Molecule 1: Serine/threonine-protein kinase pknB



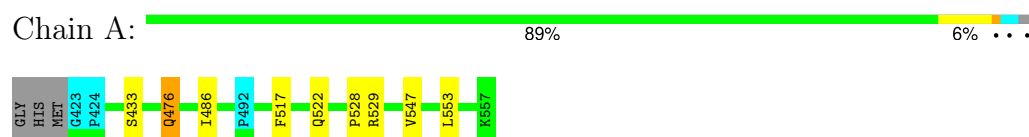
4.2.5 Score per residue for model 5

- Molecule 1: Serine/threonine-protein kinase pknB



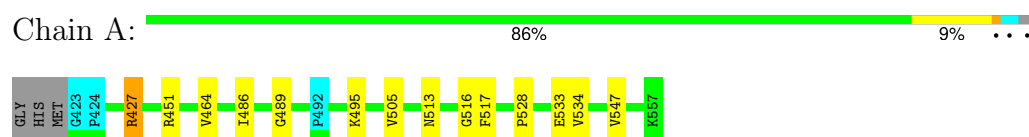
4.2.6 Score per residue for model 6

- Molecule 1: Serine/threonine-protein kinase pknB



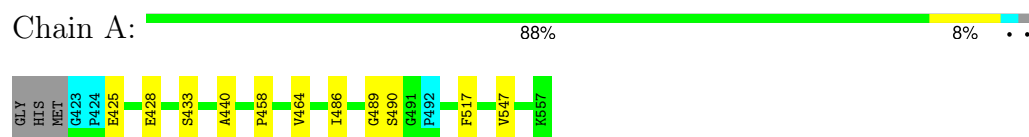
4.2.7 Score per residue for model 7

- Molecule 1: Serine/threonine-protein kinase pknB



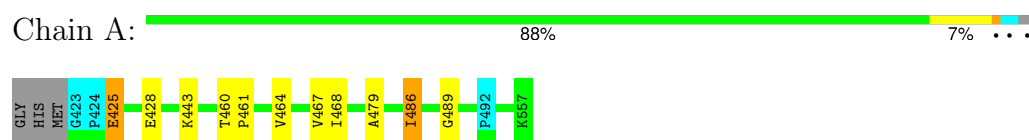
4.2.8 Score per residue for model 8

- Molecule 1: Serine/threonine-protein kinase pknB



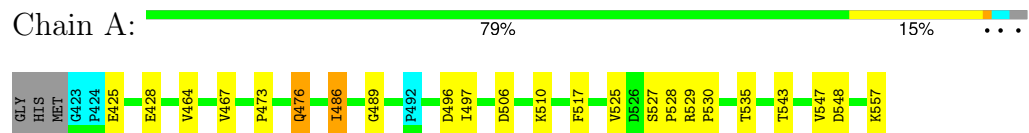
4.2.9 Score per residue for model 9

- Molecule 1: Serine/threonine-protein kinase pknB



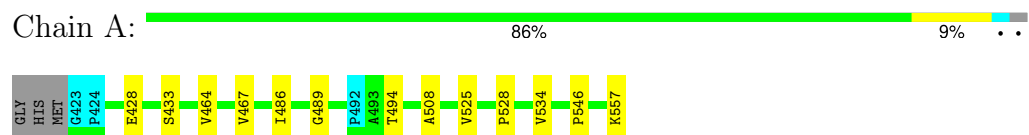
4.2.10 Score per residue for model 10

- Molecule 1: Serine/threonine-protein kinase pknB



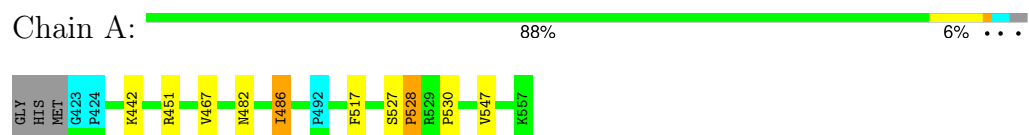
4.2.11 Score per residue for model 11

- Molecule 1: Serine/threonine-protein kinase pknB



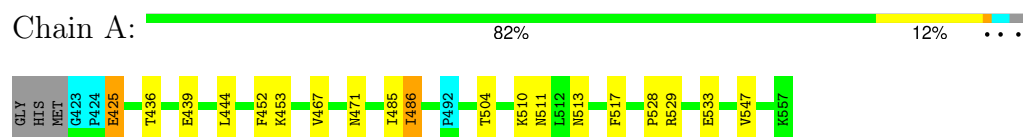
4.2.12 Score per residue for model 12

- Molecule 1: Serine/threonine-protein kinase pknB



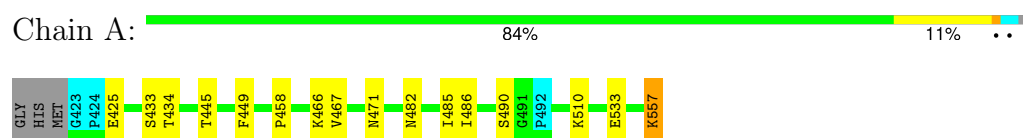
4.2.13 Score per residue for model 13

- Molecule 1: Serine/threonine-protein kinase pknB



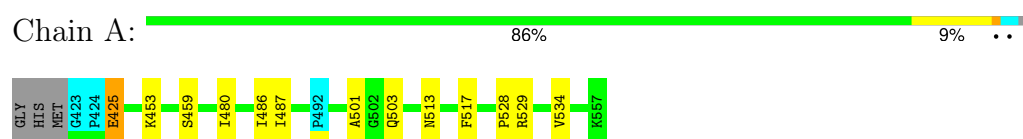
4.2.14 Score per residue for model 14

- Molecule 1: Serine/threonine-protein kinase pknB



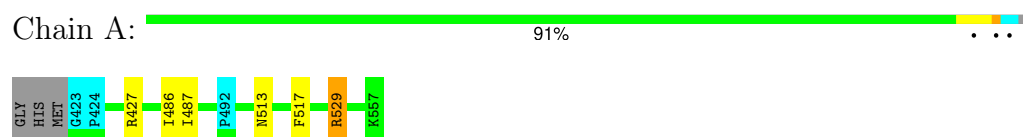
4.2.15 Score per residue for model 15

- Molecule 1: Serine/threonine-protein kinase pknB



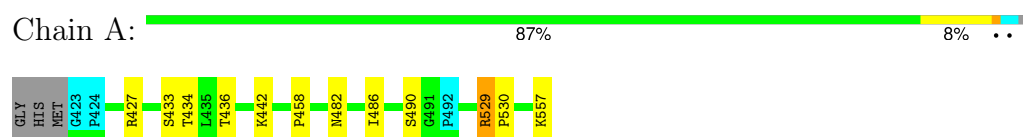
4.2.16 Score per residue for model 16

- Molecule 1: Serine/threonine-protein kinase pknB



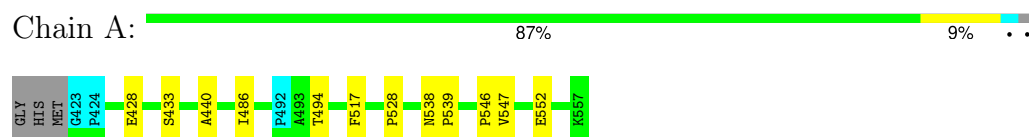
4.2.17 Score per residue for model 17

- Molecule 1: Serine/threonine-protein kinase pknB



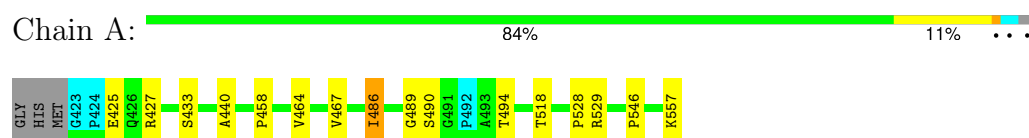
4.2.18 Score per residue for model 18

- Molecule 1: Serine/threonine-protein kinase pknB



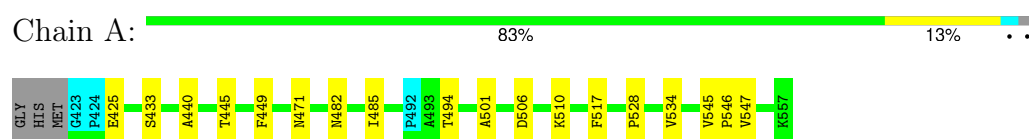
4.2.19 Score per residue for model 19

- Molecule 1: Serine/threonine-protein kinase pknB



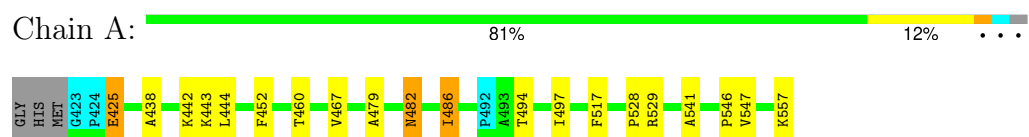
4.2.20 Score per residue for model 20

- Molecule 1: Serine/threonine-protein kinase pknB



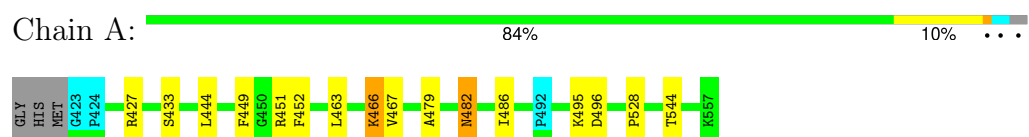
4.2.21 Score per residue for model 21

- Molecule 1: Serine/threonine-protein kinase pknB



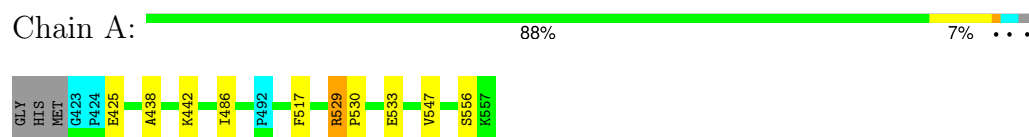
4.2.22 Score per residue for model 22

- Molecule 1: Serine/threonine-protein kinase pknB



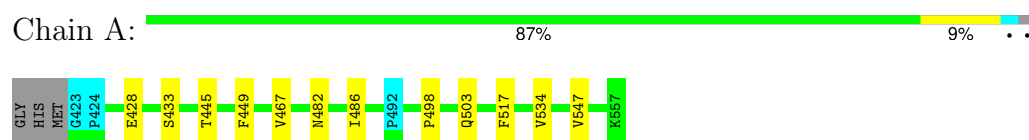
4.2.23 Score per residue for model 23

- Molecule 1: Serine/threonine-protein kinase pknB



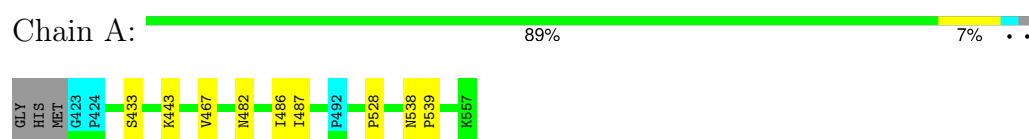
4.2.24 Score per residue for model 24

- Molecule 1: Serine/threonine-protein kinase pknB



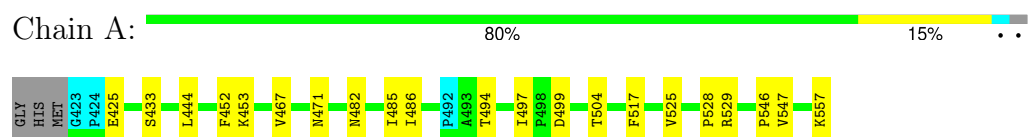
4.2.25 Score per residue for model 25

- Molecule 1: Serine/threonine-protein kinase pknB



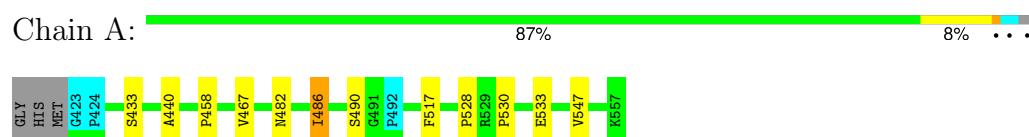
4.2.26 Score per residue for model 26

- Molecule 1: Serine/threonine-protein kinase pknB




4.2.27 Score per residue for model 27

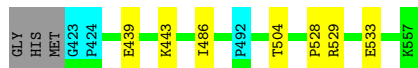
- Molecule 1: Serine/threonine-protein kinase pknB



4.2.28 Score per residue for model 28

- Molecule 1: Serine/threonine-protein kinase pknB

Chain A:  91% 5% ..



4.2.29 Score per residue for model 29


- Molecule 1: Serine/threonine-protein kinase pknB

Chain A:  90% 6% ..



4.2.30 Score per residue for model 30

- Molecule 1: Serine/threonine-protein kinase pknB

Chain A:  88% 7% ...



5 Refinement protocol and experimental data overview

The models were refined using the following method: *restrained molecular dynamics in a hydrated environment*.

Of the 30 calculated structures, 30 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	refinement	1.2

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	1422
Number of shifts mapped to atoms	1422
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	427	ARG	Sidechain	1

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	962	974	974	5±2
All	All	28860	29220	29220	146

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:433:SER:HA	1:A:440:ALA:HB2	0.62	1.72	19	7
1:A:458:PRO:HA	1:A:490:SER:O	0.58	1.99	17	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:517:PHE:CE1	1:A:547:VAL:HA	0.56	2.35	21	6
1:A:525:VAL:O	1:A:557:LYS:HG2	0.56	2.00	10	5
1:A:517:PHE:CD2	1:A:547:VAL:HA	0.56	2.36	5	5
1:A:427:ARG:NE	1:A:427:ARG:HA	0.56	2.15	19	3
1:A:517:PHE:CD1	1:A:547:VAL:HA	0.55	2.36	8	6
1:A:527:SER:HB3	1:A:530:PRO:O	0.55	2.02	12	2
1:A:464:VAL:HA	1:A:489:GLY:O	0.54	2.02	19	8
1:A:529:ARG:HA	1:A:529:ARG:NE	0.52	2.20	4	1
1:A:494:THR:HG22	1:A:546:PRO:HA	0.51	1.83	11	7
1:A:522:GLN:OE1	1:A:553:LEU:HB2	0.49	2.07	5	1
1:A:473:PRO:HG2	1:A:476:GLN:HG2	0.49	1.85	10	1
1:A:433:SER:HB3	1:A:467:VAL:HB	0.49	1.83	11	5
1:A:438:ALA:O	1:A:442:LYS:HG2	0.49	2.08	23	2
1:A:506:ASP:O	1:A:510:LYS:HD3	0.49	2.07	20	2
1:A:444:LEU:HD23	1:A:452:PHE:CE2	0.48	2.43	4	7
1:A:513:ASN:HA	1:A:517:PHE:O	0.48	2.09	7	4
1:A:467:VAL:HG22	1:A:486:ILE:HD11	0.48	1.86	27	10
1:A:517:PHE:CE2	1:A:545:VAL:HG23	0.47	2.44	20	2
1:A:433:SER:HB2	1:A:467:VAL:HB	0.47	1.87	14	1
1:A:445:THR:HA	1:A:449:PHE:O	0.47	2.09	24	3
1:A:510:LYS:O	1:A:514:VAL:HG23	0.47	2.10	2	1
1:A:517:PHE:CE2	1:A:547:VAL:HA	0.46	2.46	24	4
1:A:463:LEU:O	1:A:466:LYS:HG2	0.46	2.10	22	1
1:A:476:GLN:HE21	1:A:476:GLN:N	0.46	2.08	6	1
1:A:501:ALA:HA	1:A:534:VAL:O	0.46	2.10	20	1
1:A:427:ARG:HG2	1:A:447:ALA:O	0.46	2.10	5	1
1:A:471:ASN:CB	1:A:485:ILE:HB	0.46	2.41	14	4
1:A:433:SER:CB	1:A:467:VAL:HB	0.46	2.40	14	1
1:A:442:LYS:HE2	1:A:442:LYS:HA	0.46	1.88	17	1
1:A:439:GLU:O	1:A:443:LYS:HD3	0.46	2.10	28	1
1:A:523:ALA:HB3	1:A:554:GLN:OE1	0.45	2.12	30	1
1:A:557:LYS:HD2	1:A:557:LYS:OXT	0.45	2.12	14	1
1:A:425:GLU:O	1:A:480:ILE:HG12	0.45	2.12	15	1
1:A:479:ALA:HB3	1:A:482:ASN:ND2	0.44	2.27	22	2
1:A:436:THR:HB	1:A:439:GLU:HG2	0.44	1.89	13	1
1:A:426:GLN:HA	1:A:478:SER:O	0.43	2.13	2	1
1:A:460:THR:OG1	1:A:461:PRO:HD2	0.43	2.14	9	1
1:A:530:PRO:HA	1:A:533:GLU:OE2	0.43	2.13	27	1
1:A:476:GLN:HE21	1:A:476:GLN:CA	0.43	2.26	10	1
1:A:497:ILE:O	1:A:541:ALA:HA	0.43	2.13	21	1
1:A:425:GLU:O	1:A:479:ALA:HA	0.43	2.13	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:476:GLN:HE21	1:A:476:GLN:HA	0.43	1.72	10	1
1:A:508:ALA:CB	1:A:534:VAL:HG21	0.43	2.44	11	1
1:A:529:ARG:HB2	1:A:530:PRO:HD3	0.42	1.89	17	1
1:A:505:VAL:HA	1:A:534:VAL:CG2	0.42	2.44	7	1
1:A:522:GLN:OE1	1:A:553:LEU:HB3	0.42	2.14	6	1
1:A:496:ASP:HA	1:A:543:THR:O	0.42	2.15	10	1
1:A:427:ARG:HB3	1:A:449:PHE:CE1	0.42	2.50	22	1
1:A:503:GLN:O	1:A:534:VAL:HG12	0.42	2.15	15	3
1:A:443:LYS:HA	1:A:443:LYS:HE2	0.41	1.92	9	2
1:A:533:GLU:OE2	1:A:556:SER:HB3	0.41	2.16	23	1
1:A:453:LYS:HB2	1:A:485:ILE:HG13	0.41	1.91	26	1
1:A:538:ASN:HB3	1:A:539:PRO:HD3	0.41	1.91	25	2
1:A:529:ARG:HG3	1:A:530:PRO:HD3	0.41	1.92	23	1
1:A:529:ARG:N	1:A:530:PRO:HD2	0.41	2.30	30	1
1:A:425:GLU:CD	1:A:425:GLU:H	0.41	2.19	13	1
1:A:434:THR:O	1:A:466:LYS:HD3	0.41	2.15	14	1
1:A:501:ALA:HA	1:A:534:VAL:HG13	0.41	1.92	15	1
1:A:538:ASN:HB2	1:A:552:GLU:HB3	0.41	1.91	18	1
1:A:425:GLU:H	1:A:425:GLU:CD	0.40	2.19	21	1
1:A:496:ASP:HA	1:A:544:THR:HA	0.40	1.94	22	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	131/138 (95%)	126±2 (96±1%)	4±2 (3±2%)	1±1 (1±1%)	16	65
All	All	3930/4140 (95%)	3778 (96%)	112 (3%)	40 (1%)	16	65

All 6 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	528	PRO	22
1	A	529	ARG	14

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Mol	Chain	Res	Type	Models (Total)
1	A	500	VAL	1
1	A	516	GLY	1
1	A	460	THR	1
1	A	498	PRO	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	108/112 (96%)	104±2 (96±2%)	4±2 (4±2%)	29	82
All	All	3240/3360 (96%)	3110 (96%)	130 (4%)	29	82

All 31 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	486	ILE	29
1	A	482	ASN	15
1	A	425	GLU	14
1	A	428	GLU	9
1	A	533	GLU	7
1	A	557	LYS	5
1	A	487	ILE	5
1	A	451	ARG	5
1	A	497	ILE	3
1	A	495	LYS	3
1	A	529	ARG	3
1	A	510	LYS	3
1	A	476	GLN	3
1	A	504	THR	3
1	A	519	LYS	2
1	A	535	THR	2
1	A	511	ASN	2
1	A	433	SER	2
1	A	427	ARG	2
1	A	453	LYS	2
1	A	475	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	468	ILE	1
1	A	548	ASP	1
1	A	442	LYS	1
1	A	528	PRO	1
1	A	434	THR	1
1	A	436	THR	1
1	A	518	THR	1
1	A	466	LYS	1
1	A	443	LYS	1
1	A	499	ASP	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 84% for the well-defined parts and 83% 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	1422
Number of shifts mapped to atoms	1422
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	133	-0.14 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	121	-0.05 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	133	-0.06 ± 0.13	None needed (< 0.5 ppm)
^{15}N	122	-0.22 ± 0.31	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 84%, i.e. 1398 atoms were assigned a chemical shift out of a possible 1672. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	643/649 (99%)	262/264 (99%)	260/264 (98%)	121/121 (100%)
Sidechain	728/965 (75%)	592/632 (94%)	119/302 (39%)	17/31 (55%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	27/58 (47%)	27/28 (96%)	0/30 (0%)	0/0 (—%)
Overall	1398/1672 (84%)	881/924 (95%)	379/596 (64%)	138/152 (91%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 1420 atoms were assigned a chemical shift out of a possible 1702. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	655/661 (99%)	267/269 (99%)	266/270 (99%)	122/122 (100%)
Sidechain	738/983 (75%)	600/644 (93%)	121/308 (39%)	17/31 (55%)
Aromatic	27/58 (47%)	27/28 (96%)	0/30 (0%)	0/0 (—%)
Overall	1420/1702 (83%)	894/941 (95%)	387/608 (64%)	139/153 (91%)

7.1.4 Statistically unusual chemical shifts ⓘ

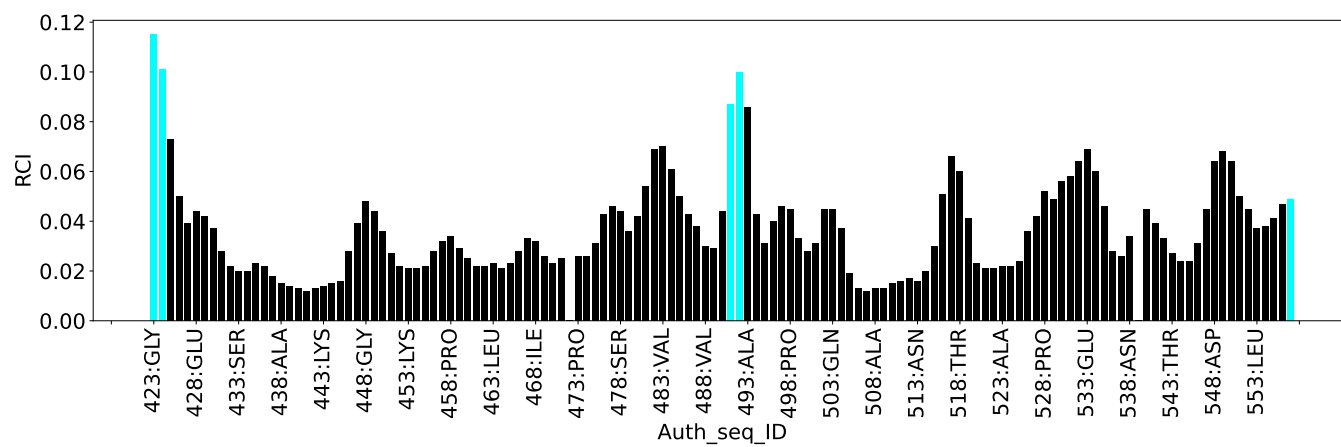
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	470	THR	HG1	6.18	0.08 – 2.19	23.9
1	A	537	THR	HG1	5.84	0.08 – 2.19	22.3

7.1.5 Random Coil Index (RCI) plots ⓘ

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1728
Intra-residue ($ i-j =0$)	357
Sequential ($ i-j =1$)	525
Medium range ($ i-j >1$ and $ i-j <5$)	228
Long range ($ i-j \geq 5$)	528
Inter-chain	0
Hydrogen bond restraints	90
Disulfide bond restraints	0
Total dihedral-angle restraints	186
Number of unmapped restraints	0
Number of restraints per residue	13.9
Number of long range restraints per residue ¹	4.1

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	5.8	0.2
0.2-0.5 (Medium)	0.1	0.38
>0.5 (Large)	0.1	1.54

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)	19.2	4.81
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis

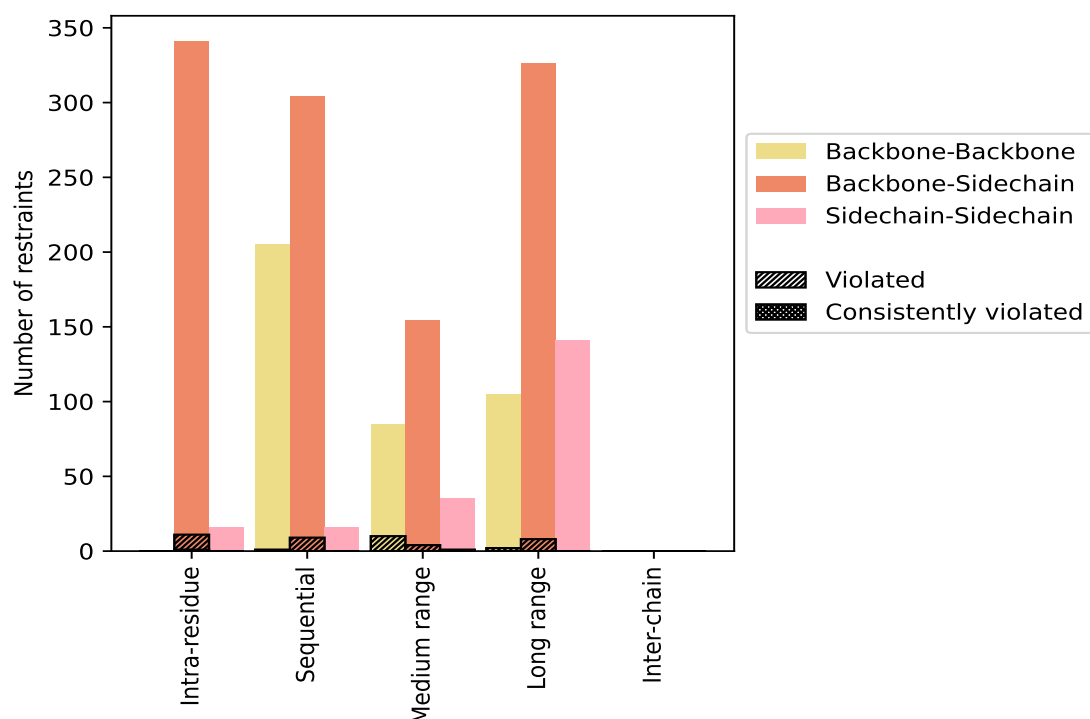
9.1 Summary of distance violations

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 ($i-j =0$)	357	20.7	11	3.1	0.6	1	0.3	0.1
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	341	19.7	11	3.2	0.6	1	0.3	0.1
Sidechain-Sidechain	16	0.9	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	525	30.4	10	1.9	0.6	0	0.0	0.0
Backbone-Backbone	205	11.9	1	0.5	0.1	0	0.0	0.0
Backbone-Sidechain	304	17.6	9	3.0	0.5	0	0.0	0.0
Sidechain-Sidechain	16	0.9	0	0.0	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	228	13.2	14	6.1	0.8	0	0.0	0.0
Backbone-Backbone	85	4.9	10	11.8	0.6	0	0.0	0.0
Backbone-Sidechain	112	6.5	3	2.7	0.2	0	0.0	0.0
Sidechain-Sidechain	31	1.8	1	3.2	0.1	0	0.0	0.0
Long range ($i-j \geq 5$)	528	30.6	10	1.9	0.6	0	0.0	0.0
Backbone-Backbone	105	6.1	2	1.9	0.1	0	0.0	0.0
Backbone-Sidechain	282	16.3	8	2.8	0.5	0	0.0	0.0
Sidechain-Sidechain	141	8.2	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	90	5.2	1	1.1	0.1	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1728	100.0	46	2.7	2.7	1	0.1	0.1
Backbone-Backbone	395	22.9	13	3.3	0.8	0	0.0	0.0
Backbone-Sidechain	1125	65.1	32	2.8	1.9	1	0.1	0.1
Sidechain-Sidechain	208	12.0	1	0.5	0.1	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 disulfide 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	2	2	0	6	0.24	0.74	0.22	0.15
2	2	0	2	2	0	6	0.12	0.15	0.02	0.12
3	3	2	3	2	0	10	0.12	0.15	0.02	0.12
4	3	1	4	1	0	9	0.14	0.18	0.02	0.13
5	2	0	0	2	0	4	0.12	0.16	0.02	0.12
6	1	2	2	0	0	5	0.14	0.26	0.06	0.13
7	1	1	4	1	0	7	0.13	0.16	0.02	0.13
8	4	1	2	1	0	8	0.14	0.18	0.02	0.14
9	1	3	3	0	0	7	0.18	0.38	0.09	0.14
10	1	1	5	4	0	11	0.24	1.13	0.29	0.17

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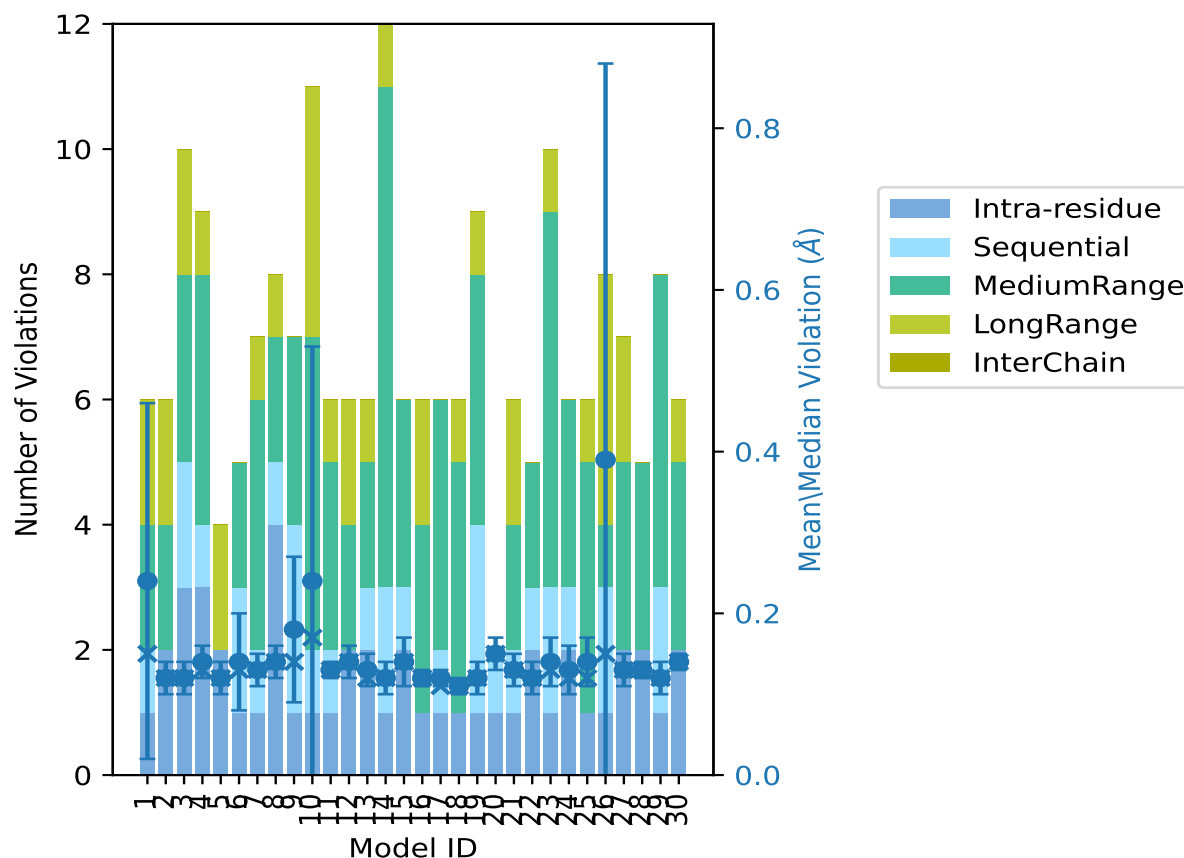
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	1	1	3	1	0	6	0.13	0.16	0.01	0.13
12	2	0	2	2	0	6	0.14	0.16	0.02	0.14
13	2	1	2	1	0	6	0.13	0.16	0.02	0.12
14	1	2	8	1	0	12	0.12	0.17	0.02	0.12
15	2	1	3	0	0	6	0.14	0.18	0.03	0.14
16	1	0	3	2	0	6	0.12	0.14	0.01	0.12
17	1	1	4	0	0	6	0.12	0.14	0.01	0.11
18	1	0	4	1	0	6	0.11	0.13	0.01	0.11
19	1	3	4	1	0	9	0.12	0.16	0.02	0.12
20	1	1	0	0	0	2	0.15	0.17	0.02	0.15
21	1	1	2	2	0	6	0.13	0.18	0.02	0.13
22	2	1	2	0	0	5	0.12	0.16	0.02	0.12
23	1	2	6	1	0	10	0.14	0.19	0.03	0.13
24	2	1	3	0	0	6	0.13	0.19	0.03	0.12
25	1	0	4	1	0	6	0.14	0.18	0.03	0.12
26	1	2	1	4	0	8	0.39	1.54	0.49	0.15
27	2	0	3	2	0	7	0.13	0.16	0.02	0.13
28	2	0	3	0	0	5	0.13	0.16	0.01	0.13
29	1	2	5	0	0	8	0.12	0.18	0.02	0.12
30	2	0	3	1	0	6	0.14	0.15	0.01	0.14

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

⁵Inter-chain restraints, ⁶Standard deviation

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1593(IR:346, SQ:515, MR:214, LR:518, 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	5	5	5	0	21	1	3.3
1	1	1	1	0	4	2	6.7
3	0	2	2	0	7	3	10.0
0	1	1	0	0	2	4	13.3
0	0	1	1	0	2	5	16.7
0	2	0	0	0	2	6	20.0

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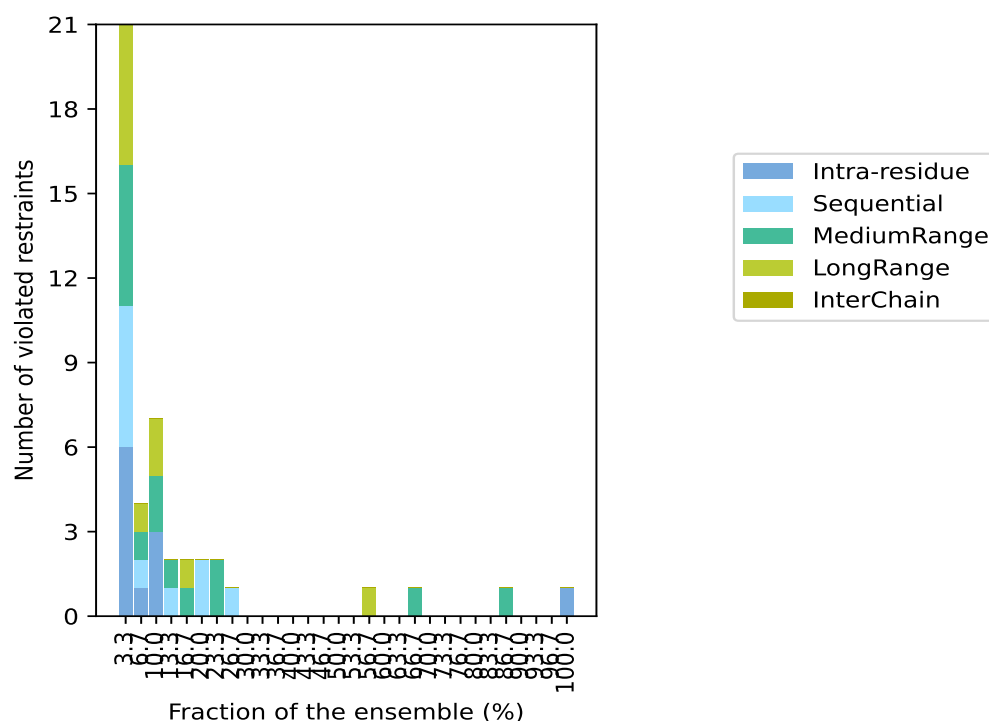
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	2	0	0	2	7	23.3
0	1	0	0	0	1	8	26.7
0	0	0	0	0	0	9	30.0
0	0	0	0	0	0	10	33.3
0	0	0	0	0	0	11	36.7
0	0	0	0	0	0	12	40.0
0	0	0	0	0	0	13	43.3
0	0	0	0	0	0	14	46.7
0	0	0	0	0	0	15	50.0
0	0	0	0	0	0	16	53.3
0	0	0	1	0	1	17	56.7
0	0	0	0	0	0	18	60.0
0	0	0	0	0	0	19	63.3
0	0	1	0	0	1	20	66.7
0	0	0	0	0	0	21	70.0
0	0	0	0	0	0	22	73.3
0	0	0	0	0	0	23	76.7
0	0	0	0	0	0	24	80.0
0	0	0	0	0	0	25	83.3
0	0	1	0	0	1	26	86.7
0	0	0	0	0	0	27	90.0
0	0	0	0	0	0	28	93.3
0	0	0	0	0	0	29	96.7
1	0	0	0	0	1	30	100.0

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

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

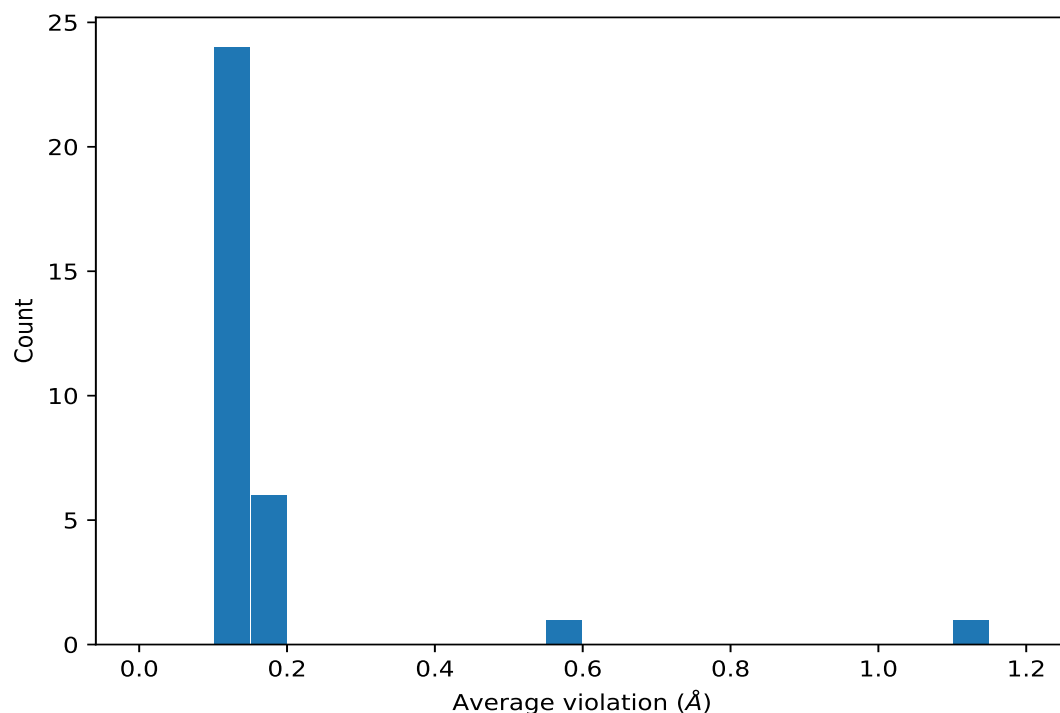
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	30	0.16	0.02	0.16
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	30	0.16	0.02	0.16
(1,999)	1:504:A:THR:H	1:507:A:VAL:HA	26	0.14	0.02	0.13
(1,313)	1:442:A:LYS:H	1:445:A:THR:HB	20	0.12	0.01	0.12
(1,838)	1:494:A:THR:HA	1:547:A:VAL:HB	17	0.13	0.02	0.12
(2,61)	1:515:A:TYR:H	1:512:A:LEU:O	10	0.11	0.01	0.12
(1,533)	1:460:A:THR:H	1:461:A:PRO:HD2	8	0.11	0.01	0.11
(1,533)	1:460:A:THR:H	1:461:A:PRO:HD3	8	0.11	0.01	0.11
(1,530)	1:460:A:THR:HA	1:462:A:GLU:H	7	0.15	0.03	0.15
(1,1176)	1:513:A:ASN:H	1:516:A:GLY:HA2	7	0.11	0.01	0.11
(1,1176)	1:513:A:ASN:H	1:516:A:GLY:HA3	7	0.11	0.01	0.11
(1,965)	1:503:A:GLN:HE21	1:504:A:THR:H	6	0.14	0.01	0.14
(1,965)	1:503:A:GLN:HE22	1:504:A:THR:H	6	0.14	0.01	0.14
(1,53)	1:427:A:ARG:HB2	1:428:A:GLU:H	6	0.11	0.01	0.11
(1,53)	1:427:A:ARG:HB3	1:428:A:GLU:H	6	0.11	0.01	0.11
(1,720)	1:479:A:ALA:H	1:482:A:ASN:HD21	5	0.13	0.01	0.13

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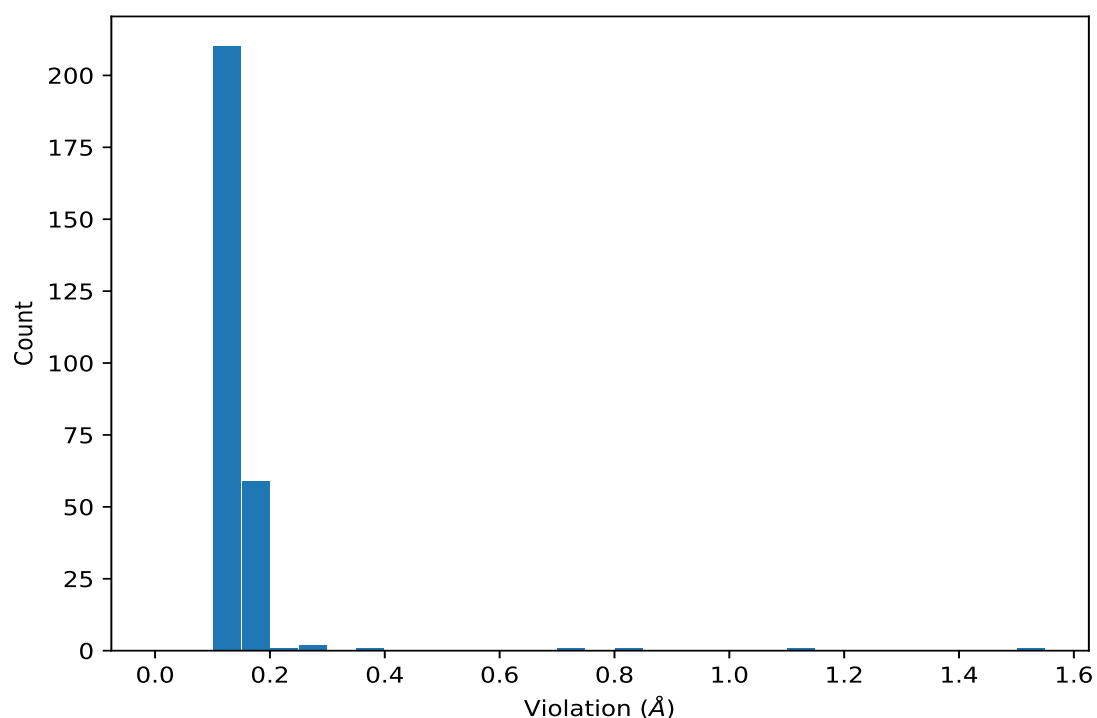
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,101)	1:429:A:ILE:H	1:475:A:ASN:H	5	0.11	0.0	0.11
(1,1607)	1:553:A:LEU:HG	1:554:A:GLN:H	4	0.14	0.03	0.13
(1,190)	1:436:A:THR:H	1:439:A:GLU:HA	4	0.12	0.01	0.12
(1,900)	1:497:A:ILE:HG13	1:543:A:THR:H	3	1.14	0.33	1.13
(1,680)	1:476:A:GLN:HA	1:476:A:GLN:HE21	3	0.15	0.02	0.16
(1,680)	1:476:A:GLN:HA	1:476:A:GLN:HE22	3	0.15	0.02	0.16
(1,745)	1:482:A:ASN:HA	1:482:A:ASN:HD22	3	0.13	0.02	0.12
(1,124)	1:431:A:ASP:H	1:433:A:SER:H	3	0.12	0.0	0.12
(1,667)	1:475:A:ASN:HA	1:475:A:ASN:HD21	3	0.12	0.0	0.12
(1,667)	1:475:A:ASN:HA	1:475:A:ASN:HD22	3	0.12	0.0	0.12
(1,992)	1:504:A:THR:HA	1:507:A:VAL:H	3	0.12	0.01	0.12
(1,25)	1:426:A:GLN:HB2	1:477:A:THR:H	3	0.11	0.01	0.1
(1,899)	1:497:A:ILE:HG13	1:541:A:ALA:H	2	0.56	0.28	0.56
(1,57)	1:427:A:ARG:HD3	1:428:A:GLU:H	2	0.18	0.08	0.18
(1,1566)	1:550:A:VAL:H	1:550:A:VAL:HB	2	0.12	0.01	0.12
(1,1598)	1:553:A:LEU:HA	1:555:A:VAL:H	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,900)	1:497:A:ILE:HG13	1:543:A:THR:H	26	1.54
(1,900)	1:497:A:ILE:HG13	1:543:A:THR:H	10	1.13
(1,899)	1:497:A:ILE:HG13	1:541:A:ALA:H	26	0.85
(1,900)	1:497:A:ILE:HG13	1:543:A:THR:H	1	0.74
(1,603)	1:468:A:ILE:HG13	1:469:A:GLY:H	9	0.38
(1,899)	1:497:A:ILE:HG13	1:541:A:ALA:H	10	0.28
(1,57)	1:427:A:ARG:HD3	1:428:A:GLU:H	6	0.26
(1,530)	1:460:A:THR:HA	1:462:A:GLU:H	9	0.2
(1,1607)	1:553:A:LEU:HG	1:554:A:GLN:H	23	0.19
(1,999)	1:504:A:THR:H	1:507:A:VAL:HA	24	0.19
(1,659)	1:473:A:PRO:HG2	1:476:A:GLN:HE21	10	0.19
(1,659)	1:473:A:PRO:HG2	1:476:A:GLN:HE22	10	0.19
(1,659)	1:473:A:PRO:HG3	1:476:A:GLN:HE21	10	0.19
(1,659)	1:473:A:PRO:HG3	1:476:A:GLN:HE22	10	0.19
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	4	0.18
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	4	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	15	0.18
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	15	0.18
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	21	0.18
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	21	0.18
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	29	0.18
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	29	0.18
(1,999)	1:504:A:THR:H	1:507:A:VAL:HA	25	0.18
(1,617)	1:469:A:GLY:H	1:486:A:ILE:HD11	8	0.18
(1,617)	1:469:A:GLY:H	1:486:A:ILE:HD12	8	0.18
(1,617)	1:469:A:GLY:H	1:486:A:ILE:HD13	8	0.18
(1,530)	1:460:A:THR:HA	1:462:A:GLU:H	10	0.18
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	1	0.17
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	1	0.17
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	10	0.17
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	10	0.17
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	14	0.17
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	14	0.17
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	20	0.17
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	20	0.17
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	23	0.17
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	23	0.17
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	25	0.17
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	25	0.17
(1,999)	1:504:A:THR:H	1:507:A:VAL:HA	10	0.17
(1,788)	1:486:A:ILE:H	1:486:A:ILE:HB	8	0.17
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	5	0.16
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	5	0.16
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	7	0.16
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	7	0.16
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	9	0.16
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	9	0.16
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	11	0.16
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	11	0.16
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	12	0.16
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	12	0.16
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	13	0.16
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	13	0.16
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	22	0.16
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	22	0.16
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	28	0.16
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	28	0.16
(1,999)	1:504:A:THR:H	1:507:A:VAL:HA	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,999)	1:504:A:THR:H	1:507:A:VAL:HA	8	0.16
(1,999)	1:504:A:THR:H	1:507:A:VAL:HA	15	0.16
(1,965)	1:503:A:GLN:HE21	1:504:A:THR:H	19	0.16
(1,965)	1:503:A:GLN:HE22	1:504:A:THR:H	19	0.16
(1,838)	1:494:A:THR:HA	1:547:A:VAL:HB	12	0.16
(1,680)	1:476:A:GLN:HA	1:476:A:GLN:HE21	4	0.16
(1,680)	1:476:A:GLN:HA	1:476:A:GLN:HE22	4	0.16
(1,680)	1:476:A:GLN:HA	1:476:A:GLN:HE21	27	0.16
(1,680)	1:476:A:GLN:HA	1:476:A:GLN:HE22	27	0.16
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	2	0.15
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	2	0.15
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	3	0.15
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	3	0.15
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	24	0.15
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	24	0.15
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	26	0.15
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	26	0.15
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	27	0.15
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	27	0.15
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	30	0.15
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	30	0.15
(1,1397)	1:529:A:ARG:H	1:529:A:ARG:HD3	3	0.15
(1,999)	1:504:A:THR:H	1:507:A:VAL:HA	1	0.15
(1,999)	1:504:A:THR:H	1:507:A:VAL:HA	26	0.15
(1,999)	1:504:A:THR:H	1:507:A:VAL:HA	27	0.15
(1,838)	1:494:A:THR:HA	1:547:A:VAL:HB	1	0.15
(1,838)	1:494:A:THR:HA	1:547:A:VAL:HB	2	0.15
(1,745)	1:482:A:ASN:HA	1:482:A:ASN:HD22	30	0.15
(1,720)	1:479:A:ALA:H	1:482:A:ASN:HD21	23	0.15
(1,530)	1:460:A:THR:HA	1:462:A:GLU:H	7	0.15
(1,530)	1:460:A:THR:HA	1:462:A:GLU:H	14	0.15
(1,313)	1:442:A:LYS:H	1:445:A:THR:HB	13	0.15
(1,299)	1:442:A:LYS:HA	1:442:A:LYS:HG2	12	0.15
(2,61)	1:515:A:TYR:H	1:512:A:LEU:O	14	0.14
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	8	0.14
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	8	0.14
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	16	0.14
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	16	0.14
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	17	0.14
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	17	0.14
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	19	0.14
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1176)	1:513:A:ASN:H	1:516:A:GLY:HA2	23	0.14
(1,1176)	1:513:A:ASN:H	1:516:A:GLY:HA3	23	0.14
(1,999)	1:504:A:THR:H	1:507:A:VAL:HA	21	0.14
(1,999)	1:504:A:THR:H	1:507:A:VAL:HA	30	0.14
(1,992)	1:504:A:THR:HA	1:507:A:VAL:H	28	0.14
(1,965)	1:503:A:GLN:HE21	1:504:A:THR:H	7	0.14
(1,965)	1:503:A:GLN:HE22	1:504:A:THR:H	7	0.14
(1,965)	1:503:A:GLN:HE21	1:504:A:THR:H	9	0.14
(1,965)	1:503:A:GLN:HE22	1:504:A:THR:H	9	0.14
(1,965)	1:503:A:GLN:HE21	1:504:A:THR:H	11	0.14
(1,965)	1:503:A:GLN:HE22	1:504:A:THR:H	11	0.14
(1,838)	1:494:A:THR:HA	1:547:A:VAL:HB	11	0.14
(1,838)	1:494:A:THR:HA	1:547:A:VAL:HB	21	0.14
(1,533)	1:460:A:THR:H	1:461:A:PRO:HD2	26	0.14
(1,533)	1:460:A:THR:H	1:461:A:PRO:HD3	26	0.14
(1,530)	1:460:A:THR:HA	1:462:A:GLU:H	15	0.14
(1,412)	1:451:A:ARG:HG2	1:452:A:PHE:H	3	0.14
(1,412)	1:451:A:ARG:HG3	1:452:A:PHE:H	3	0.14
(1,313)	1:442:A:LYS:H	1:445:A:THR:HB	30	0.14
(1,1607)	1:553:A:LEU:HG	1:554:A:GLN:H	15	0.13
(1,1607)	1:553:A:LEU:HG	1:554:A:GLN:H	29	0.13
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	6	0.13
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	6	0.13
(1,1566)	1:550:A:VAL:H	1:550:A:VAL:HB	28	0.13
(1,999)	1:504:A:THR:H	1:507:A:VAL:HA	3	0.13
(1,999)	1:504:A:THR:H	1:507:A:VAL:HA	6	0.13
(1,999)	1:504:A:THR:H	1:507:A:VAL:HA	7	0.13
(1,999)	1:504:A:THR:H	1:507:A:VAL:HA	19	0.13
(1,999)	1:504:A:THR:H	1:507:A:VAL:HA	22	0.13
(1,999)	1:504:A:THR:H	1:507:A:VAL:HA	23	0.13
(1,965)	1:503:A:GLN:HE21	1:504:A:THR:H	13	0.13
(1,965)	1:503:A:GLN:HE22	1:504:A:THR:H	13	0.13
(1,965)	1:503:A:GLN:HE21	1:504:A:THR:H	14	0.13
(1,965)	1:503:A:GLN:HE22	1:504:A:THR:H	14	0.13
(1,838)	1:494:A:THR:HA	1:547:A:VAL:HB	4	0.13
(1,838)	1:494:A:THR:HA	1:547:A:VAL:HB	10	0.13
(1,838)	1:494:A:THR:HA	1:547:A:VAL:HB	30	0.13
(1,720)	1:479:A:ALA:H	1:482:A:ASN:HD21	9	0.13
(1,720)	1:479:A:ALA:H	1:482:A:ASN:HD21	19	0.13
(1,667)	1:475:A:ASN:HA	1:475:A:ASN:HD21	8	0.13
(1,667)	1:475:A:ASN:HA	1:475:A:ASN:HD22	8	0.13
(1,530)	1:460:A:THR:HA	1:462:A:GLU:H	4	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,313)	1:442:A:LYS:H	1:445:A:THR:HB	2	0.13
(1,313)	1:442:A:LYS:H	1:445:A:THR:HB	7	0.13
(1,313)	1:442:A:LYS:H	1:445:A:THR:HB	23	0.13
(1,190)	1:436:A:THR:H	1:439:A:GLU:HA	18	0.13
(1,190)	1:436:A:THR:H	1:439:A:GLU:HA	27	0.13
(1,124)	1:431:A:ASP:H	1:433:A:SER:H	17	0.13
(1,53)	1:427:A:ARG:HB2	1:428:A:GLU:H	20	0.13
(1,53)	1:427:A:ARG:HB3	1:428:A:GLU:H	20	0.13
(2,61)	1:515:A:TYR:H	1:512:A:LEU:O	22	0.12
(2,61)	1:515:A:TYR:H	1:512:A:LEU:O	23	0.12
(2,61)	1:515:A:TYR:H	1:512:A:LEU:O	25	0.12
(2,61)	1:515:A:TYR:H	1:512:A:LEU:O	29	0.12
(1,1607)	1:553:A:LEU:HG	1:554:A:GLN:H	21	0.12
(1,1566)	1:550:A:VAL:H	1:550:A:VAL:HB	13	0.12
(1,1398)	1:529:A:ARG:H	1:529:A:ARG:HD2	5	0.12
(1,1383)	1:527:A:SER:HB3	1:557:A:LYS:H	16	0.12
(1,1176)	1:513:A:ASN:H	1:516:A:GLY:HA2	12	0.12
(1,1176)	1:513:A:ASN:H	1:516:A:GLY:HA3	12	0.12
(1,999)	1:504:A:THR:H	1:507:A:VAL:HA	11	0.12
(1,999)	1:504:A:THR:H	1:507:A:VAL:HA	12	0.12
(1,999)	1:504:A:THR:H	1:507:A:VAL:HA	14	0.12
(1,999)	1:504:A:THR:H	1:507:A:VAL:HA	16	0.12
(1,999)	1:504:A:THR:H	1:507:A:VAL:HA	18	0.12
(1,999)	1:504:A:THR:H	1:507:A:VAL:HA	29	0.12
(1,992)	1:504:A:THR:HA	1:507:A:VAL:H	14	0.12
(1,990)	1:504:A:THR:HA	1:506:A:ASP:H	28	0.12
(1,838)	1:494:A:THR:HA	1:547:A:VAL:HB	3	0.12
(1,838)	1:494:A:THR:HA	1:547:A:VAL:HB	7	0.12
(1,838)	1:494:A:THR:HA	1:547:A:VAL:HB	14	0.12
(1,838)	1:494:A:THR:HA	1:547:A:VAL:HB	19	0.12
(1,838)	1:494:A:THR:HA	1:547:A:VAL:HB	23	0.12
(1,838)	1:494:A:THR:HA	1:547:A:VAL:HB	25	0.12
(1,838)	1:494:A:THR:HA	1:547:A:VAL:HB	27	0.12
(1,745)	1:482:A:ASN:HA	1:482:A:ASN:HD22	8	0.12
(1,720)	1:479:A:ALA:H	1:482:A:ASN:HD21	11	0.12
(1,720)	1:479:A:ALA:H	1:482:A:ASN:HD21	13	0.12
(1,680)	1:476:A:GLN:HA	1:476:A:GLN:HE21	24	0.12
(1,680)	1:476:A:GLN:HA	1:476:A:GLN:HE22	24	0.12
(1,667)	1:475:A:ASN:HA	1:475:A:ASN:HD21	3	0.12
(1,667)	1:475:A:ASN:HA	1:475:A:ASN:HD22	3	0.12
(1,667)	1:475:A:ASN:HA	1:475:A:ASN:HD21	4	0.12
(1,667)	1:475:A:ASN:HA	1:475:A:ASN:HD22	4	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,313)	1:442:A:LYS:H	1:445:A:THR:HB	1	0.12
(1,313)	1:442:A:LYS:H	1:445:A:THR:HB	8	0.12
(1,313)	1:442:A:LYS:H	1:445:A:THR:HB	11	0.12
(1,313)	1:442:A:LYS:H	1:445:A:THR:HB	21	0.12
(1,313)	1:442:A:LYS:H	1:445:A:THR:HB	28	0.12
(1,313)	1:442:A:LYS:H	1:445:A:THR:HB	29	0.12
(1,190)	1:436:A:THR:H	1:439:A:GLU:HA	19	0.12
(1,124)	1:431:A:ASP:H	1:433:A:SER:H	4	0.12
(1,124)	1:431:A:ASP:H	1:433:A:SER:H	25	0.12
(1,101)	1:429:A:ILE:H	1:475:A:ASN:H	3	0.12
(1,101)	1:429:A:ILE:H	1:475:A:ASN:H	27	0.12
(1,25)	1:426:A:GLN:HB2	1:477:A:THR:H	16	0.12
(2,61)	1:515:A:TYR:H	1:512:A:LEU:O	16	0.11
(1,1598)	1:553:A:LEU:HA	1:555:A:VAL:H	14	0.11
(1,1555)	1:548:A:ASP:H	1:549:A:SER:HB2	19	0.11
(1,1554)	1:548:A:ASP:H	1:549:A:SER:HB3	14	0.11
(1,1424)	1:533:A:GLU:H	1:556:A:SER:H	21	0.11
(1,1327)	1:524:A:SER:HA	1:557:A:LYS:HB2	10	0.11
(1,1176)	1:513:A:ASN:H	1:516:A:GLY:HA2	7	0.11
(1,1176)	1:513:A:ASN:H	1:516:A:GLY:HA3	7	0.11
(1,1176)	1:513:A:ASN:H	1:516:A:GLY:HA2	16	0.11
(1,1176)	1:513:A:ASN:H	1:516:A:GLY:HA3	16	0.11
(1,1176)	1:513:A:ASN:H	1:516:A:GLY:HA2	17	0.11
(1,1176)	1:513:A:ASN:H	1:516:A:GLY:HA3	17	0.11
(1,1176)	1:513:A:ASN:H	1:516:A:GLY:HA2	29	0.11
(1,1176)	1:513:A:ASN:H	1:516:A:GLY:HA3	29	0.11
(1,999)	1:504:A:THR:H	1:507:A:VAL:HA	9	0.11
(1,999)	1:504:A:THR:H	1:507:A:VAL:HA	17	0.11
(1,992)	1:504:A:THR:HA	1:507:A:VAL:H	30	0.11
(1,913)	1:499:A:ASP:HA	1:501:A:ALA:H	24	0.11
(1,838)	1:494:A:THR:HA	1:547:A:VAL:HB	5	0.11
(1,745)	1:482:A:ASN:HA	1:482:A:ASN:HD22	15	0.11
(1,533)	1:460:A:THR:H	1:461:A:PRO:HD2	3	0.11
(1,533)	1:460:A:THR:H	1:461:A:PRO:HD3	3	0.11
(1,533)	1:460:A:THR:H	1:461:A:PRO:HD2	9	0.11
(1,533)	1:460:A:THR:H	1:461:A:PRO:HD3	9	0.11
(1,533)	1:460:A:THR:H	1:461:A:PRO:HD2	17	0.11
(1,533)	1:460:A:THR:H	1:461:A:PRO:HD3	17	0.11
(1,533)	1:460:A:THR:H	1:461:A:PRO:HD2	24	0.11
(1,533)	1:460:A:THR:H	1:461:A:PRO:HD3	24	0.11
(1,530)	1:460:A:THR:HA	1:462:A:GLU:H	23	0.11
(1,405)	1:451:A:ARG:HA	1:451:A:ARG:HD2	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,313)	1:442:A:LYS:H	1:445:A:THR:HB	3	0.11
(1,313)	1:442:A:LYS:H	1:445:A:THR:HB	4	0.11
(1,313)	1:442:A:LYS:H	1:445:A:THR:HB	10	0.11
(1,313)	1:442:A:LYS:H	1:445:A:THR:HB	17	0.11
(1,313)	1:442:A:LYS:H	1:445:A:THR:HB	18	0.11
(1,313)	1:442:A:LYS:H	1:445:A:THR:HB	24	0.11
(1,147)	1:433:A:SER:HA	1:437:A:TYR:H	14	0.11
(1,101)	1:429:A:ILE:H	1:475:A:ASN:H	5	0.11
(1,101)	1:429:A:ILE:H	1:475:A:ASN:H	12	0.11
(1,101)	1:429:A:ILE:H	1:475:A:ASN:H	26	0.11
(1,53)	1:427:A:ARG:HB2	1:428:A:GLU:H	1	0.11
(1,53)	1:427:A:ARG:HB3	1:428:A:GLU:H	1	0.11
(1,53)	1:427:A:ARG:HB2	1:428:A:GLU:H	4	0.11
(1,53)	1:427:A:ARG:HB3	1:428:A:GLU:H	4	0.11
(1,53)	1:427:A:ARG:HB2	1:428:A:GLU:H	8	0.11
(1,53)	1:427:A:ARG:HB3	1:428:A:GLU:H	8	0.11
(1,53)	1:427:A:ARG:HB2	1:428:A:GLU:H	29	0.11
(1,53)	1:427:A:ARG:HB3	1:428:A:GLU:H	29	0.11
(2,61)	1:515:A:TYR:H	1:512:A:LEU:O	6	0.1
(2,61)	1:515:A:TYR:H	1:512:A:LEU:O	10	0.1
(2,61)	1:515:A:TYR:H	1:512:A:LEU:O	18	0.1
(2,61)	1:515:A:TYR:H	1:512:A:LEU:O	19	0.1
(1,1598)	1:553:A:LEU:HA	1:555:A:VAL:H	29	0.1
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG2	18	0.1
(1,1592)	1:552:A:GLU:H	1:552:A:GLU:HG3	18	0.1
(1,1258)	1:519:A:LYS:H	1:550:A:VAL:HG21	13	0.1
(1,1258)	1:519:A:LYS:H	1:550:A:VAL:HG22	13	0.1
(1,1258)	1:519:A:LYS:H	1:550:A:VAL:HG23	13	0.1
(1,1176)	1:513:A:ASN:H	1:516:A:GLY:HA2	25	0.1
(1,1176)	1:513:A:ASN:H	1:516:A:GLY:HA3	25	0.1
(1,999)	1:504:A:THR:H	1:507:A:VAL:HA	2	0.1
(1,950)	1:502:A:GLY:H	1:503:A:GLN:HA	19	0.1
(1,838)	1:494:A:THR:HA	1:547:A:VAL:HB	26	0.1
(1,658)	1:473:A:PRO:HG2	1:475:A:ASN:H	14	0.1
(1,658)	1:473:A:PRO:HG3	1:475:A:ASN:H	14	0.1
(1,636)	1:471:A:ASN:HA	1:471:A:ASN:HD22	22	0.1
(1,533)	1:460:A:THR:H	1:461:A:PRO:HD2	6	0.1
(1,533)	1:460:A:THR:H	1:461:A:PRO:HD3	6	0.1
(1,533)	1:460:A:THR:H	1:461:A:PRO:HD2	22	0.1
(1,533)	1:460:A:THR:H	1:461:A:PRO:HD3	22	0.1
(1,533)	1:460:A:THR:H	1:461:A:PRO:HD2	23	0.1
(1,533)	1:460:A:THR:H	1:461:A:PRO:HD3	23	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,313)	1:442:A:LYS:H	1:445:A:THR:HB	14	0.1
(1,313)	1:442:A:LYS:H	1:445:A:THR:HB	15	0.1
(1,313)	1:442:A:LYS:H	1:445:A:THR:HB	27	0.1
(1,190)	1:436:A:THR:H	1:439:A:GLU:HA	3	0.1
(1,57)	1:427:A:ARG:HD3	1:428:A:GLU:H	10	0.1
(1,53)	1:427:A:ARG:HB2	1:428:A:GLU:H	26	0.1
(1,53)	1:427:A:ARG:HB3	1:428:A:GLU:H	26	0.1
(1,25)	1:426:A:GLN:HB2	1:477:A:THR:H	2	0.1
(1,25)	1:426:A:GLN:HB2	1:477:A:THR:H	18	0.1

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

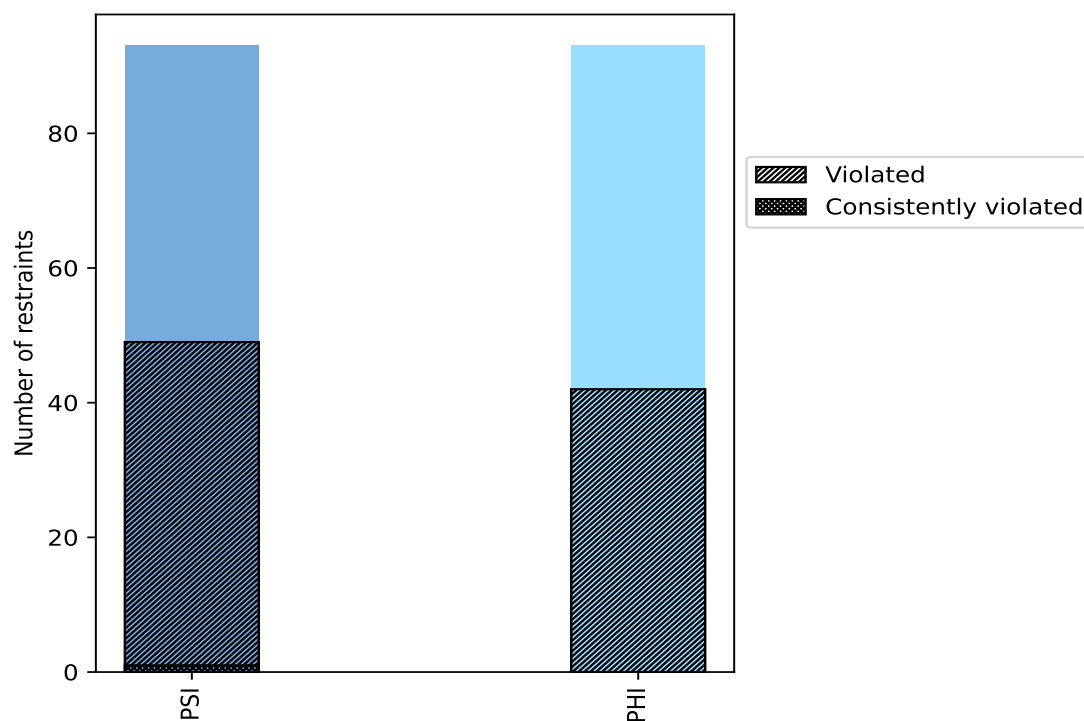
10.1 Summary of dihedral-angle violations [i](#)

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	93	50.0	49	52.7	26.3	1	1.1	0.5
PHI	93	50.0	42	45.2	22.6	0	0.0	0.0
Total	186	100.0	91	48.9	48.9	1	0.5	0.5

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](#)



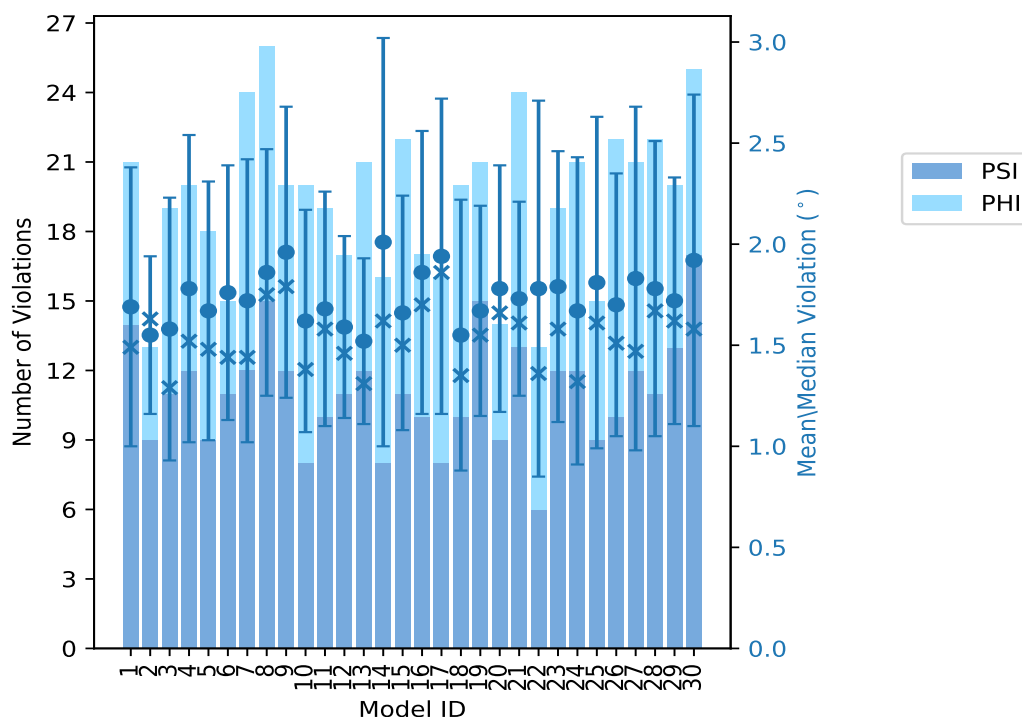
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	14	7	21	1.69	3.68	0.69	1.49
2	9	4	13	1.55	2.27	0.39	1.63
3	11	8	19	1.58	3.39	0.65	1.29
4	12	8	20	1.78	3.77	0.76	1.52
5	9	9	18	1.67	3.49	0.64	1.48
6	11	4	15	1.76	2.91	0.63	1.44
7	12	12	24	1.72	3.41	0.7	1.44
8	15	11	26	1.86	3.64	0.61	1.75
9	12	8	20	1.96	3.7	0.72	1.79
10	8	12	20	1.62	3.03	0.55	1.38
11	10	9	19	1.68	3.34	0.58	1.58
12	11	6	17	1.59	2.85	0.45	1.46
13	12	9	21	1.52	2.59	0.41	1.31
14	8	8	16	2.01	4.81	1.01	1.62
15	11	11	22	1.66	3.3	0.58	1.5
16	10	7	17	1.86	3.51	0.7	1.7
17	8	8	16	1.94	3.81	0.78	1.86
18	10	10	20	1.55	4.19	0.67	1.35
19	15	6	21	1.67	2.57	0.52	1.55
20	9	5	14	1.78	3.48	0.61	1.66
21	13	11	24	1.73	2.82	0.48	1.61
22	6	7	13	1.78	4.51	0.93	1.36
23	12	7	19	1.79	3.29	0.67	1.58
24	12	9	21	1.67	3.48	0.76	1.32
25	9	6	15	1.81	4.19	0.82	1.61
26	10	12	22	1.7	3.92	0.65	1.51
27	12	9	21	1.83	4.63	0.85	1.47
28	11	11	22	1.78	3.57	0.73	1.67
29	13	7	20	1.72	3.42	0.61	1.62
30	17	8	25	1.92	4.35	0.82	1.58

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	%
18	9	27	1	3.3
4	10	14	2	6.7
4	6	10	3	10.0
3	1	4	4	13.3
4	2	6	5	16.7
2	1	3	6	20.0
0	0	0	7	23.3
1	0	1	8	26.7
0	3	3	9	30.0
2	1	3	10	33.3
1	0	1	11	36.7

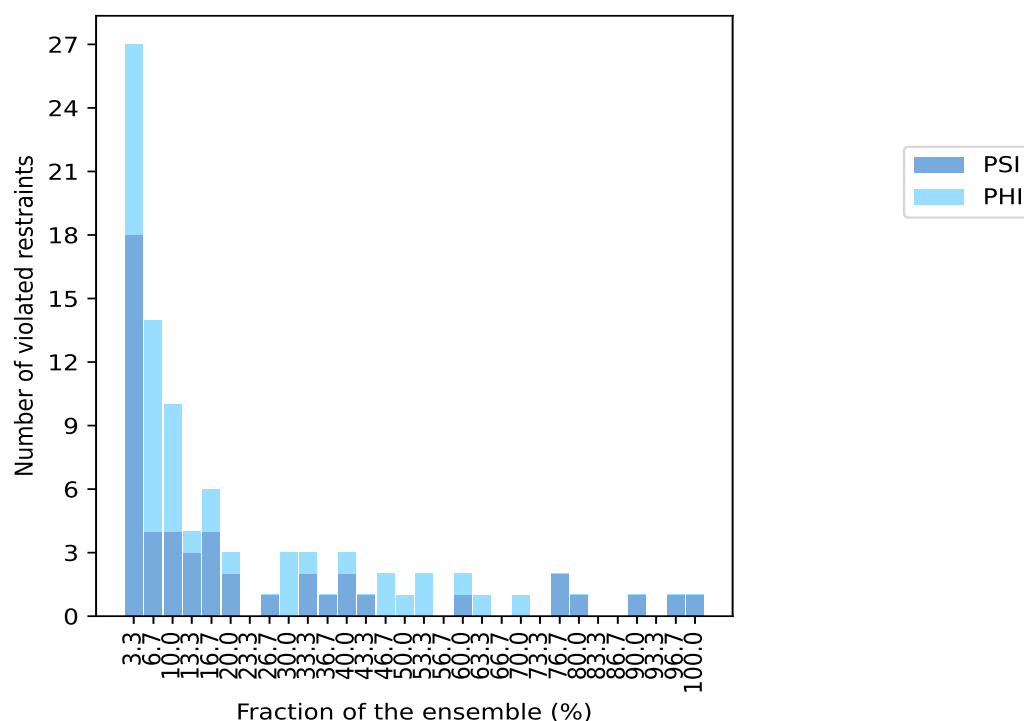
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
2	1	3	12	40.0
1	0	1	13	43.3
0	2	2	14	46.7
0	1	1	15	50.0
0	2	2	16	53.3
0	0	0	17	56.7
1	1	2	18	60.0
0	1	1	19	63.3
0	0	0	20	66.7
0	1	1	21	70.0
0	0	0	22	73.3
2	0	2	23	76.7
1	0	1	24	80.0
0	0	0	25	83.3
0	0	0	26	86.7
1	0	1	27	90.0
0	0	0	28	93.3
1	0	1	29	96.7
1	0	1	30	100.0

¹ Number of models with violations

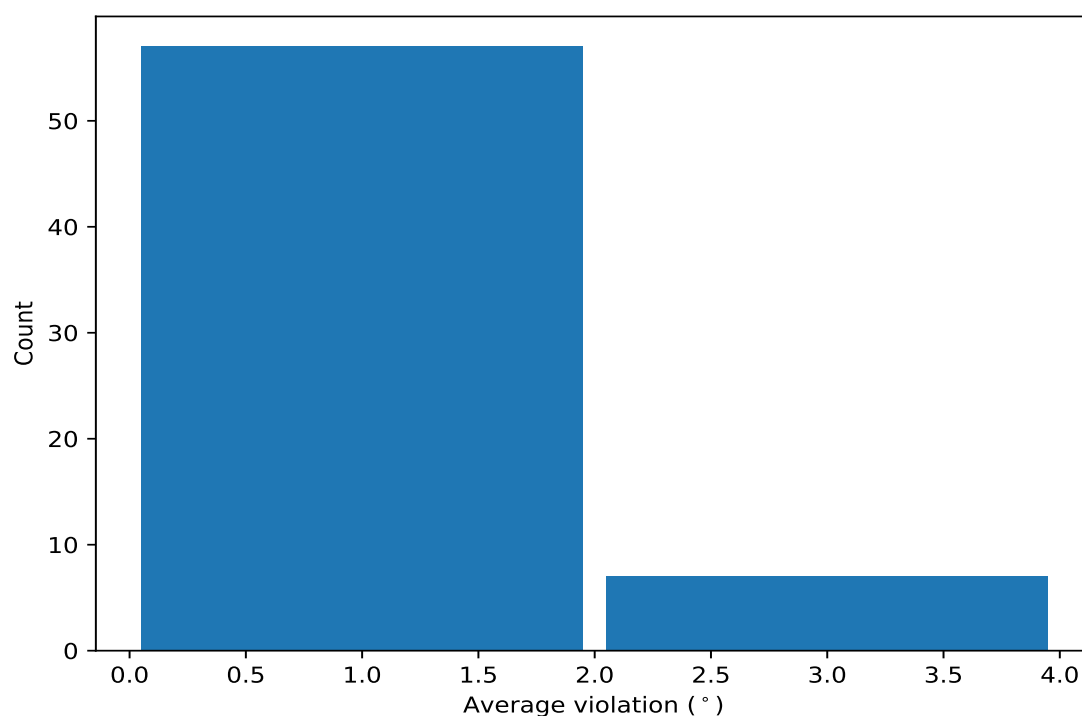
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

10.4.1 Histogram : Distribution of mean dihedral-angle 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



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
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	30	3.04	0.96	3.3
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	29	2.27	0.64	2.21
(1,100)	1:434:A:THR:N	1:434:A:THR:CA	1:434:A:THR:C	1:435:A:LEU:N	27	2.09	0.65	2.21
(1,168)	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	1:534:A:VAL:N	24	2.4	0.9	2.3
(1,148)	1:504:A:THR:N	1:504:A:THR:CA	1:504:A:THR:C	1:505:A:VAL:N	23	2.12	0.51	2.23
(1,97)	1:428:A:GLU:N	1:428:A:GLU:CA	1:428:A:GLU:C	1:429:A:ILE:N	23	1.71	0.44	1.6
(1,72)	1:524:A:SER:C	1:525:A:VAL:N	1:525:A:VAL:CA	1:525:A:VAL:C	21	1.62	0.46	1.56
(1,89)	1:551:A:ILE:C	1:552:A:GLU:N	1:552:A:GLU:CA	1:552:A:GLU:C	19	1.47	0.47	1.26
(1,113)	1:451:A:ARG:N	1:451:A:ARG:CA	1:451:A:ARG:C	1:452:A:PHE:N	18	1.63	0.6	1.38
(1,35)	1:466:A:LYS:C	1:467:A:VAL:N	1:467:A:VAL:CA	1:467:A:VAL:C	18	1.34	0.27	1.3
(1,73)	1:525:A:VAL:C	1:526:A:ASP:N	1:526:A:ASP:CA	1:526:A:ASP:C	16	1.88	0.57	1.73
(1,15)	1:442:A:LYS:C	1:443:A:LYS:N	1:443:A:LYS:CA	1:443:A:LYS:C	16	1.7	0.4	1.69
(1,29)	1:460:A:THR:C	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	15	1.61	0.5	1.42
(1,76)	1:533:A:GLU:C	1:534:A:VAL:N	1:534:A:VAL:CA	1:534:A:VAL:C	14	2.06	0.54	2.05
(1,32)	1:463:A:LEU:C	1:464:A:VAL:N	1:464:A:VAL:CA	1:464:A:VAL:C	14	1.25	0.14	1.21
(1,150)	1:506:A:ASP:N	1:506:A:ASP:CA	1:506:A:ASP:C	1:507:A:VAL:N	13	1.55	0.43	1.4
(1,69)	1:521:A:SER:C	1:522:A:GLN:N	1:522:A:GLN:CA	1:522:A:GLN:C	12	1.74	0.65	1.53
(1,178)	1:547:A:VAL:N	1:547:A:VAL:CA	1:547:A:VAL:C	1:548:A:ASP:N	12	1.71	0.43	1.73
(1,122)	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	1:462:A:GLU:N	12	1.64	0.68	1.46
(1,175)	1:544:A:THR:N	1:544:A:THR:CA	1:544:A:THR:C	1:545:A:VAL:N	11	1.34	0.21	1.32
(1,185)	1:555:A:VAL:N	1:555:A:VAL:CA	1:555:A:VAL:C	1:556:A:SER:N	10	2.02	0.84	1.77

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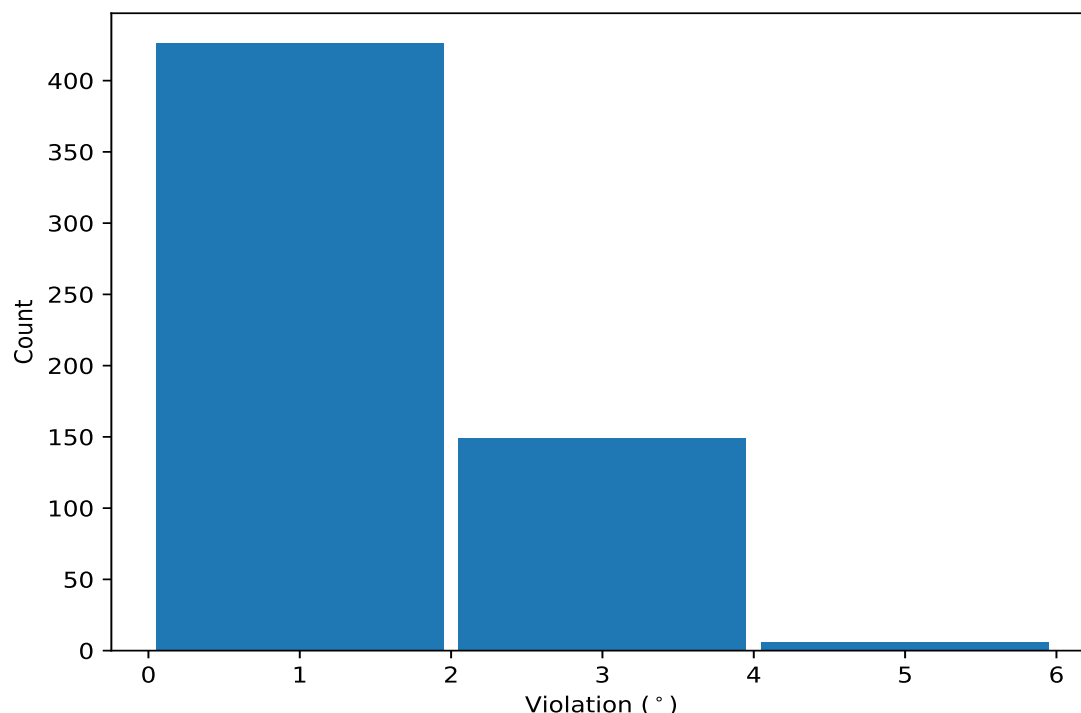
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,125)	1:464:A:VAL:N	1:464:A:VAL:CA	1:464:A:VAL:C	1:465:A:GLY:N	10	1.52	0.32	1.56
(1,75)	1:532:A:GLY:C	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	10	1.3	0.34	1.23
(1,57)	1:505:A:VAL:C	1:506:A:ASP:N	1:506:A:ASP:CA	1:506:A:ASP:C	9	1.7	0.48	1.6
(1,36)	1:467:A:VAL:C	1:468:A:ILE:N	1:468:A:ILE:CA	1:468:A:ILE:C	9	1.41	0.32	1.28
(1,27)	1:457:A:SER:C	1:458:A:PRO:N	1:458:A:PRO:CA	1:458:A:PRO:C	9	1.2	0.17	1.19
(1,121)	1:459:A:SER:N	1:459:A:SER:CA	1:459:A:SER:C	1:460:A:THR:N	8	1.42	0.28	1.37
(1,107)	1:442:A:LYS:N	1:442:A:LYS:CA	1:442:A:LYS:C	1:443:A:LYS:N	6	1.6	0.37	1.57
(1,64)	1:512:A:LEU:C	1:513:A:ASN:N	1:513:A:ASN:CA	1:513:A:ASN:C	6	1.49	0.43	1.3
(1,170)	1:537:A:THR:N	1:537:A:THR:CA	1:537:A:THR:C	1:538:A:ASN:N	6	1.43	0.24	1.42
(1,21)	1:451:A:ARG:C	1:452:A:PHE:N	1:452:A:PHE:CA	1:452:A:PHE:C	5	1.64	0.4	1.42
(1,85)	1:546:A:PRO:C	1:547:A:VAL:N	1:547:A:VAL:CA	1:547:A:VAL:C	5	1.51	0.41	1.36
(1,112)	1:447:A:ALA:N	1:447:A:ALA:CA	1:447:A:ALA:C	1:448:A:GLY:N	5	1.36	0.32	1.16
(1,167)	1:530:A:PRO:N	1:530:A:PRO:CA	1:530:A:PRO:C	1:531:A:ALA:N	5	1.35	0.32	1.24
(1,99)	1:430:A:PRO:N	1:430:A:PRO:CA	1:430:A:PRO:C	1:431:A:ASP:N	5	1.33	0.39	1.15
(1,105)	1:440:A:ALA:N	1:440:A:ALA:CA	1:440:A:ALA:C	1:441:A:VAL:N	5	1.21	0.24	1.12
(1,115)	1:453:A:LYS:N	1:453:A:LYS:CA	1:453:A:LYS:C	1:454:A:GLN:N	4	1.42	0.26	1.42
(1,165)	1:525:A:VAL:N	1:525:A:VAL:CA	1:525:A:VAL:C	1:526:A:ASP:N	4	1.34	0.3	1.2
(1,153)	1:509:A:GLN:N	1:509:A:GLN:CA	1:509:A:GLN:C	1:510:A:LYS:N	4	1.33	0.14	1.39
(1,66)	1:518:A:THR:C	1:519:A:LYS:N	1:519:A:LYS:CA	1:519:A:LYS:C	4	1.24	0.27	1.12
(1,30)	1:461:A:PRO:C	1:462:A:GLU:N	1:462:A:GLU:CA	1:462:A:GLU:C	3	1.92	0.48	1.73
(1,93)	1:555:A:VAL:C	1:556:A:SER:N	1:556:A:SER:CA	1:556:A:SER:C	3	1.88	0.24	1.76
(1,5)	1:428:A:GLU:C	1:429:A:ILE:N	1:429:A:ILE:CA	1:429:A:ILE:C	3	1.86	0.43	1.61
(1,183)	1:553:A:LEU:N	1:553:A:LEU:CA	1:553:A:LEU:C	1:554:A:GLN:N	3	1.81	0.46	1.7
(1,74)	1:529:A:ARG:C	1:530:A:PRO:N	1:530:A:PRO:CA	1:530:A:PRO:C	3	1.69	0.5	1.54
(1,120)	1:458:A:PRO:N	1:458:A:PRO:CA	1:458:A:PRO:C	1:459:A:SER:N	3	1.52	0.43	1.37
(1,177)	1:546:A:PRO:N	1:546:A:PRO:CA	1:546:A:PRO:C	1:547:A:VAL:N	3	1.45	0.33	1.45
(1,70)	1:522:A:GLN:C	1:523:A:ALA:N	1:523:A:ALA:CA	1:523:A:ALA:C	3	1.25	0.18	1.23
(1,98)	1:429:A:ILE:N	1:429:A:ILE:CA	1:429:A:ILE:C	1:430:A:PRO:N	3	1.23	0.17	1.18
(1,48)	1:487:A:ILE:C	1:488:A:VAL:N	1:488:A:VAL:CA	1:488:A:VAL:C	3	1.1	0.13	1.01
(1,45)	1:484:A:VAL:C	1:485:A:ILE:N	1:485:A:ILE:CA	1:485:A:ILE:C	2	1.68	0.49	1.68
(1,22)	1:452:A:PHE:C	1:453:A:LYS:N	1:453:A:LYS:CA	1:453:A:LYS:C	2	1.54	0.05	1.54
(1,77)	1:536:A:GLY:C	1:537:A:THR:N	1:537:A:THR:CA	1:537:A:THR:C	2	1.44	0.38	1.44
(1,124)	1:463:A:LEU:N	1:463:A:LEU:CA	1:463:A:LEU:C	1:464:A:VAL:N	2	1.36	0.11	1.36
(1,94)	1:424:A:PRO:N	1:424:A:PRO:CA	1:424:A:PRO:C	1:425:A:GLU:N	2	1.32	0.14	1.32
(1,44)	1:483:A:VAL:C	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	2	1.3	0.07	1.3
(1,133)	1:478:A:SER:N	1:478:A:SER:CA	1:478:A:SER:C	1:479:A:ALA:N	2	1.27	0.04	1.27
(1,2)	1:425:A:GLU:C	1:426:A:GLN:N	1:426:A:GLN:CA	1:426:A:GLN:C	2	1.27	0.07	1.27
(1,149)	1:505:A:VAL:N	1:505:A:VAL:CA	1:505:A:VAL:C	1:506:A:ASP:N	2	1.22	0.21	1.22
(1,59)	1:507:A:VAL:C	1:508:A:ALA:N	1:508:A:ALA:CA	1:508:A:ALA:C	2	1.19	0.07	1.19
(1,4)	1:427:A:ARG:C	1:428:A:GLU:N	1:428:A:GLU:CA	1:428:A:GLU:C	2	1.18	0.09	1.18
(1,16)	1:443:A:LYS:C	1:444:A:LEU:N	1:444:A:LEU:CA	1:444:A:LEU:C	2	1.16	0.15	1.16
(1,71)	1:523:A:ALA:C	1:524:A:SER:N	1:524:A:SER:CA	1:524:A:SER:C	2	1.14	0.02	1.14
(1,12)	1:439:A:GLU:C	1:440:A:ALA:N	1:440:A:ALA:CA	1:440:A:ALA:C	2	1.12	0.03	1.12

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 (°)
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	14	4.81
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	27	4.63
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	22	4.51
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	30	4.35
(1,168)	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	1:534:A:VAL:N	25	4.19
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	18	4.19
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	26	3.92
(1,185)	1:555:A:VAL:N	1:555:A:VAL:CA	1:555:A:VAL:C	1:556:A:SER:N	17	3.81
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	4	3.77
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	9	3.7
(1,168)	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	1:534:A:VAL:N	1	3.68
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	8	3.64
(1,168)	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	1:534:A:VAL:N	28	3.57
(1,168)	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	1:534:A:VAL:N	14	3.54

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,113)	1:451:A:ARG:N	1:451:A:ARG:CA	1:451:A:ARG:C	1:452:A:PHE:N	16	3.51
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	16	3.5
(1,122)	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	1:462:A:GLU:N	5	3.49
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	24	3.48
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	20	3.48
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	29	3.42
(1,100)	1:434:A:THR:N	1:434:A:THR:CA	1:434:A:THR:C	1:435:A:LEU:N	7	3.41
(1,100)	1:434:A:THR:N	1:434:A:THR:CA	1:434:A:THR:C	1:435:A:LEU:N	3	3.39
(1,73)	1:525:A:VAL:C	1:526:A:ASP:N	1:526:A:ASP:CA	1:526:A:ASP:C	9	3.36
(1,168)	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	1:534:A:VAL:N	27	3.34
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	11	3.34
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	28	3.32
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	7	3.31
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	24	3.31
(1,168)	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	1:534:A:VAL:N	15	3.3
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	23	3.29
(1,29)	1:460:A:THR:C	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	9	3.2
(1,185)	1:555:A:VAL:N	1:555:A:VAL:CA	1:555:A:VAL:C	1:556:A:SER:N	30	3.16
(1,97)	1:428:A:GLU:N	1:428:A:GLU:CA	1:428:A:GLU:C	1:429:A:ILE:N	30	3.16
(1,168)	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	1:534:A:VAL:N	29	3.08
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	23	3.08
(1,72)	1:524:A:SER:C	1:525:A:VAL:N	1:525:A:VAL:CA	1:525:A:VAL:C	10	3.03
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	17	3.01
(1,69)	1:521:A:SER:C	1:522:A:GLN:N	1:522:A:GLN:CA	1:522:A:GLN:C	8	3.01
(1,148)	1:504:A:THR:N	1:504:A:THR:CA	1:504:A:THR:C	1:505:A:VAL:N	7	2.99
(1,168)	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	1:534:A:VAL:N	24	2.98
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	25	2.97
(1,100)	1:434:A:THR:N	1:434:A:THR:CA	1:434:A:THR:C	1:435:A:LEU:N	14	2.96
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	6	2.91
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	1	2.88
(1,168)	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	1:534:A:VAL:N	4	2.86
(1,168)	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	1:534:A:VAL:N	12	2.85
(1,76)	1:533:A:GLU:C	1:534:A:VAL:N	1:534:A:VAL:CA	1:534:A:VAL:C	27	2.85
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	5	2.82
(1,76)	1:533:A:GLU:C	1:534:A:VAL:N	1:534:A:VAL:CA	1:534:A:VAL:C	1	2.82
(1,76)	1:533:A:GLU:C	1:534:A:VAL:N	1:534:A:VAL:CA	1:534:A:VAL:C	21	2.82
(1,176)	1:545:A:VAL:N	1:545:A:VAL:CA	1:545:A:VAL:C	1:546:A:PRO:N	28	2.79
(1,148)	1:504:A:THR:N	1:504:A:THR:CA	1:504:A:THR:C	1:505:A:VAL:N	23	2.78
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	30	2.77
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	3	2.74
(1,148)	1:504:A:THR:N	1:504:A:THR:CA	1:504:A:THR:C	1:505:A:VAL:N	6	2.72
(1,100)	1:434:A:THR:N	1:434:A:THR:CA	1:434:A:THR:C	1:435:A:LEU:N	4	2.71
(1,113)	1:451:A:ARG:N	1:451:A:ARG:CA	1:451:A:ARG:C	1:452:A:PHE:N	6	2.69
(1,73)	1:525:A:VAL:C	1:526:A:ASP:N	1:526:A:ASP:CA	1:526:A:ASP:C	4	2.68
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	22	2.67
(1,100)	1:434:A:THR:N	1:434:A:THR:CA	1:434:A:THR:C	1:435:A:LEU:N	17	2.66
(1,148)	1:504:A:THR:N	1:504:A:THR:CA	1:504:A:THR:C	1:505:A:VAL:N	30	2.65
(1,100)	1:434:A:THR:N	1:434:A:THR:CA	1:434:A:THR:C	1:435:A:LEU:N	20	2.63
(1,69)	1:521:A:SER:C	1:522:A:GLN:N	1:522:A:GLN:CA	1:522:A:GLN:C	17	2.63
(1,148)	1:504:A:THR:N	1:504:A:THR:CA	1:504:A:THR:C	1:505:A:VAL:N	3	2.59
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	13	2.59

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,150)	1:506:A:ASP:N	1:506:A:ASP:CA	1:506:A:ASP:C	1:507:A:VAL:N	30	2.58
(1,30)	1:461:A:PRO:C	1:462:A:GLU:N	1:462:A:GLU:CA	1:462:A:GLU:C	10	2.58
(1,73)	1:525:A:VAL:C	1:526:A:ASP:N	1:526:A:ASP:CA	1:526:A:ASP:C	19	2.57
(1,148)	1:504:A:THR:N	1:504:A:THR:CA	1:504:A:THR:C	1:505:A:VAL:N	11	2.56
(1,178)	1:547:A:VAL:N	1:547:A:VAL:CA	1:547:A:VAL:C	1:548:A:ASP:N	14	2.55
(1,57)	1:505:A:VAL:C	1:506:A:ASP:N	1:506:A:ASP:CA	1:506:A:ASP:C	28	2.55
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	15	2.54
(1,148)	1:504:A:THR:N	1:504:A:THR:CA	1:504:A:THR:C	1:505:A:VAL:N	8	2.53
(1,76)	1:533:A:GLU:C	1:534:A:VAL:N	1:534:A:VAL:CA	1:534:A:VAL:C	4	2.51
(1,100)	1:434:A:THR:N	1:434:A:THR:CA	1:434:A:THR:C	1:435:A:LEU:N	19	2.5
(1,168)	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	1:534:A:VAL:N	21	2.49
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	7	2.49
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	21	2.49
(1,97)	1:428:A:GLU:N	1:428:A:GLU:CA	1:428:A:GLU:C	1:429:A:ILE:N	28	2.49
(1,168)	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	1:534:A:VAL:N	8	2.48
(1,5)	1:428:A:GLU:C	1:429:A:ILE:N	1:429:A:ILE:CA	1:429:A:ILE:C	30	2.47
(1,178)	1:547:A:VAL:N	1:547:A:VAL:CA	1:547:A:VAL:C	1:548:A:ASP:N	4	2.46
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	19	2.45
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	10	2.44
(1,69)	1:521:A:SER:C	1:522:A:GLN:N	1:522:A:GLN:CA	1:522:A:GLN:C	24	2.44
(1,185)	1:555:A:VAL:N	1:555:A:VAL:CA	1:555:A:VAL:C	1:556:A:SER:N	9	2.43
(1,183)	1:553:A:LEU:N	1:553:A:LEU:CA	1:553:A:LEU:C	1:554:A:GLN:N	23	2.43
(1,100)	1:434:A:THR:N	1:434:A:THR:CA	1:434:A:THR:C	1:435:A:LEU:N	23	2.43
(1,89)	1:551:A:ILE:C	1:552:A:GLU:N	1:552:A:GLU:CA	1:552:A:GLU:C	26	2.41
(1,100)	1:434:A:THR:N	1:434:A:THR:CA	1:434:A:THR:C	1:435:A:LEU:N	1	2.4
(1,15)	1:442:A:LYS:C	1:443:A:LYS:N	1:443:A:LYS:CA	1:443:A:LYS:C	8	2.4
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	26	2.39
(1,39)	1:474:A:ALA:C	1:475:A:ASN:N	1:475:A:ASN:CA	1:475:A:ASN:C	5	2.37
(1,148)	1:504:A:THR:N	1:504:A:THR:CA	1:504:A:THR:C	1:505:A:VAL:N	22	2.36
(1,74)	1:529:A:ARG:C	1:530:A:PRO:N	1:530:A:PRO:CA	1:530:A:PRO:C	19	2.36
(1,148)	1:504:A:THR:N	1:504:A:THR:CA	1:504:A:THR:C	1:505:A:VAL:N	19	2.34
(1,100)	1:434:A:THR:N	1:434:A:THR:CA	1:434:A:THR:C	1:435:A:LEU:N	29	2.34
(1,21)	1:451:A:ARG:C	1:452:A:PHE:N	1:452:A:PHE:CA	1:452:A:PHE:C	16	2.33
(1,76)	1:533:A:GLU:C	1:534:A:VAL:N	1:534:A:VAL:CA	1:534:A:VAL:C	14	2.32
(1,64)	1:512:A:LEU:C	1:513:A:ASN:N	1:513:A:ASN:CA	1:513:A:ASN:C	8	2.32
(1,148)	1:504:A:THR:N	1:504:A:THR:CA	1:504:A:THR:C	1:505:A:VAL:N	15	2.3
(1,148)	1:504:A:THR:N	1:504:A:THR:CA	1:504:A:THR:C	1:505:A:VAL:N	25	2.3
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	14	2.3
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	6	2.3
(1,100)	1:434:A:THR:N	1:434:A:THR:CA	1:434:A:THR:C	1:435:A:LEU:N	16	2.29
(1,100)	1:434:A:THR:N	1:434:A:THR:CA	1:434:A:THR:C	1:435:A:LEU:N	26	2.29
(1,76)	1:533:A:GLU:C	1:534:A:VAL:N	1:534:A:VAL:CA	1:534:A:VAL:C	8	2.29
(1,75)	1:532:A:GLY:C	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	21	2.29
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	11	2.28
(1,89)	1:551:A:ILE:C	1:552:A:GLU:N	1:552:A:GLU:CA	1:552:A:GLU:C	27	2.28
(1,72)	1:524:A:SER:C	1:525:A:VAL:N	1:525:A:VAL:CA	1:525:A:VAL:C	24	2.28
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	2	2.27
(1,89)	1:551:A:ILE:C	1:552:A:GLU:N	1:552:A:GLU:CA	1:552:A:GLU:C	30	2.26
(1,100)	1:434:A:THR:N	1:434:A:THR:CA	1:434:A:THR:C	1:435:A:LEU:N	21	2.24
(1,148)	1:504:A:THR:N	1:504:A:THR:CA	1:504:A:THR:C	1:505:A:VAL:N	9	2.23
(1,93)	1:555:A:VAL:C	1:556:A:SER:N	1:556:A:SER:CA	1:556:A:SER:C	17	2.22

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	27	2.21
(1,100)	1:434:A:THR:N	1:434:A:THR:CA	1:434:A:THR:C	1:435:A:LEU:N	9	2.21
(1,73)	1:525:A:VAL:C	1:526:A:ASP:N	1:526:A:ASP:CA	1:526:A:ASP:C	18	2.2
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	17	2.18
(1,100)	1:434:A:THR:N	1:434:A:THR:CA	1:434:A:THR:C	1:435:A:LEU:N	15	2.18
(1,89)	1:551:A:ILE:C	1:552:A:GLU:N	1:552:A:GLU:CA	1:552:A:GLU:C	21	2.18
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	8	2.17
(1,15)	1:442:A:LYS:C	1:443:A:LYS:N	1:443:A:LYS:CA	1:443:A:LYS:C	7	2.17
(1,148)	1:504:A:THR:N	1:504:A:THR:CA	1:504:A:THR:C	1:505:A:VAL:N	28	2.16
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	3	2.16
(1,97)	1:428:A:GLU:N	1:428:A:GLU:CA	1:428:A:GLU:C	1:429:A:ILE:N	20	2.16
(1,57)	1:505:A:VAL:C	1:506:A:ASP:N	1:506:A:ASP:CA	1:506:A:ASP:C	17	2.16
(1,45)	1:484:A:VAL:C	1:485:A:ILE:N	1:485:A:ILE:CA	1:485:A:ILE:C	10	2.16
(1,15)	1:442:A:LYS:C	1:443:A:LYS:N	1:443:A:LYS:CA	1:443:A:LYS:C	13	2.16
(1,76)	1:533:A:GLU:C	1:534:A:VAL:N	1:534:A:VAL:CA	1:534:A:VAL:C	12	2.15
(1,15)	1:442:A:LYS:C	1:443:A:LYS:N	1:443:A:LYS:CA	1:443:A:LYS:C	30	2.15
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	16	2.14
(1,107)	1:442:A:LYS:N	1:442:A:LYS:CA	1:442:A:LYS:C	1:443:A:LYS:N	7	2.14
(1,29)	1:460:A:THR:C	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	15	2.14
(1,148)	1:504:A:THR:N	1:504:A:THR:CA	1:504:A:THR:C	1:505:A:VAL:N	17	2.13
(1,69)	1:521:A:SER:C	1:522:A:GLN:N	1:522:A:GLN:CA	1:522:A:GLN:C	25	2.13
(1,122)	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	1:462:A:GLU:N	9	2.12
(1,73)	1:525:A:VAL:C	1:526:A:ASP:N	1:526:A:ASP:CA	1:526:A:ASP:C	26	2.12
(1,57)	1:505:A:VAL:C	1:506:A:ASP:N	1:506:A:ASP:CA	1:506:A:ASP:C	8	2.12
(1,168)	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	1:534:A:VAL:N	11	2.11
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	19	2.11
(1,120)	1:458:A:PRO:N	1:458:A:PRO:CA	1:458:A:PRO:C	1:459:A:SER:N	5	2.11
(1,85)	1:546:A:PRO:C	1:547:A:VAL:N	1:547:A:VAL:CA	1:547:A:VAL:C	7	2.1
(1,15)	1:442:A:LYS:C	1:443:A:LYS:N	1:443:A:LYS:CA	1:443:A:LYS:C	21	2.1
(1,168)	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	1:534:A:VAL:N	30	2.08
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	12	2.08
(1,96)	1:427:A:ARG:N	1:427:A:ARG:CA	1:427:A:ARG:C	1:428:A:GLU:N	6	2.08
(1,113)	1:451:A:ARG:N	1:451:A:ARG:CA	1:451:A:ARG:C	1:452:A:PHE:N	15	2.07
(1,99)	1:430:A:PRO:N	1:430:A:PRO:CA	1:430:A:PRO:C	1:431:A:ASP:N	26	2.07
(1,150)	1:506:A:ASP:N	1:506:A:ASP:CA	1:506:A:ASP:C	1:507:A:VAL:N	9	2.06
(1,168)	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	1:534:A:VAL:N	7	2.05
(1,148)	1:504:A:THR:N	1:504:A:THR:CA	1:504:A:THR:C	1:505:A:VAL:N	27	2.05
(1,36)	1:467:A:VAL:C	1:468:A:ILE:N	1:468:A:ILE:CA	1:468:A:ILE:C	15	2.04
(1,97)	1:428:A:GLU:N	1:428:A:GLU:CA	1:428:A:GLU:C	1:429:A:ILE:N	22	2.02
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	20	1.99
(1,100)	1:434:A:THR:N	1:434:A:THR:CA	1:434:A:THR:C	1:435:A:LEU:N	24	1.99
(1,97)	1:428:A:GLU:N	1:428:A:GLU:CA	1:428:A:GLU:C	1:429:A:ILE:N	10	1.99
(1,167)	1:530:A:PRO:N	1:530:A:PRO:CA	1:530:A:PRO:C	1:531:A:ALA:N	13	1.98
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	29	1.98
(1,125)	1:464:A:VAL:N	1:464:A:VAL:CA	1:464:A:VAL:C	1:465:A:GLY:N	11	1.98
(1,72)	1:524:A:SER:C	1:525:A:VAL:N	1:525:A:VAL:CA	1:525:A:VAL:C	2	1.98
(1,139)	1:486:A:ILE:N	1:486:A:ILE:CA	1:486:A:ILE:C	1:487:A:ILE:N	8	1.97
(1,122)	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	1:462:A:GLU:N	6	1.97
(1,125)	1:464:A:VAL:N	1:464:A:VAL:CA	1:464:A:VAL:C	1:465:A:GLY:N	19	1.96
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	21	1.96
(1,185)	1:555:A:VAL:N	1:555:A:VAL:CA	1:555:A:VAL:C	1:556:A:SER:N	25	1.95

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,76)	1:533:A:GLU:C	1:534:A:VAL:N	1:534:A:VAL:CA	1:534:A:VAL:C	13	1.95
(1,100)	1:434:A:THR:N	1:434:A:THR:CA	1:434:A:THR:C	1:435:A:LEU:N	25	1.94
(1,73)	1:525:A:VAL:C	1:526:A:ASP:N	1:526:A:ASP:CA	1:526:A:ASP:C	1	1.94
(1,57)	1:505:A:VAL:C	1:506:A:ASP:N	1:506:A:ASP:CA	1:506:A:ASP:C	6	1.94
(1,122)	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	1:462:A:GLU:N	8	1.93
(1,97)	1:428:A:GLU:N	1:428:A:GLU:CA	1:428:A:GLU:C	1:429:A:ILE:N	15	1.92
(1,178)	1:547:A:VAL:N	1:547:A:VAL:CA	1:547:A:VAL:C	1:548:A:ASP:N	27	1.91
(1,107)	1:442:A:LYS:N	1:442:A:LYS:CA	1:442:A:LYS:C	1:443:A:LYS:N	21	1.9
(1,29)	1:460:A:THR:C	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	14	1.9
(1,97)	1:428:A:GLU:N	1:428:A:GLU:CA	1:428:A:GLU:C	1:429:A:ILE:N	8	1.89
(1,69)	1:521:A:SER:C	1:522:A:GLN:N	1:522:A:GLN:CA	1:522:A:GLN:C	28	1.89
(1,150)	1:506:A:ASP:N	1:506:A:ASP:CA	1:506:A:ASP:C	1:507:A:VAL:N	2	1.88
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	9	1.88
(1,122)	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	1:462:A:GLU:N	12	1.87
(1,121)	1:459:A:SER:N	1:459:A:SER:CA	1:459:A:SER:C	1:460:A:THR:N	2	1.87
(1,85)	1:546:A:PRO:C	1:547:A:VAL:N	1:547:A:VAL:CA	1:547:A:VAL:C	23	1.87
(1,76)	1:533:A:GLU:C	1:534:A:VAL:N	1:534:A:VAL:CA	1:534:A:VAL:C	28	1.87
(1,72)	1:524:A:SER:C	1:525:A:VAL:N	1:525:A:VAL:CA	1:525:A:VAL:C	29	1.87
(1,178)	1:547:A:VAL:N	1:547:A:VAL:CA	1:547:A:VAL:C	1:548:A:ASP:N	11	1.86
(1,72)	1:524:A:SER:C	1:525:A:VAL:N	1:525:A:VAL:CA	1:525:A:VAL:C	11	1.86
(1,35)	1:466:A:LYS:C	1:467:A:VAL:N	1:467:A:VAL:CA	1:467:A:VAL:C	30	1.86
(1,21)	1:451:A:ARG:C	1:452:A:PHE:N	1:452:A:PHE:CA	1:452:A:PHE:C	28	1.86
(1,177)	1:546:A:PRO:N	1:546:A:PRO:CA	1:546:A:PRO:C	1:547:A:VAL:N	23	1.85
(1,168)	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	1:534:A:VAL:N	13	1.85
(1,148)	1:504:A:THR:N	1:504:A:THR:CA	1:504:A:THR:C	1:505:A:VAL:N	26	1.85
(1,72)	1:524:A:SER:C	1:525:A:VAL:N	1:525:A:VAL:CA	1:525:A:VAL:C	21	1.85
(1,165)	1:525:A:VAL:N	1:525:A:VAL:CA	1:525:A:VAL:C	1:526:A:ASP:N	29	1.84
(1,72)	1:524:A:SER:C	1:525:A:VAL:N	1:525:A:VAL:CA	1:525:A:VAL:C	27	1.84
(1,113)	1:451:A:ARG:N	1:451:A:ARG:CA	1:451:A:ARG:C	1:452:A:PHE:N	10	1.83
(1,112)	1:447:A:ALA:N	1:447:A:ALA:CA	1:447:A:ALA:C	1:448:A:GLY:N	5	1.83
(1,107)	1:442:A:LYS:N	1:442:A:LYS:CA	1:442:A:LYS:C	1:443:A:LYS:N	18	1.83
(1,89)	1:551:A:ILE:C	1:552:A:GLU:N	1:552:A:GLU:CA	1:552:A:GLU:C	9	1.83
(1,73)	1:525:A:VAL:C	1:526:A:ASP:N	1:526:A:ASP:CA	1:526:A:ASP:C	29	1.83
(1,72)	1:524:A:SER:C	1:525:A:VAL:N	1:525:A:VAL:CA	1:525:A:VAL:C	26	1.83
(1,15)	1:442:A:LYS:C	1:443:A:LYS:N	1:443:A:LYS:CA	1:443:A:LYS:C	16	1.83
(1,178)	1:547:A:VAL:N	1:547:A:VAL:CA	1:547:A:VAL:C	1:548:A:ASP:N	2	1.82
(1,121)	1:459:A:SER:N	1:459:A:SER:CA	1:459:A:SER:C	1:460:A:THR:N	29	1.82
(1,185)	1:555:A:VAL:N	1:555:A:VAL:CA	1:555:A:VAL:C	1:556:A:SER:N	16	1.81
(1,77)	1:536:A:GLY:C	1:537:A:THR:N	1:537:A:THR:CA	1:537:A:THR:C	4	1.81
(1,150)	1:506:A:ASP:N	1:506:A:ASP:CA	1:506:A:ASP:C	1:507:A:VAL:N	23	1.79
(1,97)	1:428:A:GLU:N	1:428:A:GLU:CA	1:428:A:GLU:C	1:429:A:ILE:N	16	1.79
(1,15)	1:442:A:LYS:C	1:443:A:LYS:N	1:443:A:LYS:CA	1:443:A:LYS:C	1	1.79
(1,178)	1:547:A:VAL:N	1:547:A:VAL:CA	1:547:A:VAL:C	1:548:A:ASP:N	19	1.78
(1,175)	1:544:A:THR:N	1:544:A:THR:CA	1:544:A:THR:C	1:545:A:VAL:N	8	1.77
(1,125)	1:464:A:VAL:N	1:464:A:VAL:CA	1:464:A:VAL:C	1:465:A:GLY:N	18	1.77
(1,113)	1:451:A:ARG:N	1:451:A:ARG:CA	1:451:A:ARG:C	1:452:A:PHE:N	28	1.77
(1,100)	1:434:A:THR:N	1:434:A:THR:CA	1:434:A:THR:C	1:435:A:LEU:N	28	1.77
(1,29)	1:460:A:THR:C	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	24	1.77
(1,170)	1:537:A:THR:N	1:537:A:THR:CA	1:537:A:THR:C	1:538:A:ASN:N	13	1.76
(1,168)	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	1:534:A:VAL:N	5	1.76
(1,97)	1:428:A:GLU:N	1:428:A:GLU:CA	1:428:A:GLU:C	1:429:A:ILE:N	24	1.76

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,93)	1:555:A:VAL:C	1:556:A:SER:N	1:556:A:SER:CA	1:556:A:SER:C	30	1.76
(1,73)	1:525:A:VAL:C	1:526:A:ASP:N	1:526:A:ASP:CA	1:526:A:ASP:C	7	1.75
(1,64)	1:512:A:LEU:C	1:513:A:ASN:N	1:513:A:ASN:CA	1:513:A:ASN:C	13	1.75
(1,35)	1:466:A:LYS:C	1:467:A:VAL:N	1:467:A:VAL:CA	1:467:A:VAL:C	9	1.75
(1,185)	1:555:A:VAL:N	1:555:A:VAL:CA	1:555:A:VAL:C	1:556:A:SER:N	19	1.73
(1,38)	1:472:A:PRO:C	1:473:A:PRO:N	1:473:A:PRO:CA	1:473:A:PRO:C	8	1.73
(1,30)	1:461:A:PRO:C	1:462:A:GLU:N	1:462:A:GLU:CA	1:462:A:GLU:C	5	1.73
(1,185)	1:555:A:VAL:N	1:555:A:VAL:CA	1:555:A:VAL:C	1:556:A:SER:N	8	1.71
(1,148)	1:504:A:THR:N	1:504:A:THR:CA	1:504:A:THR:C	1:505:A:VAL:N	20	1.71
(1,113)	1:451:A:ARG:N	1:451:A:ARG:CA	1:451:A:ARG:C	1:452:A:PHE:N	21	1.71
(1,73)	1:525:A:VAL:C	1:526:A:ASP:N	1:526:A:ASP:CA	1:526:A:ASP:C	27	1.71
(1,66)	1:518:A:THR:C	1:519:A:LYS:N	1:519:A:LYS:CA	1:519:A:LYS:C	21	1.71
(1,183)	1:553:A:LEU:N	1:553:A:LEU:CA	1:553:A:LEU:C	1:554:A:GLN:N	15	1.7
(1,168)	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	1:534:A:VAL:N	26	1.7
(1,116)	1:454:A:GLN:N	1:454:A:GLN:CA	1:454:A:GLN:C	1:455:A:ALA:N	12	1.7
(1,72)	1:524:A:SER:C	1:525:A:VAL:N	1:525:A:VAL:CA	1:525:A:VAL:C	16	1.7
(1,113)	1:451:A:ARG:N	1:451:A:ARG:CA	1:451:A:ARG:C	1:452:A:PHE:N	19	1.69
(1,76)	1:533:A:GLU:C	1:534:A:VAL:N	1:534:A:VAL:CA	1:534:A:VAL:C	29	1.69
(1,36)	1:467:A:VAL:C	1:468:A:ILE:N	1:468:A:ILE:CA	1:468:A:ILE:C	29	1.69
(1,15)	1:442:A:LYS:C	1:443:A:LYS:N	1:443:A:LYS:CA	1:443:A:LYS:C	11	1.69
(1,15)	1:442:A:LYS:C	1:443:A:LYS:N	1:443:A:LYS:CA	1:443:A:LYS:C	20	1.69
(1,178)	1:547:A:VAL:N	1:547:A:VAL:CA	1:547:A:VAL:C	1:548:A:ASP:N	12	1.68
(1,150)	1:506:A:ASP:N	1:506:A:ASP:CA	1:506:A:ASP:C	1:507:A:VAL:N	16	1.68
(1,115)	1:453:A:LYS:N	1:453:A:LYS:CA	1:453:A:LYS:C	1:454:A:GLN:N	1	1.68
(1,15)	1:442:A:LYS:C	1:443:A:LYS:N	1:443:A:LYS:CA	1:443:A:LYS:C	10	1.68
(1,170)	1:537:A:THR:N	1:537:A:THR:CA	1:537:A:THR:C	1:538:A:ASN:N	20	1.67
(1,105)	1:440:A:ALA:N	1:440:A:ALA:CA	1:440:A:ALA:C	1:441:A:VAL:N	8	1.67
(1,93)	1:555:A:VAL:C	1:556:A:SER:N	1:556:A:SER:CA	1:556:A:SER:C	9	1.67
(1,73)	1:525:A:VAL:C	1:526:A:ASP:N	1:526:A:ASP:CA	1:526:A:ASP:C	10	1.67
(1,36)	1:467:A:VAL:C	1:468:A:ILE:N	1:468:A:ILE:CA	1:468:A:ILE:C	14	1.67
(1,125)	1:464:A:VAL:N	1:464:A:VAL:CA	1:464:A:VAL:C	1:465:A:GLY:N	27	1.66
(1,115)	1:453:A:LYS:N	1:453:A:LYS:CA	1:453:A:LYS:C	1:454:A:GLN:N	2	1.66
(1,100)	1:434:A:THR:N	1:434:A:THR:CA	1:434:A:THR:C	1:435:A:LEU:N	13	1.66
(1,148)	1:504:A:THR:N	1:504:A:THR:CA	1:504:A:THR:C	1:505:A:VAL:N	1	1.65
(1,112)	1:447:A:ALA:N	1:447:A:ALA:CA	1:447:A:ALA:C	1:448:A:GLY:N	12	1.65
(1,35)	1:466:A:LYS:C	1:467:A:VAL:N	1:467:A:VAL:CA	1:467:A:VAL:C	3	1.65
(1,35)	1:466:A:LYS:C	1:467:A:VAL:N	1:467:A:VAL:CA	1:467:A:VAL:C	20	1.65
(1,175)	1:544:A:THR:N	1:544:A:THR:CA	1:544:A:THR:C	1:545:A:VAL:N	22	1.64
(1,148)	1:504:A:THR:N	1:504:A:THR:CA	1:504:A:THR:C	1:505:A:VAL:N	4	1.64
(1,97)	1:428:A:GLU:N	1:428:A:GLU:CA	1:428:A:GLU:C	1:429:A:ILE:N	9	1.64
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	2	1.63
(1,125)	1:464:A:VAL:N	1:464:A:VAL:CA	1:464:A:VAL:C	1:465:A:GLY:N	23	1.63
(1,69)	1:521:A:SER:C	1:522:A:GLN:N	1:522:A:GLN:CA	1:522:A:GLN:C	18	1.63
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	25	1.62
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	1	1.62
(1,97)	1:428:A:GLU:N	1:428:A:GLU:CA	1:428:A:GLU:C	1:429:A:ILE:N	12	1.61
(1,73)	1:525:A:VAL:C	1:526:A:ASP:N	1:526:A:ASP:CA	1:526:A:ASP:C	11	1.61
(1,72)	1:524:A:SER:C	1:525:A:VAL:N	1:525:A:VAL:CA	1:525:A:VAL:C	25	1.61
(1,5)	1:428:A:GLU:C	1:429:A:ILE:N	1:429:A:ILE:CA	1:429:A:ILE:C	18	1.61
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	18	1.6
(1,97)	1:428:A:GLU:N	1:428:A:GLU:CA	1:428:A:GLU:C	1:429:A:ILE:N	7	1.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,57)	1:505:A:VAL:C	1:506:A:ASP:N	1:506:A:ASP:CA	1:506:A:ASP:C	7	1.6
(1,168)	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	1:534:A:VAL:N	17	1.59
(1,76)	1:533:A:GLU:C	1:534:A:VAL:N	1:534:A:VAL:CA	1:534:A:VAL:C	15	1.59
(1,27)	1:457:A:SER:C	1:458:A:PRO:N	1:458:A:PRO:CA	1:458:A:PRO:C	1	1.59
(1,22)	1:452:A:PHE:C	1:453:A:LYS:N	1:453:A:LYS:CA	1:453:A:LYS:C	15	1.59
(1,163)	1:523:A:ALA:N	1:523:A:ALA:CA	1:523:A:ALA:C	1:524:A:SER:N	30	1.58
(1,150)	1:506:A:ASP:N	1:506:A:ASP:CA	1:506:A:ASP:C	1:507:A:VAL:N	11	1.58
(1,73)	1:525:A:VAL:C	1:526:A:ASP:N	1:526:A:ASP:CA	1:526:A:ASP:C	30	1.58
(1,29)	1:460:A:THR:C	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	23	1.58
(1,29)	1:460:A:THR:C	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	26	1.58
(1,180)	1:550:A:VAL:N	1:550:A:VAL:CA	1:550:A:VAL:C	1:551:A:ILE:N	28	1.57
(1,89)	1:551:A:ILE:C	1:552:A:GLU:N	1:552:A:GLU:CA	1:552:A:GLU:C	10	1.57
(1,35)	1:466:A:LYS:C	1:467:A:VAL:N	1:467:A:VAL:CA	1:467:A:VAL:C	14	1.57
(1,35)	1:466:A:LYS:C	1:467:A:VAL:N	1:467:A:VAL:CA	1:467:A:VAL:C	17	1.57
(1,72)	1:524:A:SER:C	1:525:A:VAL:N	1:525:A:VAL:CA	1:525:A:VAL:C	4	1.56
(1,97)	1:428:A:GLU:N	1:428:A:GLU:CA	1:428:A:GLU:C	1:429:A:ILE:N	19	1.55
(1,97)	1:428:A:GLU:N	1:428:A:GLU:CA	1:428:A:GLU:C	1:429:A:ILE:N	29	1.55
(1,89)	1:551:A:ILE:C	1:552:A:GLU:N	1:552:A:GLU:CA	1:552:A:GLU:C	13	1.55
(1,29)	1:460:A:THR:C	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	5	1.55
(1,15)	1:442:A:LYS:C	1:443:A:LYS:N	1:443:A:LYS:CA	1:443:A:LYS:C	18	1.55
(1,140)	1:487:A:ILE:N	1:487:A:ILE:CA	1:487:A:ILE:C	1:488:A:VAL:N	20	1.54
(1,74)	1:529:A:ARG:C	1:530:A:PRO:N	1:530:A:PRO:CA	1:530:A:PRO:C	26	1.54
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	4	1.53
(1,97)	1:428:A:GLU:N	1:428:A:GLU:CA	1:428:A:GLU:C	1:429:A:ILE:N	3	1.53
(1,175)	1:544:A:THR:N	1:544:A:THR:CA	1:544:A:THR:C	1:545:A:VAL:N	4	1.52
(1,127)	1:466:A:LYS:N	1:466:A:LYS:CA	1:466:A:LYS:C	1:467:A:VAL:N	30	1.51
(1,113)	1:451:A:ARG:N	1:451:A:ARG:CA	1:451:A:ARG:C	1:452:A:PHE:N	22	1.51
(1,36)	1:467:A:VAL:C	1:468:A:ILE:N	1:468:A:ILE:CA	1:468:A:ILE:C	16	1.51
(1,32)	1:463:A:LEU:C	1:464:A:VAL:N	1:464:A:VAL:CA	1:464:A:VAL:C	9	1.51
(1,5)	1:428:A:GLU:C	1:429:A:ILE:N	1:429:A:ILE:CA	1:429:A:ILE:C	21	1.51
(1,170)	1:537:A:THR:N	1:537:A:THR:CA	1:537:A:THR:C	1:538:A:ASN:N	29	1.5
(1,125)	1:464:A:VAL:N	1:464:A:VAL:CA	1:464:A:VAL:C	1:465:A:GLY:N	3	1.5
(1,97)	1:428:A:GLU:N	1:428:A:GLU:CA	1:428:A:GLU:C	1:429:A:ILE:N	13	1.5
(1,32)	1:463:A:LEU:C	1:464:A:VAL:N	1:464:A:VAL:CA	1:464:A:VAL:C	11	1.5
(1,148)	1:504:A:THR:N	1:504:A:THR:CA	1:504:A:THR:C	1:505:A:VAL:N	29	1.49
(1,122)	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	1:462:A:GLU:N	29	1.49
(1,121)	1:459:A:SER:N	1:459:A:SER:CA	1:459:A:SER:C	1:460:A:THR:N	1	1.49
(1,100)	1:434:A:THR:N	1:434:A:THR:CA	1:434:A:THR:C	1:435:A:LEU:N	5	1.49
(1,22)	1:452:A:PHE:C	1:453:A:LYS:N	1:453:A:LYS:CA	1:453:A:LYS:C	18	1.49
(1,97)	1:428:A:GLU:N	1:428:A:GLU:CA	1:428:A:GLU:C	1:429:A:ILE:N	26	1.48
(1,124)	1:463:A:LEU:N	1:463:A:LEU:CA	1:463:A:LEU:C	1:464:A:VAL:N	30	1.47
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	5	1.47
(1,97)	1:428:A:GLU:N	1:428:A:GLU:CA	1:428:A:GLU:C	1:429:A:ILE:N	27	1.47
(1,72)	1:524:A:SER:C	1:525:A:VAL:N	1:525:A:VAL:CA	1:525:A:VAL:C	8	1.47
(1,70)	1:522:A:GLN:C	1:523:A:ALA:N	1:523:A:ALA:CA	1:523:A:ALA:C	11	1.47
(1,121)	1:459:A:SER:N	1:459:A:SER:CA	1:459:A:SER:C	1:460:A:THR:N	21	1.46
(1,98)	1:429:A:ILE:N	1:429:A:ILE:CA	1:429:A:ILE:C	1:430:A:PRO:N	12	1.46
(1,94)	1:424:A:PRO:N	1:424:A:PRO:CA	1:424:A:PRO:C	1:425:A:GLU:N	1	1.46
(1,72)	1:524:A:SER:C	1:525:A:VAL:N	1:525:A:VAL:CA	1:525:A:VAL:C	12	1.46
(1,177)	1:546:A:PRO:N	1:546:A:PRO:CA	1:546:A:PRO:C	1:547:A:VAL:N	7	1.45
(1,174)	1:543:A:THR:N	1:543:A:THR:CA	1:543:A:THR:C	1:544:A:THR:N	21	1.45

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,73)	1:525:A:VAL:C	1:526:A:ASP:N	1:526:A:ASP:CA	1:526:A:ASP:C	21	1.45
(1,30)	1:461:A:PRO:C	1:462:A:GLU:N	1:462:A:GLU:CA	1:462:A:GLU:C	21	1.45
(1,153)	1:509:A:GLN:N	1:509:A:GLN:CA	1:509:A:GLN:C	1:510:A:LYS:N	9	1.44
(1,148)	1:504:A:THR:N	1:504:A:THR:CA	1:504:A:THR:C	1:505:A:VAL:N	14	1.44
(1,147)	1:497:A:ILE:N	1:497:A:ILE:CA	1:497:A:ILE:C	1:498:A:PRO:N	6	1.44
(1,100)	1:434:A:THR:N	1:434:A:THR:CA	1:434:A:THR:C	1:435:A:LEU:N	27	1.44
(1,149)	1:505:A:VAL:N	1:505:A:VAL:CA	1:505:A:VAL:C	1:506:A:ASP:N	23	1.43
(1,76)	1:533:A:GLU:C	1:534:A:VAL:N	1:534:A:VAL:CA	1:534:A:VAL:C	7	1.43
(1,69)	1:521:A:SER:C	1:522:A:GLN:N	1:522:A:GLN:CA	1:522:A:GLN:C	3	1.43
(1,153)	1:509:A:GLN:N	1:509:A:GLN:CA	1:509:A:GLN:C	1:510:A:LYS:N	26	1.42
(1,122)	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	1:462:A:GLU:N	27	1.42
(1,29)	1:460:A:THR:C	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	11	1.42
(1,29)	1:460:A:THR:C	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	25	1.42
(1,21)	1:451:A:ARG:C	1:452:A:PHE:N	1:452:A:PHE:CA	1:452:A:PHE:C	15	1.42
(1,178)	1:547:A:VAL:N	1:547:A:VAL:CA	1:547:A:VAL:C	1:548:A:ASP:N	8	1.41
(1,178)	1:547:A:VAL:N	1:547:A:VAL:CA	1:547:A:VAL:C	1:548:A:ASP:N	9	1.4
(1,175)	1:544:A:THR:N	1:544:A:THR:CA	1:544:A:THR:C	1:545:A:VAL:N	10	1.4
(1,150)	1:506:A:ASP:N	1:506:A:ASP:CA	1:506:A:ASP:C	1:507:A:VAL:N	12	1.4
(1,113)	1:451:A:ARG:N	1:451:A:ARG:CA	1:451:A:ARG:C	1:452:A:PHE:N	20	1.4
(1,108)	1:443:A:LYS:N	1:443:A:LYS:CA	1:443:A:LYS:C	1:444:A:LEU:N	3	1.4
(1,99)	1:430:A:PRO:N	1:430:A:PRO:CA	1:430:A:PRO:C	1:431:A:ASP:N	21	1.4
(1,72)	1:524:A:SER:C	1:525:A:VAL:N	1:525:A:VAL:CA	1:525:A:VAL:C	9	1.4
(1,168)	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	1:534:A:VAL:N	19	1.39
(1,97)	1:428:A:GLU:N	1:428:A:GLU:CA	1:428:A:GLU:C	1:429:A:ILE:N	2	1.39
(1,97)	1:428:A:GLU:N	1:428:A:GLU:CA	1:428:A:GLU:C	1:429:A:ILE:N	14	1.39
(1,72)	1:524:A:SER:C	1:525:A:VAL:N	1:525:A:VAL:CA	1:525:A:VAL:C	1	1.39
(1,35)	1:466:A:LYS:C	1:467:A:VAL:N	1:467:A:VAL:CA	1:467:A:VAL:C	26	1.39
(1,29)	1:460:A:THR:C	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	8	1.39
(1,100)	1:434:A:THR:N	1:434:A:THR:CA	1:434:A:THR:C	1:435:A:LEU:N	12	1.38
(1,89)	1:551:A:ILE:C	1:552:A:GLU:N	1:552:A:GLU:CA	1:552:A:GLU:C	16	1.38
(1,72)	1:524:A:SER:C	1:525:A:VAL:N	1:525:A:VAL:CA	1:525:A:VAL:C	23	1.38
(1,6)	1:429:A:ILE:C	1:430:A:PRO:N	1:430:A:PRO:CA	1:430:A:PRO:C	17	1.38
(1,120)	1:458:A:PRO:N	1:458:A:PRO:CA	1:458:A:PRO:C	1:459:A:SER:N	4	1.37
(1,44)	1:483:A:VAL:C	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	10	1.37
(1,35)	1:466:A:LYS:C	1:467:A:VAL:N	1:467:A:VAL:CA	1:467:A:VAL:C	29	1.37
(1,32)	1:463:A:LEU:C	1:464:A:VAL:N	1:464:A:VAL:CA	1:464:A:VAL:C	23	1.37
(1,156)	1:512:A:LEU:N	1:512:A:LEU:CA	1:512:A:LEU:C	1:513:A:ASN:N	8	1.36
(1,153)	1:509:A:GLN:N	1:509:A:GLN:CA	1:509:A:GLN:C	1:510:A:LYS:N	6	1.36
(1,150)	1:506:A:ASP:N	1:506:A:ASP:CA	1:506:A:ASP:C	1:507:A:VAL:N	27	1.36
(1,113)	1:451:A:ARG:N	1:451:A:ARG:CA	1:451:A:ARG:C	1:452:A:PHE:N	8	1.36
(1,89)	1:551:A:ILE:C	1:552:A:GLU:N	1:552:A:GLU:CA	1:552:A:GLU:C	22	1.36
(1,85)	1:546:A:PRO:C	1:547:A:VAL:N	1:547:A:VAL:CA	1:547:A:VAL:C	22	1.36
(1,29)	1:460:A:THR:C	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	7	1.36
(1,113)	1:451:A:ARG:N	1:451:A:ARG:CA	1:451:A:ARG:C	1:452:A:PHE:N	4	1.35
(1,32)	1:463:A:LEU:C	1:464:A:VAL:N	1:464:A:VAL:CA	1:464:A:VAL:C	18	1.35
(1,175)	1:544:A:THR:N	1:544:A:THR:CA	1:544:A:THR:C	1:545:A:VAL:N	19	1.34
(1,168)	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	1:534:A:VAL:N	18	1.34
(1,142)	1:490:A:SER:N	1:490:A:SER:CA	1:490:A:SER:C	1:491:A:GLY:N	25	1.34
(1,57)	1:505:A:VAL:C	1:506:A:ASP:N	1:506:A:ASP:CA	1:506:A:ASP:C	5	1.34
(1,57)	1:505:A:VAL:C	1:506:A:ASP:N	1:506:A:ASP:CA	1:506:A:ASP:C	26	1.34
(1,29)	1:460:A:THR:C	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	10	1.34

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,170)	1:537:A:THR:N	1:537:A:THR:CA	1:537:A:THR:C	1:538:A:ASN:N	28	1.33
(1,100)	1:434:A:THR:N	1:434:A:THR:CA	1:434:A:THR:C	1:435:A:LEU:N	30	1.33
(1,75)	1:532:A:GLY:C	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	28	1.33
(1,35)	1:466:A:LYS:C	1:467:A:VAL:N	1:467:A:VAL:CA	1:467:A:VAL:C	16	1.33
(1,2)	1:425:A:GLU:C	1:426:A:GLN:N	1:426:A:GLN:CA	1:426:A:GLN:C	22	1.33
(1,175)	1:544:A:THR:N	1:544:A:THR:CA	1:544:A:THR:C	1:545:A:VAL:N	24	1.32
(1,125)	1:464:A:VAL:N	1:464:A:VAL:CA	1:464:A:VAL:C	1:465:A:GLY:N	24	1.32
(1,113)	1:451:A:ARG:N	1:451:A:ARG:CA	1:451:A:ARG:C	1:452:A:PHE:N	24	1.32
(1,64)	1:512:A:LEU:C	1:513:A:ASN:N	1:513:A:ASN:CA	1:513:A:ASN:C	17	1.32
(1,27)	1:457:A:SER:C	1:458:A:PRO:N	1:458:A:PRO:CA	1:458:A:PRO:C	7	1.32
(1,183)	1:553:A:LEU:N	1:553:A:LEU:CA	1:553:A:LEU:C	1:554:A:GLN:N	21	1.31
(1,133)	1:478:A:SER:N	1:478:A:SER:CA	1:478:A:SER:C	1:479:A:ALA:N	23	1.31
(1,125)	1:464:A:VAL:N	1:464:A:VAL:CA	1:464:A:VAL:C	1:465:A:GLY:N	13	1.31
(1,107)	1:442:A:LYS:N	1:442:A:LYS:CA	1:442:A:LYS:C	1:443:A:LYS:N	30	1.31
(1,73)	1:525:A:VAL:C	1:526:A:ASP:N	1:526:A:ASP:CA	1:526:A:ASP:C	8	1.31
(1,113)	1:451:A:ARG:N	1:451:A:ARG:CA	1:451:A:ARG:C	1:452:A:PHE:N	13	1.3
(1,81)	1:542:A:GLY:C	1:543:A:THR:N	1:543:A:THR:CA	1:543:A:THR:C	26	1.3
(1,21)	1:451:A:ARG:C	1:452:A:PHE:N	1:452:A:PHE:CA	1:452:A:PHE:C	6	1.3
(1,16)	1:443:A:LYS:C	1:444:A:LEU:N	1:444:A:LEU:CA	1:444:A:LEU:C	20	1.3
(1,185)	1:555:A:VAL:N	1:555:A:VAL:CA	1:555:A:VAL:C	1:556:A:SER:N	7	1.29
(1,170)	1:537:A:THR:N	1:537:A:THR:CA	1:537:A:THR:C	1:538:A:ASN:N	3	1.29
(1,167)	1:530:A:PRO:N	1:530:A:PRO:CA	1:530:A:PRO:C	1:531:A:ALA:N	18	1.29
(1,76)	1:533:A:GLU:C	1:534:A:VAL:N	1:534:A:VAL:CA	1:534:A:VAL:C	25	1.29
(1,32)	1:463:A:LEU:C	1:464:A:VAL:N	1:464:A:VAL:CA	1:464:A:VAL:C	12	1.29
(1,150)	1:506:A:ASP:N	1:506:A:ASP:CA	1:506:A:ASP:C	1:507:A:VAL:N	1	1.28
(1,121)	1:459:A:SER:N	1:459:A:SER:CA	1:459:A:SER:C	1:460:A:THR:N	10	1.28
(1,121)	1:459:A:SER:N	1:459:A:SER:CA	1:459:A:SER:C	1:460:A:THR:N	16	1.28
(1,113)	1:451:A:ARG:N	1:451:A:ARG:CA	1:451:A:ARG:C	1:452:A:PHE:N	5	1.28
(1,48)	1:487:A:ILE:C	1:488:A:VAL:N	1:488:A:VAL:CA	1:488:A:VAL:C	4	1.28
(1,36)	1:467:A:VAL:C	1:468:A:ILE:N	1:468:A:ILE:CA	1:468:A:ILE:C	3	1.28
(1,32)	1:463:A:LEU:C	1:464:A:VAL:N	1:464:A:VAL:CA	1:464:A:VAL:C	19	1.28
(1,27)	1:457:A:SER:C	1:458:A:PRO:N	1:458:A:PRO:CA	1:458:A:PRO:C	13	1.28
(1,21)	1:451:A:ARG:C	1:452:A:PHE:N	1:452:A:PHE:CA	1:452:A:PHE:C	10	1.28
(1,15)	1:442:A:LYS:C	1:443:A:LYS:N	1:443:A:LYS:CA	1:443:A:LYS:C	28	1.28
(1,161)	1:521:A:SER:N	1:521:A:SER:CA	1:521:A:SER:C	1:522:A:GLN:N	15	1.27
(1,113)	1:451:A:ARG:N	1:451:A:ARG:CA	1:451:A:ARG:C	1:452:A:PHE:N	29	1.27
(1,97)	1:428:A:GLU:N	1:428:A:GLU:CA	1:428:A:GLU:C	1:429:A:ILE:N	23	1.27
(1,76)	1:533:A:GLU:C	1:534:A:VAL:N	1:534:A:VAL:CA	1:534:A:VAL:C	26	1.27
(1,75)	1:532:A:GLY:C	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	15	1.27
(1,64)	1:512:A:LEU:C	1:513:A:ASN:N	1:513:A:ASN:CA	1:513:A:ASN:C	21	1.27
(1,4)	1:427:A:ARG:C	1:428:A:GLU:N	1:428:A:GLU:CA	1:428:A:GLU:C	5	1.27
(1,168)	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	1:534:A:VAL:N	16	1.26
(1,100)	1:434:A:THR:N	1:434:A:THR:CA	1:434:A:THR:C	1:435:A:LEU:N	8	1.26
(1,89)	1:551:A:ILE:C	1:552:A:GLU:N	1:552:A:GLU:CA	1:552:A:GLU:C	3	1.26
(1,59)	1:507:A:VAL:C	1:508:A:ALA:N	1:508:A:ALA:CA	1:508:A:ALA:C	27	1.26
(1,36)	1:467:A:VAL:C	1:468:A:ILE:N	1:468:A:ILE:CA	1:468:A:ILE:C	7	1.26
(1,35)	1:466:A:LYS:C	1:467:A:VAL:N	1:467:A:VAL:CA	1:467:A:VAL:C	15	1.26
(1,178)	1:547:A:VAL:N	1:547:A:VAL:CA	1:547:A:VAL:C	1:548:A:ASP:N	1	1.25
(1,175)	1:544:A:THR:N	1:544:A:THR:CA	1:544:A:THR:C	1:545:A:VAL:N	14	1.25
(1,148)	1:504:A:THR:N	1:504:A:THR:CA	1:504:A:THR:C	1:505:A:VAL:N	24	1.25
(1,124)	1:463:A:LEU:N	1:463:A:LEU:CA	1:463:A:LEU:C	1:464:A:VAL:N	21	1.25

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,101)	1:435:A:LEU:N	1:435:A:LEU:CA	1:435:A:LEU:C	1:436:A:THR:N	13	1.25
(1,75)	1:532:A:GLY:C	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	27	1.25
(1,167)	1:530:A:PRO:N	1:530:A:PRO:CA	1:530:A:PRO:C	1:531:A:ALA:N	25	1.24
(1,165)	1:525:A:VAL:N	1:525:A:VAL:CA	1:525:A:VAL:C	1:526:A:ASP:N	19	1.24
(1,133)	1:478:A:SER:N	1:478:A:SER:CA	1:478:A:SER:C	1:479:A:ALA:N	27	1.24
(1,72)	1:524:A:SER:C	1:525:A:VAL:N	1:525:A:VAL:CA	1:525:A:VAL:C	13	1.24
(1,15)	1:442:A:LYS:C	1:443:A:LYS:N	1:443:A:LYS:CA	1:443:A:LYS:C	2	1.24
(1,178)	1:547:A:VAL:N	1:547:A:VAL:CA	1:547:A:VAL:C	1:548:A:ASP:N	6	1.23
(1,175)	1:544:A:THR:N	1:544:A:THR:CA	1:544:A:THR:C	1:545:A:VAL:N	2	1.23
(1,75)	1:532:A:GLY:C	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	14	1.23
(1,70)	1:522:A:GLN:C	1:523:A:ALA:N	1:523:A:ALA:CA	1:523:A:ALA:C	18	1.23
(1,44)	1:483:A:VAL:C	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	13	1.23
(1,27)	1:457:A:SER:C	1:458:A:PRO:N	1:458:A:PRO:CA	1:458:A:PRO:C	15	1.23
(1,105)	1:440:A:ALA:N	1:440:A:ALA:CA	1:440:A:ALA:C	1:441:A:VAL:N	19	1.22
(1,75)	1:532:A:GLY:C	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	10	1.22
(1,73)	1:525:A:VAL:C	1:526:A:ASP:N	1:526:A:ASP:CA	1:526:A:ASP:C	12	1.22
(1,69)	1:521:A:SER:C	1:522:A:GLN:N	1:522:A:GLN:CA	1:522:A:GLN:C	15	1.22
(1,64)	1:512:A:LEU:C	1:513:A:ASN:N	1:513:A:ASN:CA	1:513:A:ASN:C	10	1.22
(1,35)	1:466:A:LYS:C	1:467:A:VAL:N	1:467:A:VAL:CA	1:467:A:VAL:C	24	1.22
(1,29)	1:460:A:THR:C	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	20	1.22
(1,178)	1:547:A:VAL:N	1:547:A:VAL:CA	1:547:A:VAL:C	1:548:A:ASP:N	30	1.21
(1,107)	1:442:A:LYS:N	1:442:A:LYS:CA	1:442:A:LYS:C	1:443:A:LYS:N	20	1.21
(1,57)	1:505:A:VAL:C	1:506:A:ASP:N	1:506:A:ASP:CA	1:506:A:ASP:C	20	1.21
(1,32)	1:463:A:LEU:C	1:464:A:VAL:N	1:464:A:VAL:CA	1:464:A:VAL:C	5	1.21
(1,32)	1:463:A:LEU:C	1:464:A:VAL:N	1:464:A:VAL:CA	1:464:A:VAL:C	27	1.21
(1,32)	1:463:A:LEU:C	1:464:A:VAL:N	1:464:A:VAL:CA	1:464:A:VAL:C	3	1.2
(1,32)	1:463:A:LEU:C	1:464:A:VAL:N	1:464:A:VAL:CA	1:464:A:VAL:C	7	1.2
(1,2)	1:425:A:GLU:C	1:426:A:GLN:N	1:426:A:GLN:CA	1:426:A:GLN:C	23	1.2
(1,107)	1:442:A:LYS:N	1:442:A:LYS:CA	1:442:A:LYS:C	1:443:A:LYS:N	13	1.19
(1,94)	1:424:A:PRO:N	1:424:A:PRO:CA	1:424:A:PRO:C	1:425:A:GLU:N	23	1.19
(1,89)	1:551:A:ILE:C	1:552:A:GLU:N	1:552:A:GLU:CA	1:552:A:GLU:C	18	1.19
(1,45)	1:484:A:VAL:C	1:485:A:ILE:N	1:485:A:ILE:CA	1:485:A:ILE:C	15	1.19
(1,27)	1:457:A:SER:C	1:458:A:PRO:N	1:458:A:PRO:CA	1:458:A:PRO:C	6	1.19
(1,15)	1:442:A:LYS:C	1:443:A:LYS:N	1:443:A:LYS:CA	1:443:A:LYS:C	17	1.19
(1,98)	1:429:A:ILE:N	1:429:A:ILE:CA	1:429:A:ILE:C	1:430:A:PRO:N	19	1.18
(1,89)	1:551:A:ILE:C	1:552:A:GLU:N	1:552:A:GLU:CA	1:552:A:GLU:C	4	1.18
(1,15)	1:442:A:LYS:C	1:443:A:LYS:N	1:443:A:LYS:CA	1:443:A:LYS:C	3	1.18
(1,115)	1:453:A:LYS:N	1:453:A:LYS:CA	1:453:A:LYS:C	1:454:A:GLN:N	21	1.17
(1,100)	1:434:A:THR:N	1:434:A:THR:CA	1:434:A:THR:C	1:435:A:LEU:N	11	1.17
(1,75)	1:532:A:GLY:C	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	30	1.17
(1,74)	1:529:A:ARG:C	1:530:A:PRO:N	1:530:A:PRO:CA	1:530:A:PRO:C	16	1.17
(1,71)	1:523:A:ALA:C	1:524:A:SER:N	1:524:A:SER:CA	1:524:A:SER:C	30	1.17
(1,35)	1:466:A:LYS:C	1:467:A:VAL:N	1:467:A:VAL:CA	1:467:A:VAL:C	28	1.17
(1,185)	1:555:A:VAL:N	1:555:A:VAL:CA	1:555:A:VAL:C	1:556:A:SER:N	11	1.16
(1,167)	1:530:A:PRO:N	1:530:A:PRO:CA	1:530:A:PRO:C	1:531:A:ALA:N	28	1.16
(1,165)	1:525:A:VAL:N	1:525:A:VAL:CA	1:525:A:VAL:C	1:526:A:ASP:N	30	1.16
(1,151)	1:507:A:VAL:N	1:507:A:VAL:CA	1:507:A:VAL:C	1:508:A:ALA:N	9	1.16
(1,112)	1:447:A:ALA:N	1:447:A:ALA:CA	1:447:A:ALA:C	1:448:A:GLY:N	18	1.16
(1,100)	1:434:A:THR:N	1:434:A:THR:CA	1:434:A:THR:C	1:435:A:LEU:N	18	1.16
(1,85)	1:546:A:PRO:C	1:547:A:VAL:N	1:547:A:VAL:CA	1:547:A:VAL:C	26	1.16
(1,66)	1:518:A:THR:C	1:519:A:LYS:N	1:519:A:LYS:CA	1:519:A:LYS:C	22	1.16

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,35)	1:466:A:LYS:C	1:467:A:VAL:N	1:467:A:VAL:CA	1:467:A:VAL:C	7	1.16
(1,12)	1:439:A:GLU:C	1:440:A:ALA:N	1:440:A:ALA:CA	1:440:A:ALA:C	27	1.16
(1,150)	1:506:A:ASP:N	1:506:A:ASP:CA	1:506:A:ASP:C	1:507:A:VAL:N	6	1.15
(1,115)	1:453:A:LYS:N	1:453:A:LYS:CA	1:453:A:LYS:C	1:454:A:GLN:N	19	1.15
(1,99)	1:430:A:PRO:N	1:430:A:PRO:CA	1:430:A:PRO:C	1:431:A:ASP:N	11	1.15
(1,97)	1:428:A:GLU:N	1:428:A:GLU:CA	1:428:A:GLU:C	1:429:A:ILE:N	4	1.15
(1,89)	1:551:A:ILE:C	1:552:A:GLU:N	1:552:A:GLU:CA	1:552:A:GLU:C	25	1.15
(1,36)	1:467:A:VAL:C	1:468:A:ILE:N	1:468:A:ILE:CA	1:468:A:ILE:C	17	1.15
(1,29)	1:460:A:THR:C	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	28	1.15
(1,175)	1:544:A:THR:N	1:544:A:THR:CA	1:544:A:THR:C	1:545:A:VAL:N	1	1.14
(1,113)	1:451:A:ARG:N	1:451:A:ARG:CA	1:451:A:ARG:C	1:452:A:PHE:N	1	1.14
(1,112)	1:447:A:ALA:N	1:447:A:ALA:CA	1:447:A:ALA:C	1:448:A:GLY:N	2	1.14
(1,89)	1:551:A:ILE:C	1:552:A:GLU:N	1:552:A:GLU:CA	1:552:A:GLU:C	11	1.14
(1,69)	1:521:A:SER:C	1:522:A:GLN:N	1:522:A:GLN:CA	1:522:A:GLN:C	5	1.14
(1,32)	1:463:A:LEU:C	1:464:A:VAL:N	1:464:A:VAL:CA	1:464:A:VAL:C	14	1.14
(1,175)	1:544:A:THR:N	1:544:A:THR:CA	1:544:A:THR:C	1:545:A:VAL:N	9	1.13
(1,168)	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	1:534:A:VAL:N	3	1.13
(1,150)	1:506:A:ASP:N	1:506:A:ASP:CA	1:506:A:ASP:C	1:507:A:VAL:N	3	1.13
(1,100)	1:434:A:THR:N	1:434:A:THR:CA	1:434:A:THR:C	1:435:A:LEU:N	10	1.13
(1,75)	1:532:A:GLY:C	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	26	1.13
(1,59)	1:507:A:VAL:C	1:508:A:ALA:N	1:508:A:ALA:CA	1:508:A:ALA:C	21	1.13
(1,29)	1:460:A:THR:C	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	19	1.13
(1,122)	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	1:462:A:GLU:N	24	1.12
(1,105)	1:440:A:ALA:N	1:440:A:ALA:CA	1:440:A:ALA:C	1:441:A:VAL:N	13	1.12
(1,73)	1:525:A:VAL:C	1:526:A:ASP:N	1:526:A:ASP:CA	1:526:A:ASP:C	13	1.12
(1,72)	1:524:A:SER:C	1:525:A:VAL:N	1:525:A:VAL:CA	1:525:A:VAL:C	22	1.12
(1,71)	1:523:A:ALA:C	1:524:A:SER:N	1:524:A:SER:CA	1:524:A:SER:C	8	1.12
(1,69)	1:521:A:SER:C	1:522:A:GLN:N	1:522:A:GLN:CA	1:522:A:GLN:C	1	1.12
(1,69)	1:521:A:SER:C	1:522:A:GLN:N	1:522:A:GLN:CA	1:522:A:GLN:C	14	1.12
(1,15)	1:442:A:LYS:C	1:443:A:LYS:N	1:443:A:LYS:CA	1:443:A:LYS:C	24	1.12
(1,185)	1:555:A:VAL:N	1:555:A:VAL:CA	1:555:A:VAL:C	1:556:A:SER:N	1	1.11
(1,179)	1:548:A:ASP:N	1:548:A:ASP:CA	1:548:A:ASP:C	1:549:A:SER:N	18	1.11
(1,150)	1:506:A:ASP:N	1:506:A:ASP:CA	1:506:A:ASP:C	1:507:A:VAL:N	8	1.11
(1,150)	1:506:A:ASP:N	1:506:A:ASP:CA	1:506:A:ASP:C	1:507:A:VAL:N	29	1.11
(1,125)	1:464:A:VAL:N	1:464:A:VAL:CA	1:464:A:VAL:C	1:465:A:GLY:N	7	1.11
(1,113)	1:451:A:ARG:N	1:451:A:ARG:CA	1:451:A:ARG:C	1:452:A:PHE:N	26	1.11
(1,63)	1:511:A:ASN:C	1:512:A:LEU:N	1:512:A:LEU:CA	1:512:A:LEU:C	24	1.11
(1,62)	1:510:A:LYS:C	1:511:A:ASN:N	1:511:A:ASN:CA	1:511:A:ASN:C	18	1.11
(1,32)	1:463:A:LEU:C	1:464:A:VAL:N	1:464:A:VAL:CA	1:464:A:VAL:C	24	1.11
(1,165)	1:525:A:VAL:N	1:525:A:VAL:CA	1:525:A:VAL:C	1:526:A:ASP:N	27	1.1
(1,97)	1:428:A:GLU:N	1:428:A:GLU:CA	1:428:A:GLU:C	1:429:A:ILE:N	18	1.1
(1,27)	1:457:A:SER:C	1:458:A:PRO:N	1:458:A:PRO:CA	1:458:A:PRO:C	29	1.1
(1,167)	1:530:A:PRO:N	1:530:A:PRO:CA	1:530:A:PRO:C	1:531:A:ALA:N	30	1.09
(1,153)	1:509:A:GLN:N	1:509:A:GLN:CA	1:509:A:GLN:C	1:510:A:LYS:N	16	1.09
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	12	1.09
(1,122)	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	1:462:A:GLU:N	4	1.09
(1,122)	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	1:462:A:GLU:N	26	1.09
(1,122)	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	1:462:A:GLU:N	30	1.09
(1,121)	1:459:A:SER:N	1:459:A:SER:CA	1:459:A:SER:C	1:460:A:THR:N	13	1.09
(1,120)	1:458:A:PRO:N	1:458:A:PRO:CA	1:458:A:PRO:C	1:459:A:SER:N	15	1.09
(1,118)	1:456:A:ASN:N	1:456:A:ASN:CA	1:456:A:ASN:C	1:457:A:SER:N	24	1.09

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,89)	1:551:A:ILE:C	1:552:A:GLU:N	1:552:A:GLU:CA	1:552:A:GLU:C	15	1.09
(1,12)	1:439:A:GLU:C	1:440:A:ALA:N	1:440:A:ALA:CA	1:440:A:ALA:C	28	1.09
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	28	1.08
(1,36)	1:467:A:VAL:C	1:468:A:ILE:N	1:468:A:ILE:CA	1:468:A:ILE:C	5	1.08
(1,4)	1:427:A:ARG:C	1:428:A:GLU:N	1:428:A:GLU:CA	1:428:A:GLU:C	12	1.08
(1,168)	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	1:534:A:VAL:N	10	1.07
(1,137)	1:484:A:VAL:N	1:484:A:VAL:CA	1:484:A:VAL:C	1:485:A:ILE:N	10	1.07
(1,113)	1:451:A:ARG:N	1:451:A:ARG:CA	1:451:A:ARG:C	1:452:A:PHE:N	7	1.07
(1,69)	1:521:A:SER:C	1:522:A:GLN:N	1:522:A:GLN:CA	1:522:A:GLN:C	6	1.07
(1,66)	1:518:A:THR:C	1:519:A:LYS:N	1:519:A:LYS:CA	1:519:A:LYS:C	24	1.07
(1,27)	1:457:A:SER:C	1:458:A:PRO:N	1:458:A:PRO:CA	1:458:A:PRO:C	27	1.07
(1,148)	1:504:A:THR:N	1:504:A:THR:CA	1:504:A:THR:C	1:505:A:VAL:N	5	1.06
(1,121)	1:459:A:SER:N	1:459:A:SER:CA	1:459:A:SER:C	1:460:A:THR:N	30	1.06
(1,77)	1:536:A:GLY:C	1:537:A:THR:N	1:537:A:THR:CA	1:537:A:THR:C	24	1.06
(1,75)	1:532:A:GLY:C	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	5	1.06
(1,72)	1:524:A:SER:C	1:525:A:VAL:N	1:525:A:VAL:CA	1:525:A:VAL:C	7	1.06
(1,68)	1:520:A:PHE:C	1:521:A:SER:N	1:521:A:SER:CA	1:521:A:SER:C	23	1.06
(1,64)	1:512:A:LEU:C	1:513:A:ASN:N	1:513:A:ASN:CA	1:513:A:ASN:C	12	1.06
(1,32)	1:463:A:LEU:C	1:464:A:VAL:N	1:464:A:VAL:CA	1:464:A:VAL:C	8	1.06
(1,177)	1:546:A:PRO:N	1:546:A:PRO:CA	1:546:A:PRO:C	1:547:A:VAL:N	24	1.05
(1,175)	1:544:A:THR:N	1:544:A:THR:CA	1:544:A:THR:C	1:545:A:VAL:N	17	1.05
(1,99)	1:430:A:PRO:N	1:430:A:PRO:CA	1:430:A:PRO:C	1:431:A:ASP:N	7	1.05
(1,85)	1:546:A:PRO:C	1:547:A:VAL:N	1:547:A:VAL:CA	1:547:A:VAL:C	3	1.05
(1,33)	1:464:A:VAL:C	1:465:A:GLY:N	1:465:A:GLY:CA	1:465:A:GLY:C	10	1.05
(1,170)	1:537:A:THR:N	1:537:A:THR:CA	1:537:A:THR:C	1:538:A:ASN:N	15	1.04
(1,146)	1:496:A:ASP:N	1:496:A:ASP:CA	1:496:A:ASP:C	1:497:A:ILE:N	6	1.04
(1,122)	1:461:A:PRO:N	1:461:A:PRO:CA	1:461:A:PRO:C	1:462:A:GLU:N	15	1.04
(1,98)	1:429:A:ILE:N	1:429:A:ILE:CA	1:429:A:ILE:C	1:430:A:PRO:N	21	1.04
(1,72)	1:524:A:SER:C	1:525:A:VAL:N	1:525:A:VAL:CA	1:525:A:VAL:C	3	1.04
(1,70)	1:522:A:GLN:C	1:523:A:ALA:N	1:523:A:ALA:CA	1:523:A:ALA:C	22	1.04
(1,57)	1:505:A:VAL:C	1:506:A:ASP:N	1:506:A:ASP:CA	1:506:A:ASP:C	14	1.04
(1,36)	1:467:A:VAL:C	1:468:A:ILE:N	1:468:A:ILE:CA	1:468:A:ILE:C	4	1.04
(1,105)	1:440:A:ALA:N	1:440:A:ALA:CA	1:440:A:ALA:C	1:441:A:VAL:N	1	1.03
(1,105)	1:440:A:ALA:N	1:440:A:ALA:CA	1:440:A:ALA:C	1:441:A:VAL:N	3	1.03
(1,66)	1:518:A:THR:C	1:519:A:LYS:N	1:519:A:LYS:CA	1:519:A:LYS:C	1	1.03
(1,35)	1:466:A:LYS:C	1:467:A:VAL:N	1:467:A:VAL:CA	1:467:A:VAL:C	4	1.03
(1,35)	1:466:A:LYS:C	1:467:A:VAL:N	1:467:A:VAL:CA	1:467:A:VAL:C	22	1.03
(1,27)	1:457:A:SER:C	1:458:A:PRO:N	1:458:A:PRO:CA	1:458:A:PRO:C	28	1.03
(1,75)	1:532:A:GLY:C	1:533:A:GLU:N	1:533:A:GLU:CA	1:533:A:GLU:C	11	1.02
(1,72)	1:524:A:SER:C	1:525:A:VAL:N	1:525:A:VAL:CA	1:525:A:VAL:C	18	1.02
(1,35)	1:466:A:LYS:C	1:467:A:VAL:N	1:467:A:VAL:CA	1:467:A:VAL:C	11	1.02
(1,35)	1:466:A:LYS:C	1:467:A:VAL:N	1:467:A:VAL:CA	1:467:A:VAL:C	19	1.02
(1,3)	1:426:A:GLN:C	1:427:A:ARG:N	1:427:A:ARG:CA	1:427:A:ARG:C	2	1.02
(1,149)	1:505:A:VAL:N	1:505:A:VAL:CA	1:505:A:VAL:C	1:506:A:ASP:N	4	1.01
(1,125)	1:464:A:VAL:N	1:464:A:VAL:CA	1:464:A:VAL:C	1:465:A:GLY:N	17	1.01
(1,112)	1:447:A:ALA:N	1:447:A:ALA:CA	1:447:A:ALA:C	1:448:A:GLY:N	25	1.01
(1,89)	1:551:A:ILE:C	1:552:A:GLU:N	1:552:A:GLU:CA	1:552:A:GLU:C	2	1.01
(1,89)	1:551:A:ILE:C	1:552:A:GLU:N	1:552:A:GLU:CA	1:552:A:GLU:C	19	1.01
(1,48)	1:487:A:ILE:C	1:488:A:VAL:N	1:488:A:VAL:CA	1:488:A:VAL:C	7	1.01
(1,48)	1:487:A:ILE:C	1:488:A:VAL:N	1:488:A:VAL:CA	1:488:A:VAL:C	26	1.01
(1,35)	1:466:A:LYS:C	1:467:A:VAL:N	1:467:A:VAL:CA	1:467:A:VAL:C	23	1.01

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,32)	1:463:A:LEU:C	1:464:A:VAL:N	1:464:A:VAL:CA	1:464:A:VAL:C	13	1.01
(1,16)	1:443:A:LYS:C	1:444:A:LEU:N	1:444:A:LEU:CA	1:444:A:LEU:C	9	1.01
(1,99)	1:430:A:PRO:N	1:430:A:PRO:CA	1:430:A:PRO:C	1:431:A:ASP:N	29	1.0
(1,89)	1:551:A:ILE:C	1:552:A:GLU:N	1:552:A:GLU:CA	1:552:A:GLU:C	28	1.0
(1,89)	1:551:A:ILE:C	1:552:A:GLU:N	1:552:A:GLU:CA	1:552:A:GLU:C	29	1.0
(1,27)	1:457:A:SER:C	1:458:A:PRO:N	1:458:A:PRO:CA	1:458:A:PRO:C	25	1.0