Full wwPDB NMR Structure Validation Report (i)

Jun 6, 2023 – 08:27 pm BST

PDB ID	:	6EY3
BMRB ID	:	34198
Title	:	mf2
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Deposited on	:	2017-11-10

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 (i) 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 (1)) were used in the production of this report:

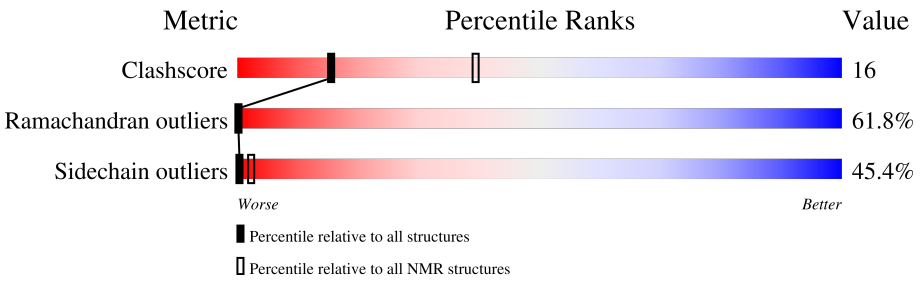
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 50%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	9	22% 33% 44%

2 Ensemble composition and analysis (i)

This entry contains 40 models.

Cyrange was unable to find well-defined residues.

Error message: The number of core atoms (2) was below the domain threshold value (8).

NmrClust was unable to cluster the ensemble.

Error message: Wrapper check: not enough residues in core to run NmrClust

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 132 atoms, of which 64 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	9	132	43	64	13	10	2	0

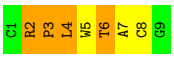
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 22% 33% 44%



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

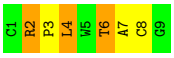
• Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 44% 11% 44%

4.2.2 Score per residue for model 2

• Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 33% 33% 33%



4.2.3 Score per residue for model 3

• Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 44% 22% 11% 22%

C1 R2 P3 L4 W5 T6 A7 C8 G9

4.2.4 Score per residue for model 4

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 22% 33% 33% 11%

C1 R2 P3 L4 W5 T6 A7 C8 G9

4.2.5 Score per residue for model 5

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 22% 56% 22%

C1 R2 P3 L4 W5 T6 A7 C8 G9

4.2.6 Score per residue for model 6

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 33% 33% 11% 22%

C1 R2 P3 L4 W5 T6 A7 C8 G9

4.2.7 Score per residue for model 7

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 22% 44% 33%

C1 R2 P3 L4 W5 T6 A7 C8 G9

4.2.8 Score per residue for model 8

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 33% 33% 33%

4.2.9 Score per residue for model 9

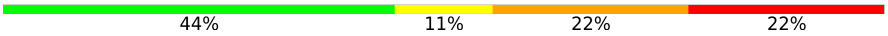
• Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

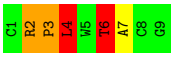
Chain A:

4.2.10 Score per residue for model 10

• Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A:

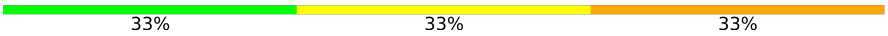


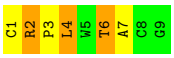


4.2.11 Score per residue for model 11

• Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A:

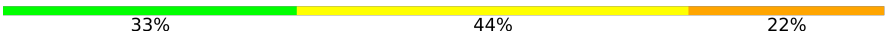




4.2.12 Score per residue for model 12

• Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A:

4.2.14 Score per residue for model 14

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 22% 56% 22%

C1 R2 P3 L4 W5 T6 A7 C8 G9

4.2.15 Score per residue for model 15

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 22% 22% 44% 11%

C1 R2 P3 L4 W5 T6 A7 C8 G9

4.2.16 Score per residue for model 16

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 33% 22% 44%

C1 R2 P3 L4 W5 T6 A7 C8 G9

4.2.17 Score per residue for model 17

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 33% 33% 33%

C1 R2 P3 L4 W5 T6 A7 C8 G9

4.2.18 Score per residue for model 18

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 22% 44% 22% 11%

C1 R2 P3 L4 W5 T6 A7 C8 G9

4.2.19 Score per residue for model 19

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 22% 56% 22%

4.2.20 Score per residue for model 20

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 22% 11% 56% 11%

4.2.21 Score per residue for model 21

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 11% 67% 22%

4.2.22 Score per residue for model 22

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 11% 56% 33%

4.2.23 Score per residue for model 23

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 33% 33% 33%

4.2.24 Score per residue for model 24

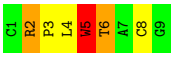
- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 44% 44% 11%

4.2.25 Score per residue for model 25

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 33% 33% 22% 11%



4.2.26 Score per residue for model 26

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 22% 56% 11% 11%

4.2.27 Score per residue for model 27

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 11% 22% 56% 11%

4.2.28 Score per residue for model 28

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 22% 33% 22% 22%

4.2.29 Score per residue for model 29

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 22% 33% 33% 11%

4.2.30 Score per residue for model 30

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 22% 56% 22%

4.2.31 Score per residue for model 31

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 22% 33% 44%

4.2.32 Score per residue for model 32

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 22% 22% 33% 22%

4.2.33 Score per residue for model 33

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 22% 22% 33% 22%

4.2.34 Score per residue for model 34

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 22% 22% 44% 11%

C1 R2 P3 L4 W5 T6 A7 C8 G9

4.2.35 Score per residue for model 35

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 22% 33% 44%

C1 R2 P3 L4 W5 T6 A7 C8 G9

4.2.36 Score per residue for model 36

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 22% 56% 22%

C1 R2 P3 L4 W5 T6 A7 C8 G9

4.2.37 Score per residue for model 37

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 22% 33% 22% 22%

C1 R2 P3 L4 W5 T6 A7 C8 G9

4.2.38 Score per residue for model 38

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

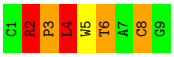
Chain A: 22% 33% 33% 11%

C1 R2 P3 L4 W5 T6 A7 C8 G9

4.2.39 Score per residue for model 39

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 33% 11% 33% 22%



4.2.40 Score per residue for model 40

- Molecule 1: CYS-ARG-PRO-LEU-TRP-THR-ALA-CYS-GLY

Chain A: 11% 44% 22% 22%

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *distance geometry*.

Of the 100 calculated structures, 40 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	57
Number of shifts mapped to atoms	57
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	50%

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	7.0±0.0	0.0±0.0
All	All	280	0

There are no bond-length outliers.

There are no bond-angle outliers.

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

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	2	ARG	CA	40
1	A	3	PRO	CA	40
1	A	4	LEU	CA	40
1	A	5	TRP	CA	40
1	A	6	THR	CA,CB	40
1	A	7	ALA	CA	40

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	68	64	66	2±2
All	All	2720	2560	2640	88

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:LEU:HD23	1:A:7:ALA:HB2	0.90	1.41	27	1
1:A:5:TRP:O	1:A:6:THR:HG22	0.84	1.73	40	1
1:A:4:LEU:O	1:A:5:TRP:C	0.72	2.28	32	1
1:A:3:PRO:O	1:A:4:LEU:HD12	0.65	1.92	39	2
1:A:3:PRO:O	1:A:4:LEU:HD23	0.63	1.93	18	2
1:A:4:LEU:HD13	1:A:8:CYS:O	0.61	1.95	20	1
1:A:3:PRO:C	1:A:4:LEU:HD12	0.60	2.16	28	3
1:A:3:PRO:O	1:A:4:LEU:HD13	0.59	1.97	10	1
1:A:7:ALA:O	1:A:8:CYS:C	0.59	2.41	33	1
1:A:6:THR:O	1:A:7:ALA:HB2	0.59	1.98	38	2
1:A:2:ARG:CB	1:A:3:PRO:HD2	0.56	2.31	37	18
1:A:4:LEU:O	1:A:5:TRP:CB	0.54	2.56	18	2
1:A:2:ARG:O	1:A:4:LEU:HD23	0.54	2.02	35	1
1:A:5:TRP:C	1:A:6:THR:OG1	0.54	2.45	40	1
1:A:4:LEU:CD2	1:A:7:ALA:HB2	0.53	2.25	27	1
1:A:4:LEU:C	1:A:6:THR:H	0.53	2.07	38	2
1:A:5:TRP:O	1:A:6:THR:CG2	0.52	2.53	40	1
1:A:5:TRP:CG	1:A:5:TRP:O	0.52	2.62	1	2
1:A:4:LEU:HD23	1:A:6:THR:CG2	0.52	2.35	6	2
1:A:2:ARG:HD3	1:A:4:LEU:HD13	0.50	1.81	3	1
1:A:2:ARG:HB3	1:A:3:PRO:HD2	0.49	1.83	37	1
1:A:5:TRP:O	1:A:6:THR:CB	0.49	2.60	25	3
1:A:4:LEU:HD23	1:A:9:GLY:HA3	0.49	1.85	4	1
1:A:4:LEU:C	1:A:6:THR:N	0.47	2.68	40	2
1:A:4:LEU:HD12	1:A:4:LEU:N	0.46	2.25	37	1
1:A:6:THR:O	1:A:7:ALA:HB3	0.46	2.09	34	2
1:A:2:ARG:CB	1:A:3:PRO:CD	0.46	2.94	34	5
1:A:2:ARG:N	1:A:3:PRO:CD	0.46	2.79	31	15
1:A:6:THR:O	1:A:6:THR:HG22	0.45	2.10	20	1
1:A:4:LEU:HD23	1:A:6:THR:HG21	0.45	1.88	6	1
1:A:5:TRP:O	1:A:6:THR:C	0.45	2.55	39	1
1:A:6:THR:O	1:A:7:ALA:CB	0.45	2.64	38	1
1:A:1:CYS:C	1:A:2:ARG:HG3	0.45	2.32	37	1
1:A:4:LEU:O	1:A:6:THR:HG22	0.43	2.14	3	1
1:A:3:PRO:C	1:A:4:LEU:HG	0.42	2.34	37	1
1:A:2:ARG:HB3	1:A:7:ALA:HB2	0.41	1.90	15	1
1:A:2:ARG:C	1:A:4:LEU:H	0.41	2.19	24	1
1:A:4:LEU:O	1:A:6:THR:N	0.40	2.53	32	1
1:A:4:LEU:HB3	1:A:6:THR:HG23	0.40	1.92	28	1
1:A:3:PRO:O	1:A:4:LEU:O	0.40	2.39	37	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	7/9 (78%)	1±1 (20±12%)	1±1 (18±13%)	4±1 (62±13%)	0 0
All	All	280/360 (78%)	57 (20%)	50 (18%)	173 (62%)	0 0

All 7 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	3	PRO	40
1	A	4	LEU	32
1	A	7	ALA	32
1	A	2	ARG	24
1	A	6	THR	20
1	A	5	TRP	15
1	A	8	CYS	10

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	7/7 (100%)	4±1 (55±10%)	3±1 (45±10%)	0 2
All	All	280/280 (100%)	153 (55%)	127 (45%)	0 2

All 6 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	2	ARG	37
1	A	4	LEU	29
1	A	5	TRP	24

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Mol	Chain	Res	Type	Models (Total)
1	A	8	CYS	21
1	A	1	CYS	11
1	A	6	THR	5

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 monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 50% for the well-defined parts and 50% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *ciclo1.str*

7.1.1 Bookkeeping (i)

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

Total number of shifts	57
Number of shifts mapped to atoms	57
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing (i)

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

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 50%, i.e. 57 atoms were assigned a chemical shift out of a possible 115. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}**H**	^{13}**C**	^{15}**N**
Backbone	17/44 (39%)	17/18 (94%)	0/18 (0%)	0/8 (0%)
Sidechain	35/59 (59%)	35/39 (90%)	0/17 (0%)	0/3 (0%)
Aromatic	5/12 (42%)	5/6 (83%)	0/5 (0%)	0/1 (0%)
Overall	57/115 (50%)	57/63 (90%)	0/40 (0%)	0/12 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 50%, i.e. 57 atoms were assigned a chemical shift out of a possible 115. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	17/44 (39%)	17/18 (94%)	0/18 (0%)	0/8 (0%)
Sidechain	35/59 (59%)	35/39 (90%)	0/17 (0%)	0/3 (0%)
Aromatic	5/12 (42%)	5/6 (83%)	0/5 (0%)	0/1 (0%)
Overall	57/115 (50%)	57/63 (90%)	0/40 (0%)	0/12 (0%)

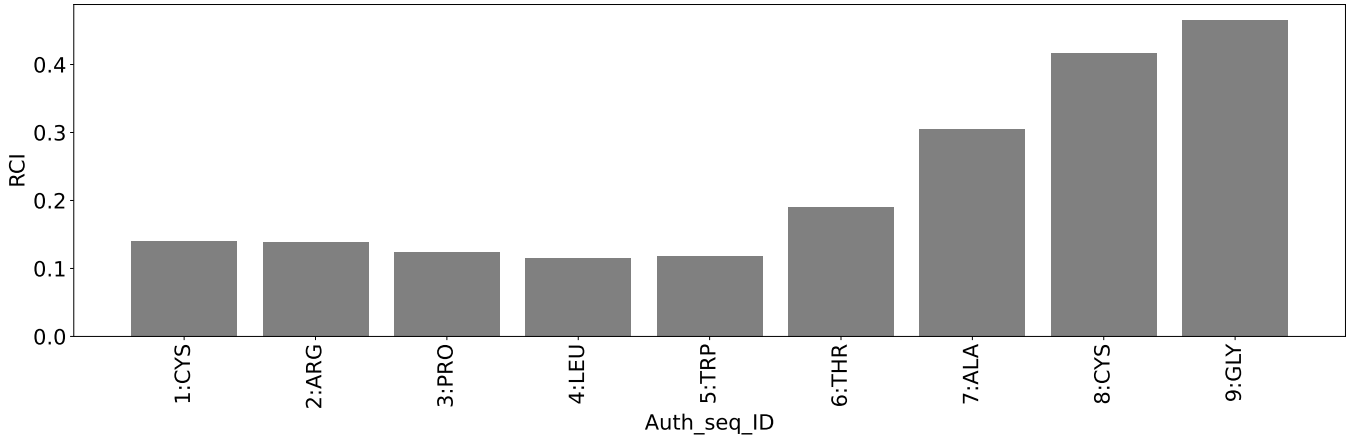
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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	75
Intra-residue (|i-j|=0)	59
Sequential (|i-j|=1)	14
Medium range (|i-j|>1 and |i-j|<5)	2
Long range (|i-j|≥5)	0
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	8.3
Number of long range restraints per residue[1]	0.0

[1]Long 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 (i)

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 (i)

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)	1.1	0.2
0.2-0.5 (Medium)	1.2	0.5
>0.5 (Large)	1.9	3.88

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

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

9 Distance violation analysis (i)

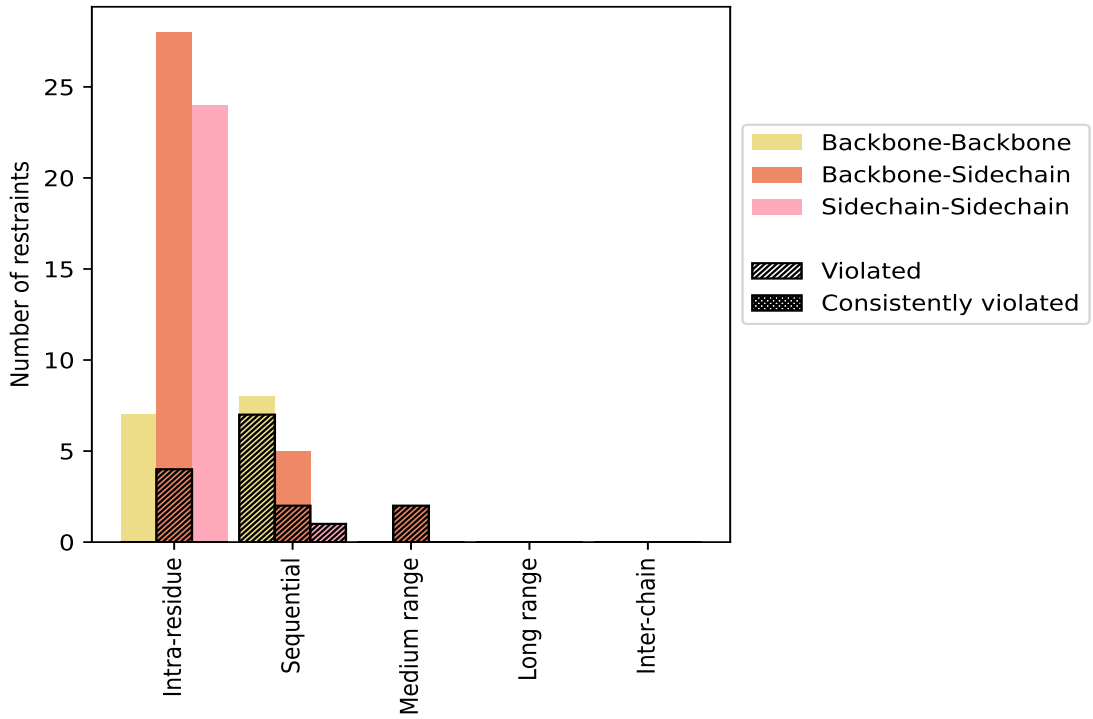
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	59	78.7	4	6.8	5.3	0	0.0	0.0
Backbone-Backbone	7	9.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	28	37.3	4	14.3	5.3	0	0.0	0.0
Sidechain-Sidechain	24	32.0	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	14	18.7	10	71.4	13.3	0	0.0	0.0
Backbone-Backbone	8	10.7	7	87.5	9.3	0	0.0	0.0
Backbone-Sidechain	5	6.7	2	40.0	2.7	0	0.0	0.0
Sidechain-Sidechain	1	1.3	1	100.0	1.3	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	2	2.7	2	100.0	2.7	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	2	2.7	2	100.0	2.7	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	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
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	75	100.0	16	21.3	21.3	0	0.0	0.0
Backbone-Backbone	15	20.0	7	46.7	9.3	0	0.0	0.0
Backbone-Sidechain	35	46.7	8	22.9	10.7	0	0.0	0.0
Sidechain-Sidechain	25	33.3	1	4.0	1.3	0	0.0	0.0

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

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



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

9.2 Distance violation statistics for each model (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	2	1	0	0	3	0.43	0.68	0.18	0.38
2	0	2	1	0	0	3	0.83	1.94	0.79	0.37
3	0	2	1	0	0	3	1.04	2.52	1.05	0.42
4	1	3	0	0	0	4	1.31	3.84	1.48	0.62
5	0	1	1	0	0	2	0.29	0.38	0.09	0.29
6	0	2	2	0	0	4	0.77	2.52	1.01	0.22
7	0	1	0	0	0	1	0.2	0.2	0.0	0.2
8	0	3	2	0	0	5	0.56	1.66	0.58	0.2
9	0	3	1	0	0	4	1.05	2.75	1.05	0.65
10	0	2	1	0	0	3	1.1	2.56	1.04	0.48
11	0	2	1	0	0	3	1.49	3.82	1.65	0.46

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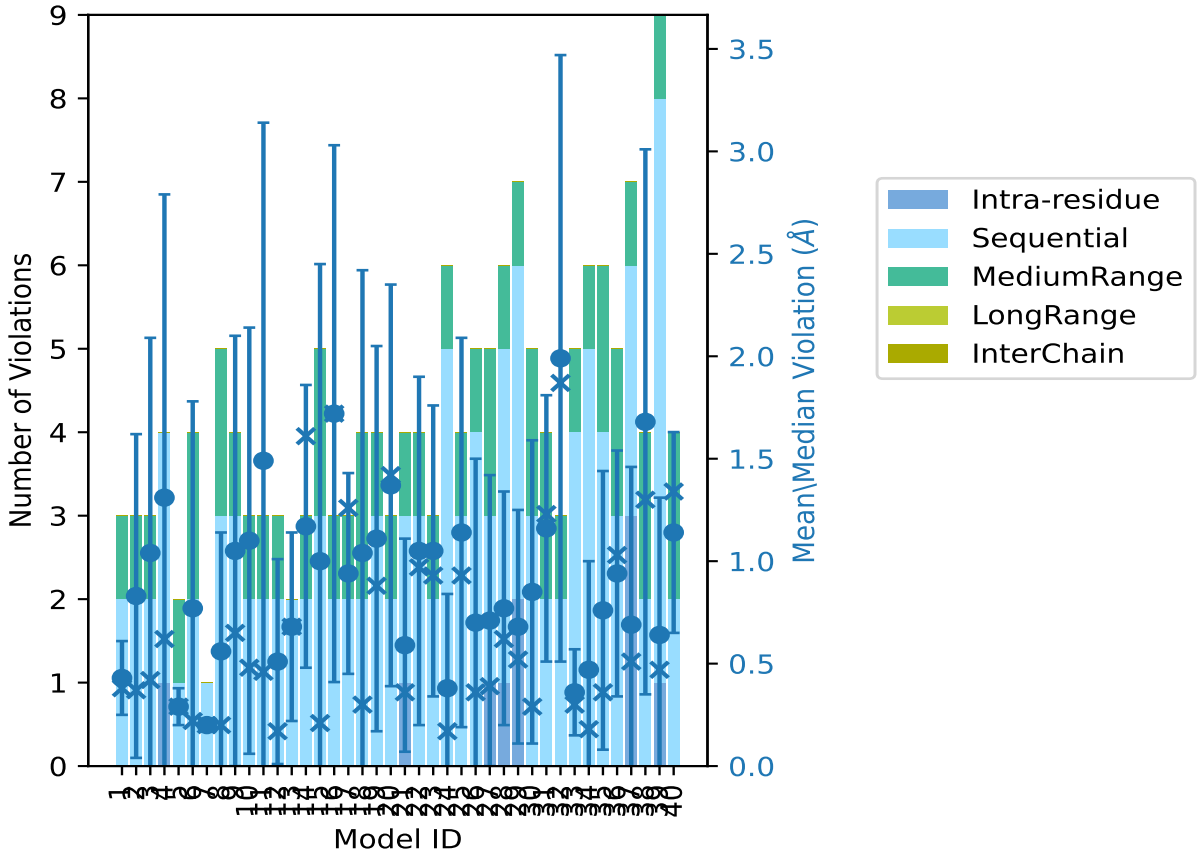
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	2	1	0	0	3	0.51	1.22	0.5	0.17
13	0	2	0	0	0	2	0.68	1.14	0.46	0.68
14	0	2	1	0	0	3	1.17	1.71	0.69	1.61
15	0	3	2	0	0	5	1.0	3.88	1.45	0.21
16	0	2	1	0	0	3	1.72	3.33	1.31	1.72
17	0	2	1	0	0	3	0.94	1.31	0.49	1.26
18	0	2	2	0	0	4	1.04	3.42	1.38	0.3
19	0	3	1	0	0	4	1.11	2.5	0.94	0.88
20	0	2	1	0	0	3	1.37	2.55	0.98	1.42
21	1	2	1	0	0	4	0.59	1.47	0.52	0.36
22	0	3	1	0	0	4	1.05	2.13	0.85	0.97
23	0	2	1	0	0	3	1.05	1.97	0.71	0.93
24	0	5	1	0	0	6	0.38	1.39	0.46	0.17
25	0	3	1	0	0	4	1.14	2.54	0.95	0.93
26	0	4	1	0	0	5	0.7	2.28	0.8	0.36
27	1	2	2	0	0	5	0.71	2.06	0.71	0.39
28	1	4	1	0	0	6	0.77	1.99	0.57	0.62
29	2	4	1	0	0	7	0.68	1.99	0.57	0.52
30	0	3	2	0	0	5	0.85	1.99	0.74	0.29
31	0	2	2	0	0	4	1.16	2.0	0.65	1.23
32	0	2	1	0	0	3	1.99	3.87	1.48	1.87
33	0	4	1	0	0	5	0.36	0.73	0.21	0.3
34	0	5	1	0	0	6	0.47	1.6	0.53	0.18
35	0	4	2	0	0	6	0.76	1.92	0.68	0.36
36	0	3	2	0	0	5	0.94	1.86	0.6	1.03
37	3	3	1	0	0	7	0.69	2.55	0.77	0.51
38	0	2	2	0	0	4	1.68	3.85	1.33	1.3
39	1	7	1	0	0	9	0.64	2.46	0.67	0.47
40	0	2	2	0	0	4	1.14	1.55	0.49	1.34

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard 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, 59(IR:55, SQ:4, MR:0, LR:0, 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]	%
2	1	0	0	0	3	1	2.5
0	1	0	0	0	1	2	5.0
1	1	0	0	0	2	3	7.5
0	0	0	0	0	0	4	10.0
1	1	0	0	0	2	5	12.5
0	0	0	0	0	0	6	15.0

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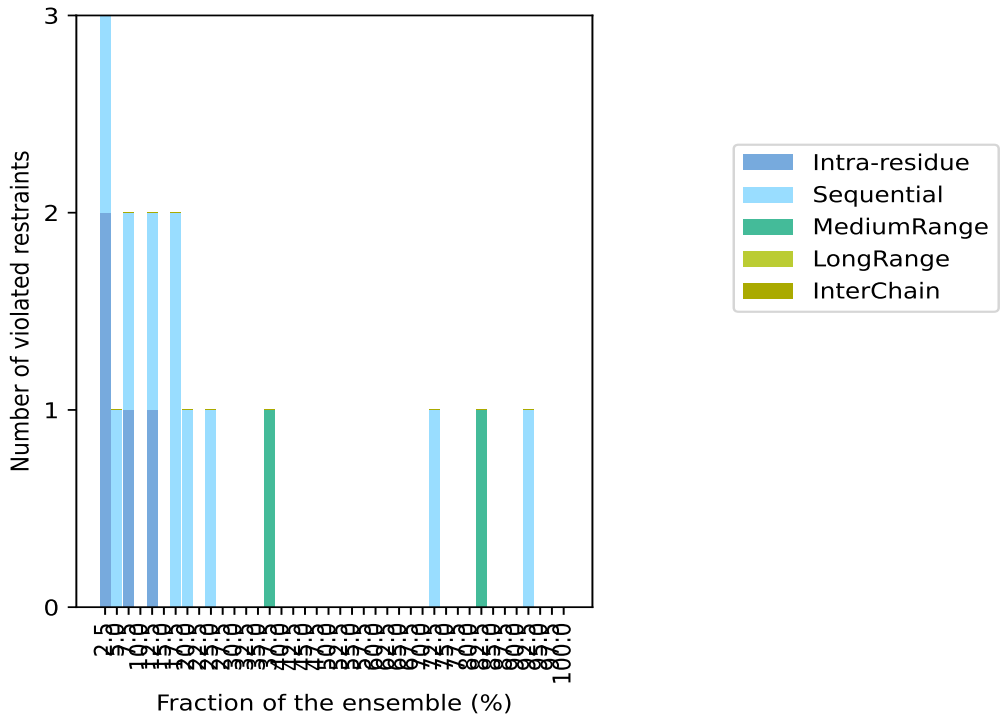
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	2	0	0	0	2	7	17.5
0	1	0	0	0	1	8	20.0
0	0	0	0	0	0	9	22.5
0	1	0	0	0	1	10	25.0
0	0	0	0	0	0	11	27.5
0	0	0	0	0	0	12	30.0
0	0	0	0	0	0	13	32.5
0	0	0	0	0	0	14	35.0
0	0	1	0	0	1	15	37.5
0	0	0	0	0	0	16	40.0
0	0	0	0	0	0	17	42.5
0	0	0	0	0	0	18	45.0
0	0	0	0	0	0	19	47.5
0	0	0	0	0	0	20	50.0
0	0	0	0	0	0	21	52.5
0	0	0	0	0	0	22	55.0
0	0	0	0	0	0	23	57.5
0	0	0	0	0	0	24	60.0
0	0	0	0	0	0	25	62.5
0	0	0	0	0	0	26	65.0
0	0	0	0	0	0	27	67.5
0	0	0	0	0	0	28	70.0
0	1	0	0	0	1	29	72.5
0	0	0	0	0	0	30	75.0
0	0	0	0	0	0	31	77.5
0	0	0	0	0	0	32	80.0
0	0	1	0	0	1	33	82.5
0	0	0	0	0	0	34	85.0
0	0	0	0	0	0	35	87.5
0	0	0	0	0	0	36	90.0
0	1	0	0	0	1	37	92.5
0	0	0	0	0	0	38	95.0
0	0	0	0	0	0	39	97.5
0	0	0	0	0	0	40	100.0

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

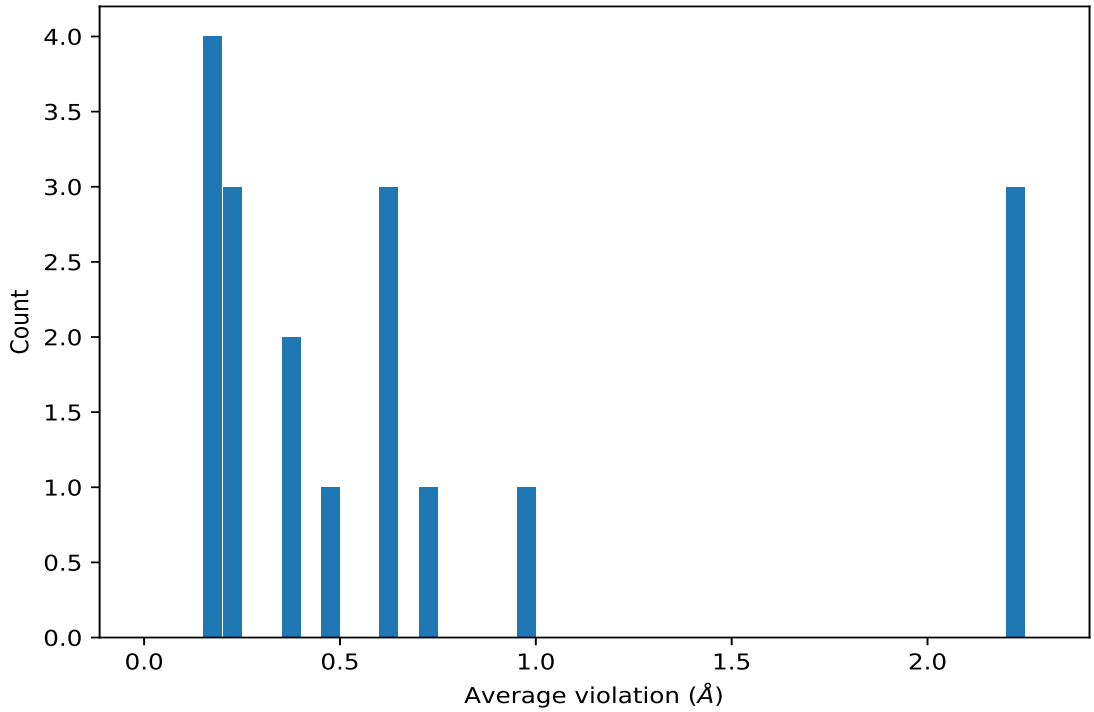
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	37	2.24	0.92	2.06
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	37	2.24	0.92	2.06
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	37	2.24	0.92	2.06
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	33	0.98	0.53	1.07
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	29	0.19	0.03	0.2
(1,50)	1:A:4:LEU:HG	1:A:6:THR:H	15	0.24	0.12	0.21
(1,42)	1:A:4:LEU:HB2	1:A:5:TRP:H	10	0.71	0.37	0.68
(1,31)	1:A:4:LEU:H	1:A:5:TRP:H	8	0.35	0.12	0.34
(1,9)	1:A:3:PRO:HA	1:A:4:LEU:H	7	0.47	0.23	0.37
(1,67)	1:A:7:ALA:HA	1:A:8:CYS:H	7	0.37	0.08	0.33
(1,40)	1:A:4:LEU:HA	1:A:4:LEU:HD21	5	0.62	0.12	0.69
(1,40)	1:A:4:LEU:HA	1:A:4:LEU:HD22	5	0.62	0.12	0.69
(1,40)	1:A:4:LEU:HA	1:A:4:LEU:HD23	5	0.62	0.12	0.69
(1,56)	1:A:5:TRP:HA	1:A:6:THR:H	5	0.15	0.01	0.15
(1,62)	1:A:6:THR:H	1:A:7:ALA:H	3	0.24	0.11	0.19
(1,70)	1:A:8:CYS:H	1:A:8:CYS:HB2	3	0.17	0.01	0.17

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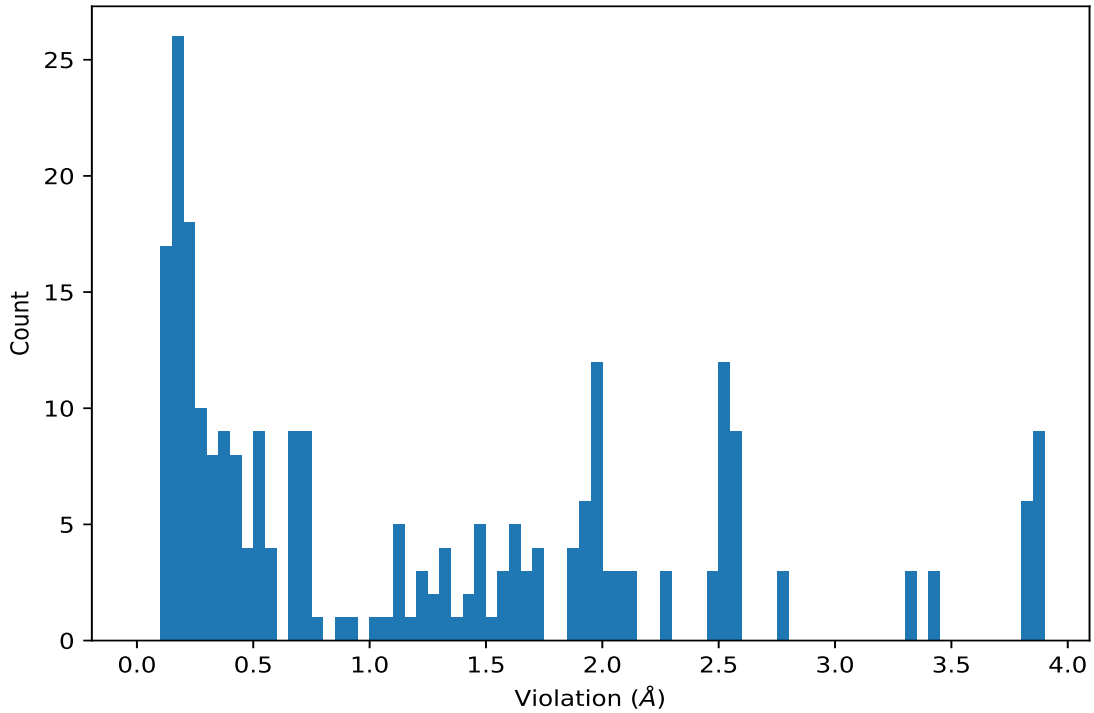
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,70)	1:A:8:CYS:H	1:A:8:CYS:HB3	3	0.17	0.01	0.17
(1,2)	1:A:1:CYS:HA	1:A:2:ARG:H	2	0.24	0.1	0.24

[1]Number of violated models, [2]Standard 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)
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	15	3.88
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	15	3.88

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	15	3.88
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	32	3.87
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	32	3.87
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	32	3.87
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	38	3.85
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	38	3.85
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	38	3.85
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	4	3.84
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	4	3.84
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	4	3.84
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	11	3.82
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	11	3.82
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	11	3.82
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	18	3.42
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	18	3.42
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	18	3.42
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	16	3.33
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	16	3.33
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	16	3.33
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	9	2.75
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	9	2.75
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	9	2.75
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	10	2.56
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	10	2.56
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	10	2.56
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	20	2.55
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	20	2.55
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	20	2.55
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	37	2.55
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	37	2.55
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	37	2.55
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	25	2.54
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	25	2.54
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	25	2.54
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	3	2.52
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	3	2.52
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	3	2.52
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	6	2.52
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	6	2.52
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	6	2.52
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	19	2.5
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	19	2.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	19	2.5
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	39	2.46
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	39	2.46
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	39	2.46
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	26	2.28
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	26	2.28
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	26	2.28
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	22	2.13
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	22	2.13
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	22	2.13
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	27	2.06
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	27	2.06
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	27	2.06
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	31	2.0
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	31	2.0
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	31	2.0
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	28	1.99
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	28	1.99
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	28	1.99
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	29	1.99
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	29	1.99
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	29	1.99
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	30	1.99
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	30	1.99
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	30	1.99
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	23	1.97
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	23	1.97
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	23	1.97
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	2	1.94
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	2	1.94
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	2	1.94
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	35	1.92
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	35	1.92
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	35	1.92
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	32	1.87
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	36	1.86
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	36	1.86
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	36	1.86
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	16	1.72
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	14	1.71
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	14	1.71
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	14	1.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	8	1.66
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	8	1.66
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	8	1.66
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	22	1.62
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	14	1.61
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	34	1.6
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	34	1.6
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	34	1.6
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	40	1.55
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	40	1.55
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	40	1.55
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	35	1.5
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	40	1.49
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	38	1.48
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	21	1.47
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	25	1.47
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	30	1.47
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	19	1.43
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	20	1.42
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	24	1.39
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	31	1.32
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	17	1.31
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	17	1.31
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	17	1.31
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	17	1.26
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	36	1.25
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	12	1.22
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	12	1.22
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	12	1.22
(1,42)	1:A:4:LEU:HB2	1:A:5:TRP:H	40	1.18
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	13	1.14
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	13	1.14
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	13	1.14
(1,42)	1:A:4:LEU:HB2	1:A:5:TRP:H	31	1.14
(1,42)	1:A:4:LEU:HB2	1:A:5:TRP:H	38	1.12
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	9	1.07
(1,42)	1:A:4:LEU:HB2	1:A:5:TRP:H	36	1.03
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	23	0.93
(1,42)	1:A:4:LEU:HB2	1:A:5:TRP:H	4	0.85
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	27	0.76
(1,9)	1:A:3:PRO:HA	1:A:4:LEU:H	29	0.74
(1,9)	1:A:3:PRO:HA	1:A:4:LEU:H	28	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	33	0.73
(1,40)	1:A:4:LEU:HA	1:A:4:LEU:HD21	28	0.72
(1,40)	1:A:4:LEU:HA	1:A:4:LEU:HD22	28	0.72
(1,40)	1:A:4:LEU:HA	1:A:4:LEU:HD23	28	0.72
(1,40)	1:A:4:LEU:HA	1:A:4:LEU:HD21	39	0.7
(1,40)	1:A:4:LEU:HA	1:A:4:LEU:HD22	39	0.7
(1,40)	1:A:4:LEU:HA	1:A:4:LEU:HD23	39	0.7
(1,40)	1:A:4:LEU:HA	1:A:4:LEU:HD21	29	0.69
(1,40)	1:A:4:LEU:HA	1:A:4:LEU:HD22	29	0.69
(1,40)	1:A:4:LEU:HA	1:A:4:LEU:HD23	29	0.69
(1,9)	1:A:3:PRO:HA	1:A:4:LEU:H	39	0.68
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	1	0.68
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	1	0.68
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	1	0.68
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	8	0.66
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	15	0.65
(1,40)	1:A:4:LEU:HA	1:A:4:LEU:HD21	37	0.58
(1,40)	1:A:4:LEU:HA	1:A:4:LEU:HD22	37	0.58
(1,40)	1:A:4:LEU:HA	1:A:4:LEU:HD23	37	0.58
(1,67)	1:A:7:ALA:HA	1:A:8:CYS:H	34	0.55
(1,8)	1:A:2:ARG:H	1:A:2:ARG:HH11	37	0.52
(1,8)	1:A:2:ARG:H	1:A:2:ARG:HH12	37	0.52
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	21	0.52
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	21	0.52
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	21	0.52
(1,42)	1:A:4:LEU:HB2	1:A:5:TRP:H	29	0.52
(1,31)	1:A:4:LEU:H	1:A:5:TRP:H	28	0.52
(1,50)	1:A:4:LEU:HG	1:A:6:THR:H	37	0.51
(1,31)	1:A:4:LEU:H	1:A:5:TRP:H	39	0.5
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	10	0.48
(1,50)	1:A:4:LEU:HG	1:A:6:THR:H	39	0.47
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	11	0.46
(1,42)	1:A:4:LEU:HB2	1:A:5:TRP:H	28	0.46
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	3	0.42
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	18	0.42
(1,31)	1:A:4:LEU:H	1:A:5:TRP:H	33	0.42
(1,67)	1:A:7:ALA:HA	1:A:8:CYS:H	36	0.41
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	26	0.4
(1,40)	1:A:4:LEU:HA	1:A:4:LEU:HD21	4	0.4
(1,40)	1:A:4:LEU:HA	1:A:4:LEU:HD22	4	0.4
(1,40)	1:A:4:LEU:HA	1:A:4:LEU:HD23	4	0.4
(1,62)	1:A:6:THR:H	1:A:7:ALA:H	25	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,50)	1:A:4:LEU:HG	1:A:6:THR:H	27	0.39
(1,31)	1:A:4:LEU:H	1:A:5:TRP:H	29	0.39
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	1	0.38
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	5	0.38
(1,9)	1:A:3:PRO:HA	1:A:4:LEU:H	35	0.37
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	2	0.37
(1,9)	1:A:3:PRO:HA	1:A:4:LEU:H	26	0.36
(1,42)	1:A:4:LEU:HB2	1:A:5:TRP:H	37	0.36
(1,67)	1:A:7:ALA:HA	1:A:8:CYS:H	35	0.34
(1,67)	1:A:7:ALA:HA	1:A:8:CYS:H	19	0.33
(1,67)	1:A:7:ALA:HA	1:A:8:CYS:H	26	0.33
(1,50)	1:A:4:LEU:HG	1:A:6:THR:H	40	0.33
(1,2)	1:A:1:CYS:HA	1:A:2:ARG:H	39	0.33
(1,67)	1:A:7:ALA:HA	1:A:8:CYS:H	22	0.31
(1,42)	1:A:4:LEU:HB2	1:A:5:TRP:H	39	0.31
(1,67)	1:A:7:ALA:HA	1:A:8:CYS:H	33	0.3
(1,31)	1:A:4:LEU:H	1:A:5:TRP:H	30	0.29
(1,50)	1:A:4:LEU:HG	1:A:6:THR:H	38	0.27
(1,31)	1:A:4:LEU:H	1:A:5:TRP:H	35	0.27
(1,9)	1:A:3:PRO:HA	1:A:4:LEU:H	30	0.26
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG21	24	0.26
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG22	24	0.26
(1,59)	1:A:5:TRP:HD1	1:A:6:THR:HG23	24	0.26
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	6	0.25
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	10	0.25
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	17	0.25
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	1	0.24
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	23	0.24
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	32	0.24
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	9	0.23
(1,50)	1:A:4:LEU:HG	1:A:6:THR:H	29	0.22
(1,50)	1:A:4:LEU:HG	1:A:6:THR:H	30	0.22
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	34	0.22
(1,50)	1:A:4:LEU:HG	1:A:6:THR:H	28	0.21
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	13	0.21
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	15	0.21
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	21	0.21
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	33	0.21
(1,31)	1:A:4:LEU:H	1:A:5:TRP:H	37	0.21
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	5	0.2
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	7	0.2
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	8	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	11	0.2
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	14	0.2
(1,62)	1:A:6:THR:H	1:A:7:ALA:H	39	0.19
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	3	0.19
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	6	0.19
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	27	0.19
(1,70)	1:A:8:CYS:H	1:A:8:CYS:HB2	29	0.18
(1,70)	1:A:8:CYS:H	1:A:8:CYS:HB3	29	0.18
(1,50)	1:A:4:LEU:HG	1:A:6:THR:H	31	0.18
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	2	0.18
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	18	0.18
(1,70)	1:A:8:CYS:H	1:A:8:CYS:HB2	21	0.17
(1,70)	1:A:8:CYS:H	1:A:8:CYS:HB3	21	0.17
(1,56)	1:A:5:TRP:HA	1:A:6:THR:H	24	0.17
(1,50)	1:A:4:LEU:HG	1:A:6:THR:H	35	0.17
(1,50)	1:A:4:LEU:HG	1:A:6:THR:H	36	0.17
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	12	0.17
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	19	0.17
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	25	0.17
(1,31)	1:A:4:LEU:H	1:A:5:TRP:H	24	0.17
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	4	0.16
(1,70)	1:A:8:CYS:H	1:A:8:CYS:HB2	27	0.15
(1,70)	1:A:8:CYS:H	1:A:8:CYS:HB3	27	0.15
(1,56)	1:A:5:TRP:HA	1:A:6:THR:H	9	0.15
(1,56)	1:A:5:TRP:HA	1:A:6:THR:H	15	0.15
(1,49)	1:A:4:LEU:HB3	1:A:6:THR:H	12	0.15
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	20	0.15
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	34	0.15
(1,9)	1:A:3:PRO:HA	1:A:4:LEU:H	24	0.14
(1,56)	1:A:5:TRP:HA	1:A:6:THR:H	8	0.14
(1,56)	1:A:5:TRP:HA	1:A:6:THR:H	33	0.14
(1,42)	1:A:4:LEU:HB2	1:A:5:TRP:H	34	0.14
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	22	0.14
(1,2)	1:A:1:CYS:HA	1:A:2:ARG:H	34	0.14
(1,62)	1:A:6:THR:H	1:A:7:ALA:H	24	0.13
(1,50)	1:A:4:LEU:HG	1:A:6:THR:H	8	0.13
(1,50)	1:A:4:LEU:HG	1:A:6:THR:H	18	0.13
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	26	0.13
(1,74)	1:A:8:CYS:HB2	1:A:9:GLY:H	39	0.12
(1,74)	1:A:8:CYS:HB3	1:A:9:GLY:H	39	0.12
(1,50)	1:A:4:LEU:HG	1:A:6:THR:H	6	0.12
(1,50)	1:A:4:LEU:HG	1:A:6:THR:H	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,41)	1:A:4:LEU:HA	1:A:5:TRP:H	16	0.12
(1,13)	1:A:2:ARG:HA	1:A:2:ARG:HH11	37	0.12
(1,13)	1:A:2:ARG:HA	1:A:2:ARG:HH12	37	0.12

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found