



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 08:10 PM UTC

PDB ID : 2W9W / pdb_00002w9w
BMRB ID : 16152
Title : Solution structure of jerdostatin mutant R24K from *Trimeresurus jerdonii* with end C-terminal residues N45G46 deleted
Authors : Carbajo, R.J.; Sanz, L.; Mosulen, S.; Calvete, J.J.; Pineda-Lucena, A.
Deposited on : 2009-01-29

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

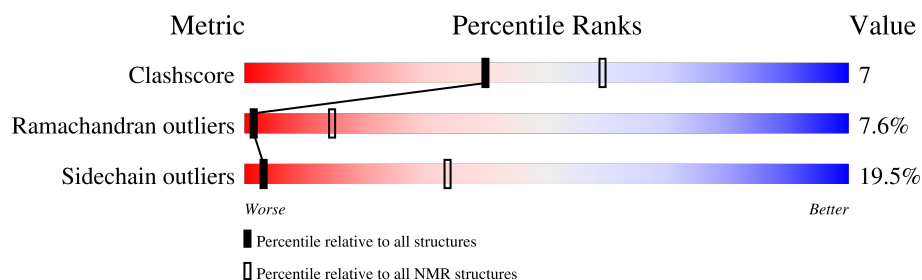
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 82%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	44	

2 Ensemble composition and analysis

This entry contains 40 models. Model 25 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:4-A:44 (41)	1.11	25

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 5 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 4, 5, 8, 11, 12, 14, 15, 17, 18, 19, 21, 24, 25, 26, 27, 29, 30, 34, 38, 39
2	7, 9, 10, 13, 16, 22, 23, 33, 36, 37, 40
3	6, 28
4	31, 35
5	3, 32
Single-model clusters	20

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 620 atoms, of which 299 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SHORT DISINTEGRIN JERDOSTATIN.

Mol	Chain	Residues	Atoms							Trace
1	A	44	Total	C	H	N	O	S		0
			620	192	299	57	63	9		

There is a discrepancy between the modelled and reference sequences:

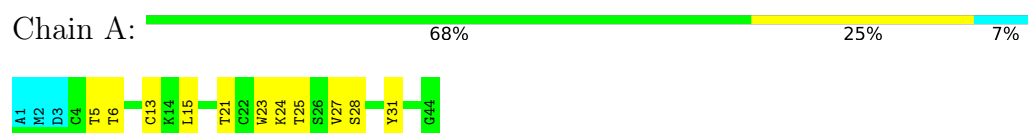
Chain	Residue	Modelled	Actual	Comment	Reference
A	24	LYS	ARG	engineered mutation	UNP Q7ZZM2

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: SHORT DISINTEGRIN JERDOSTATIN

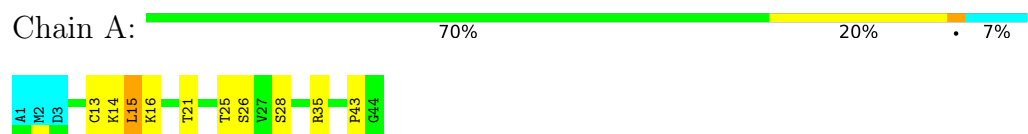


4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

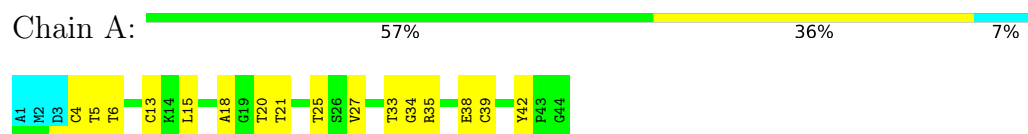
4.2.1 Score per residue for model 1

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



4.2.2 Score per residue for model 2

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



4.2.3 Score per residue for model 3

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN

Chain A:  52% 34% 7% 7%



4.2.4 Score per residue for model 4

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN

Chain A:  73% 18% 7%



4.2.5 Score per residue for model 5

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN

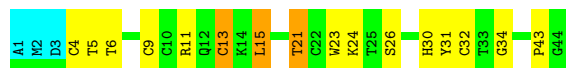
Chain A:  66% 25% 7%



4.2.6 Score per residue for model 6

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN

Chain A:  57% 30% 7% 7%



4.2.7 Score per residue for model 7

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN

Chain A:  64% 30% 7%



4.2.8 Score per residue for model 8

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN

Chain A:  68% 25% 7%



4.2.9 Score per residue for model 9

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN

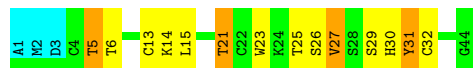
Chain A:  70% 18% . . 7%



4.2.10 Score per residue for model 10

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN

Chain A:  61% 23% 9% 7%



4.2.11 Score per residue for model 11

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN

Chain A:  75% 14% 5% 7%



4.2.12 Score per residue for model 12

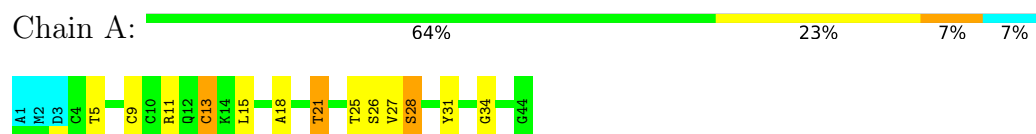
- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN

Chain A:  68% 20% 5% 7%



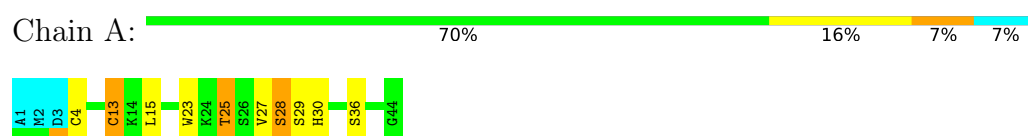
4.2.13 Score per residue for model 13

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



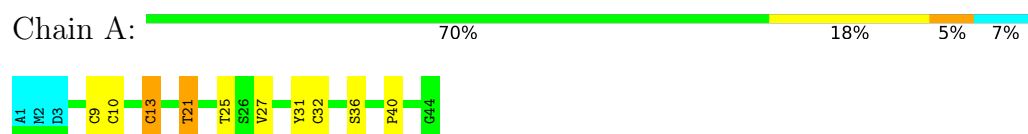
4.2.14 Score per residue for model 14

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



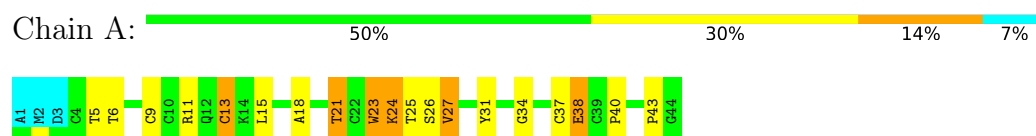
4.2.15 Score per residue for model 15

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



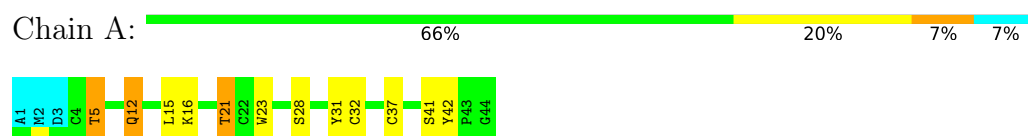
4.2.16 Score per residue for model 16

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



4.2.17 Score per residue for model 17

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



4.2.18 Score per residue for model 18

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN

Chain A:  59% 27% 7% 7%



4.2.19 Score per residue for model 19

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN

Chain A:  59% 30% 5% 7%



4.2.20 Score per residue for model 20

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN

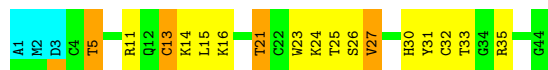
Chain A:  68% 20% 5% 7%



4.2.21 Score per residue for model 21

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN

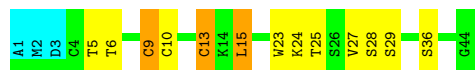
Chain A:  55% 30% 9% 7%



4.2.22 Score per residue for model 22

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN

Chain A:  64% 23% 7% 7%



4.2.23 Score per residue for model 23

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN

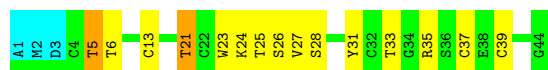
Chain A:  55% 36% 7%



4.2.24 Score per residue for model 24

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN

Chain A:  59% 30% 5% 7%



4.2.25 Score per residue for model 25 (medoid)

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN

Chain A:  59% 27% 7% 7%



4.2.26 Score per residue for model 26

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN

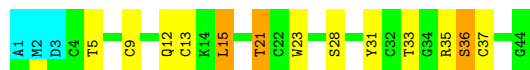
Chain A:  70% 20% 7%



4.2.27 Score per residue for model 27

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN

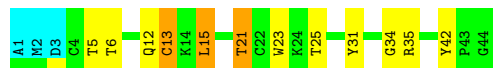
Chain A:  64% 23% 7% 7%



4.2.28 Score per residue for model 28

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN

Chain A:  66% 20% 7% 7%



4.2.29 Score per residue for model 29

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN

Chain A:  59% 30% 5% 7%



4.2.30 Score per residue for model 30

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN

Chain A:  70% 20% 7%



4.2.31 Score per residue for model 31

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN

Chain A:  70% 18% 5% 7%



4.2.32 Score per residue for model 32

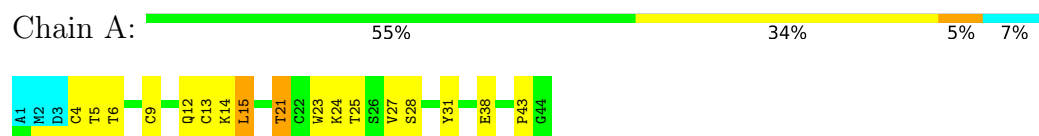
- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN

Chain A:  61% 27% 5% 7%



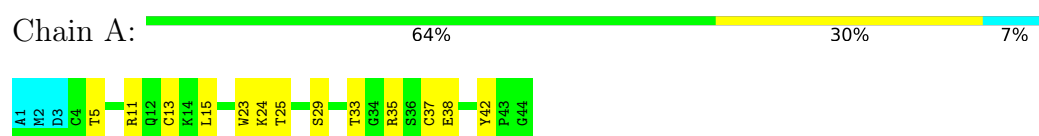
4.2.33 Score per residue for model 33

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



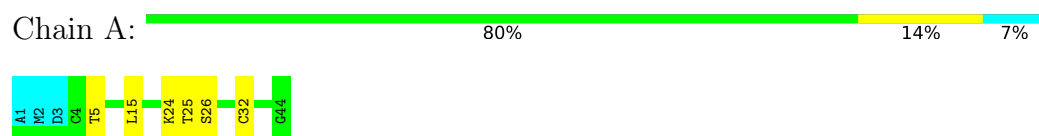
4.2.34 Score per residue for model 34

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



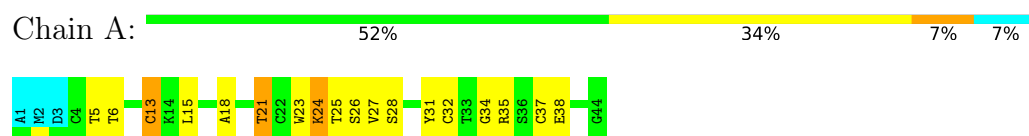
4.2.35 Score per residue for model 35

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



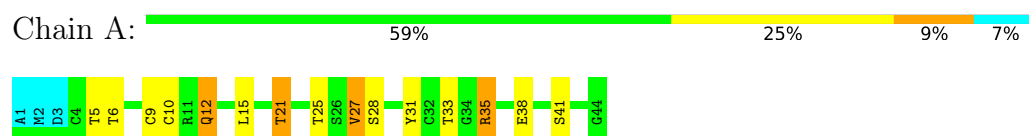
4.2.36 Score per residue for model 36

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



4.2.37 Score per residue for model 37

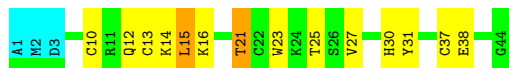
- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



4.2.38 Score per residue for model 38

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN

Chain A:  61% 27% 5% 7%



4.2.39 Score per residue for model 39

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN

Chain A:  64% 25% 5% 7%



4.2.40 Score per residue for model 40

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN

Chain A:  70% 16% 7% 7%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *CNS*.

Of the 50 calculated structures, 40 were deposited, based on the following criterion: *LOWEST TOTAL ENERGY*.

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

Software name	Classification	Version
CNS	refinement	
Sparky	structure solution	

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	421
Number of shifts mapped to atoms	421
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	300	279	278	4±2
All	All	12000	11160	11120	163

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:THR:HG23	1:A:31:TYR:CE2	0.85	2.05	33	8
1:A:21:THR:HG23	1:A:31:TYR:CE1	0.81	2.10	16	12
1:A:25:THR:HG22	1:A:28:SER:O	0.75	1.82	29	1
1:A:21:THR:HG23	1:A:31:TYR:CZ	0.71	2.19	28	17
1:A:26:SER:O	1:A:27:VAL:HG13	0.66	1.91	9	2
1:A:15:LEU:HD11	1:A:36:SER:C	0.65	2.16	25	3
1:A:10:CYS:SG	1:A:15:LEU:HD22	0.64	2.32	22	2
1:A:15:LEU:HD12	1:A:34:GLY:HA2	0.64	1.70	32	5
1:A:21:THR:HG23	1:A:31:TYR:CD1	0.63	2.29	39	1
1:A:33:THR:HG23	1:A:35:ARG:HB2	0.62	1.72	25	12
1:A:18:ALA:HB2	1:A:34:GLY:HA3	0.62	1.72	23	9
1:A:15:LEU:N	1:A:15:LEU:HD13	0.61	2.11	33	1
1:A:15:LEU:HD12	1:A:16:LYS:O	0.60	1.97	21	4
1:A:5:THR:HG23	1:A:37:CYS:SG	0.59	2.37	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:LEU:HD11	1:A:35:ARG:C	0.56	2.26	3	1
1:A:25:THR:HG23	1:A:27:VAL:HG22	0.56	1.78	22	1
1:A:23:TRP:CD1	1:A:25:THR:HG1	0.56	2.19	11	1
1:A:23:TRP:CZ2	1:A:25:THR:HG21	0.55	2.37	5	3
1:A:23:TRP:CH2	1:A:25:THR:HG21	0.55	2.37	5	2
1:A:15:LEU:HD11	1:A:36:SER:CA	0.53	2.33	25	2
1:A:15:LEU:O	1:A:15:LEU:HD22	0.52	2.04	33	1
1:A:27:VAL:O	1:A:27:VAL:HG12	0.51	2.06	16	3
1:A:25:THR:HG23	1:A:25:THR:O	0.50	2.07	13	1
1:A:23:TRP:CE2	1:A:25:THR:HG21	0.50	2.41	30	2
1:A:15:LEU:HD13	1:A:16:LYS:N	0.49	2.22	38	1
1:A:25:THR:HG23	1:A:27:VAL:CG2	0.48	2.37	22	1
1:A:5:THR:HG22	1:A:37:CYS:SG	0.48	2.48	17	2
1:A:23:TRP:CE3	1:A:25:THR:HG22	0.47	2.44	10	1
1:A:15:LEU:HD11	1:A:36:SER:O	0.47	2.09	22	1
1:A:15:LEU:HD11	1:A:36:SER:HA	0.47	1.86	27	1
1:A:5:THR:HG22	1:A:37:CYS:HB2	0.47	1.85	24	1
1:A:15:LEU:HD12	1:A:15:LEU:C	0.47	2.35	36	5
1:A:21:THR:HG22	1:A:29:SER:CB	0.46	2.40	10	1
1:A:23:TRP:CE2	1:A:25:THR:HG23	0.45	2.46	18	1
1:A:23:TRP:CZ2	1:A:25:THR:CG2	0.45	3.00	24	1
1:A:23:TRP:CD1	1:A:25:THR:CG2	0.45	3.00	30	1
1:A:23:TRP:CH2	1:A:25:THR:CG2	0.44	3.01	31	2
1:A:21:THR:CG2	1:A:31:TYR:CZ	0.44	3.00	21	3
1:A:23:TRP:CE2	1:A:25:THR:CG2	0.44	3.00	36	1
1:A:23:TRP:CE3	1:A:25:THR:CG2	0.44	3.00	10	2
1:A:42:TYR:O	1:A:42:TYR:CD2	0.44	2.71	2	3
1:A:30:HIS:CD2	1:A:30:HIS:N	0.44	2.85	26	3
1:A:25:THR:O	1:A:27:VAL:HG22	0.43	2.13	9	1
1:A:25:THR:CG2	1:A:27:VAL:HG22	0.43	2.43	22	1
1:A:26:SER:C	1:A:27:VAL:HG22	0.43	2.39	9	1
1:A:27:VAL:HG13	1:A:28:SER:N	0.43	2.28	18	7
1:A:23:TRP:CZ3	1:A:25:THR:CG2	0.43	3.02	10	1
1:A:42:TYR:CD2	1:A:42:TYR:N	0.43	2.86	26	2
1:A:15:LEU:HD23	1:A:16:LYS:O	0.43	2.14	25	1
1:A:27:VAL:HG23	1:A:28:SER:N	0.43	2.29	33	2
1:A:23:TRP:CE3	1:A:30:HIS:CD2	0.42	3.07	10	2
1:A:15:LEU:N	1:A:15:LEU:CD1	0.42	2.82	33	1
1:A:15:LEU:HD13	1:A:15:LEU:H	0.42	1.71	33	1
1:A:21:THR:HG22	1:A:30:HIS:O	0.42	2.15	26	2
1:A:16:LYS:HE3	1:A:20:THR:HG21	0.42	1.91	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:TYR:O	1:A:42:TYR:CD1	0.41	2.73	30	3
1:A:42:TYR:O	1:A:42:TYR:CG	0.41	2.74	17	2
1:A:15:LEU:HD23	1:A:15:LEU:N	0.41	2.31	1	1
1:A:27:VAL:HG12	1:A:27:VAL:O	0.41	2.16	37	1
1:A:30:HIS:CE1	1:A:40:PRO:O	0.40	2.74	4	2
1:A:30:HIS:N	1:A:30:HIS:CD2	0.40	2.89	32	1
1:A:23:TRP:CD1	1:A:25:THR:OG1	0.40	2.74	28	1
1:A:25:THR:CG2	1:A:27:VAL:CG2	0.40	3.00	22	1
1:A:30:HIS:C	1:A:31:TYR:CD1	0.40	3.00	3	1
1:A:30:HIS:C	1:A:31:TYR:CD2	0.40	3.00	12	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	40/44 (91%)	30±2 (76±6%)	7±2 (16±6%)	3±1 (8±4%)	1	14
All	All	1600/1760 (91%)	1216 (76%)	263 (16%)	121 (8%)	1	14

All 14 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	13	CYS	31
1	A	27	VAL	16
1	A	24	LYS	13
1	A	11	ARG	12
1	A	5	THR	10
1	A	40	PRO	8
1	A	4	CYS	7
1	A	9	CYS	6
1	A	12	GLN	6
1	A	43	PRO	5
1	A	38	GLU	4
1	A	31	TYR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	28	SER	1
1	A	29	SER	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	36/38 (95%)	29±2 (80±5%)	7±2 (20±5%)	3	33
All	All	1440/1520 (95%)	1159 (80%)	281 (20%)	3	33

All 27 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	21	THR	30
1	A	15	LEU	27
1	A	6	THR	21
1	A	25	THR	20
1	A	5	THR	19
1	A	32	CYS	17
1	A	23	TRP	14
1	A	13	CYS	14
1	A	28	SER	13
1	A	26	SER	12
1	A	9	CYS	11
1	A	24	LYS	11
1	A	14	LYS	9
1	A	29	SER	9
1	A	12	GLN	9
1	A	11	ARG	7
1	A	37	CYS	7
1	A	35	ARG	5
1	A	36	SER	5
1	A	38	GLU	5
1	A	10	CYS	4
1	A	16	LYS	3
1	A	41	SER	3

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Mol	Chain	Res	Type	Models (Total)
1	A	39	CYS	2
1	A	33	THR	2
1	A	20	THR	1
1	A	27	VAL	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 82% for the well-defined parts and 82% 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	421
Number of shifts mapped to atoms	421
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
$^{13}\text{C}_\alpha$	42	0.42 ± 0.43	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	38	-0.01 ± 0.21	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	39	0.75 ± 0.99	None needed (imprecise)

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 82%, i.e. 394 atoms were assigned a chemical shift out of a possible 481. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	158/201 (79%)	82/82 (100%)	39/82 (48%)	37/37 (100%)
Sidechain	219/242 (90%)	147/157 (94%)	69/75 (92%)	3/10 (30%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	17/38 (45%)	16/18 (89%)	0/17 (0%)	1/3 (33%)
Overall	394/481 (82%)	245/257 (95%)	108/174 (62%)	41/50 (82%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 421 atoms were assigned a chemical shift out of a possible 514. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	168/216 (78%)	87/88 (99%)	42/88 (48%)	39/40 (98%)
Sidechain	236/260 (91%)	159/169 (94%)	74/81 (91%)	3/10 (30%)
Aromatic	17/38 (45%)	16/18 (89%)	0/17 (0%)	1/3 (33%)
Overall	421/514 (82%)	262/275 (95%)	116/186 (62%)	43/53 (81%)

7.1.4 Statistically unusual chemical shifts ⓘ

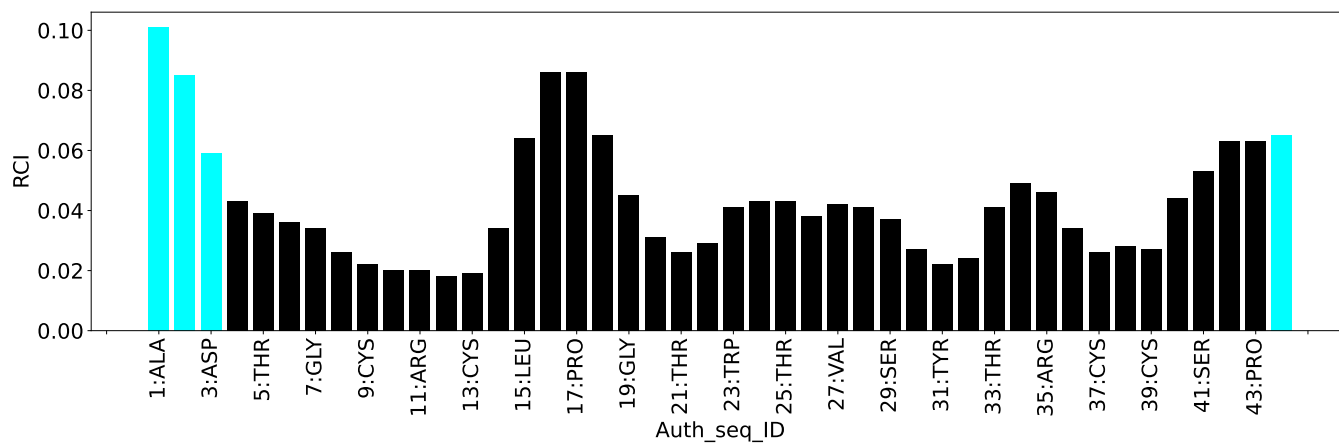
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	35	ARG	NE	109.90	76.53 – 92.65	15.7
1	A	11	ARG	NE	109.20	76.53 – 92.65	15.3

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	518
Intra-residue ($ i-j =0$)	96
Sequential ($ i-j =1$)	174
Medium range ($ i-j >1$ and $ i-j <5$)	72
Long range ($ i-j \geq 5$)	174
Inter-chain	0
Hydrogen bond restraints	2
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	11.8
Number of long range restraints per residue ¹	4.0

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)	1.1	0.2
0.2-0.5 (Medium)	1.2	0.49
>0.5 (Large)	1.4	1.47

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 ⓘ

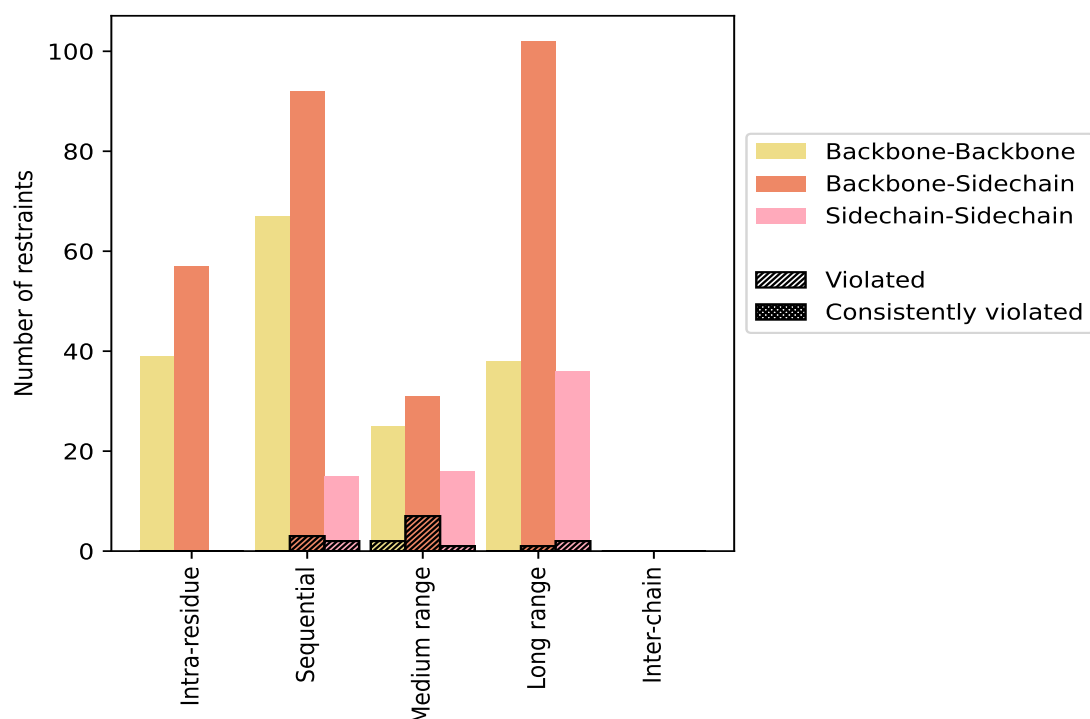
9.1 Summary of distance violations ⓘ

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$)	96	18.5	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	39	7.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	57	11.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ($ i-j =1$)	174	33.6	5	2.9	1.0	0	0.0	0.0
Backbone-Backbone	67	12.9	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	92	17.8	3	3.3	0.6	0	0.0	0.0
Sidechain-Sidechain	15	2.9	2	13.3	0.4	0	0.0	0.0
Medium range ($ i-j >1$ & $ i-j <5$)	72	13.9	10	13.9	1.9	0	0.0	0.0
Backbone-Backbone	25	4.8	2	8.0	0.4	0	0.0	0.0
Backbone-Sidechain	31	6.0	7	22.6	1.4	0	0.0	0.0
Sidechain-Sidechain	16	3.1	1	6.2	0.2	0	0.0	0.0
Long range ($ i-j \geq 5$)	174	33.6	3	1.7	0.6	0	0.0	0.0
Backbone-Backbone	38	7.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	100	19.3	1	1.0	0.2	0	0.0	0.0
Sidechain-Sidechain	36	6.9	2	5.6	0.4	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	2	0.4	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	518	100.0	18	3.5	3.5	0	0.0	0.0
Backbone-Backbone	169	32.6	2	1.2	0.4	0	0.0	0.0
Backbone-Sidechain	282	54.4	11	3.9	2.1	0	0.0	0.0
Sidechain-Sidechain	67	12.9	5	7.5	1.0	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	1	2	1	0	4	0.34	0.55	0.15	0.34
2	0	0	2	1	0	3	0.74	0.9	0.22	0.89
3	0	1	1	2	0	4	0.64	1.27	0.45	0.6
4	0	0	2	0	0	2	0.14	0.15	0.01	0.14
5	0	0	1	0	0	1	0.13	0.13	0.0	0.13
6	0	0	1	1	0	2	0.78	1.31	0.52	0.78
7	0	1	1	4	0	6	0.6	1.26	0.39	0.43
8	0	1	2	1	0	4	0.56	1.08	0.32	0.48
9	0	0	1	2	0	3	0.54	0.75	0.29	0.74
10	0	1	1	1	0	3	0.39	0.81	0.3	0.19

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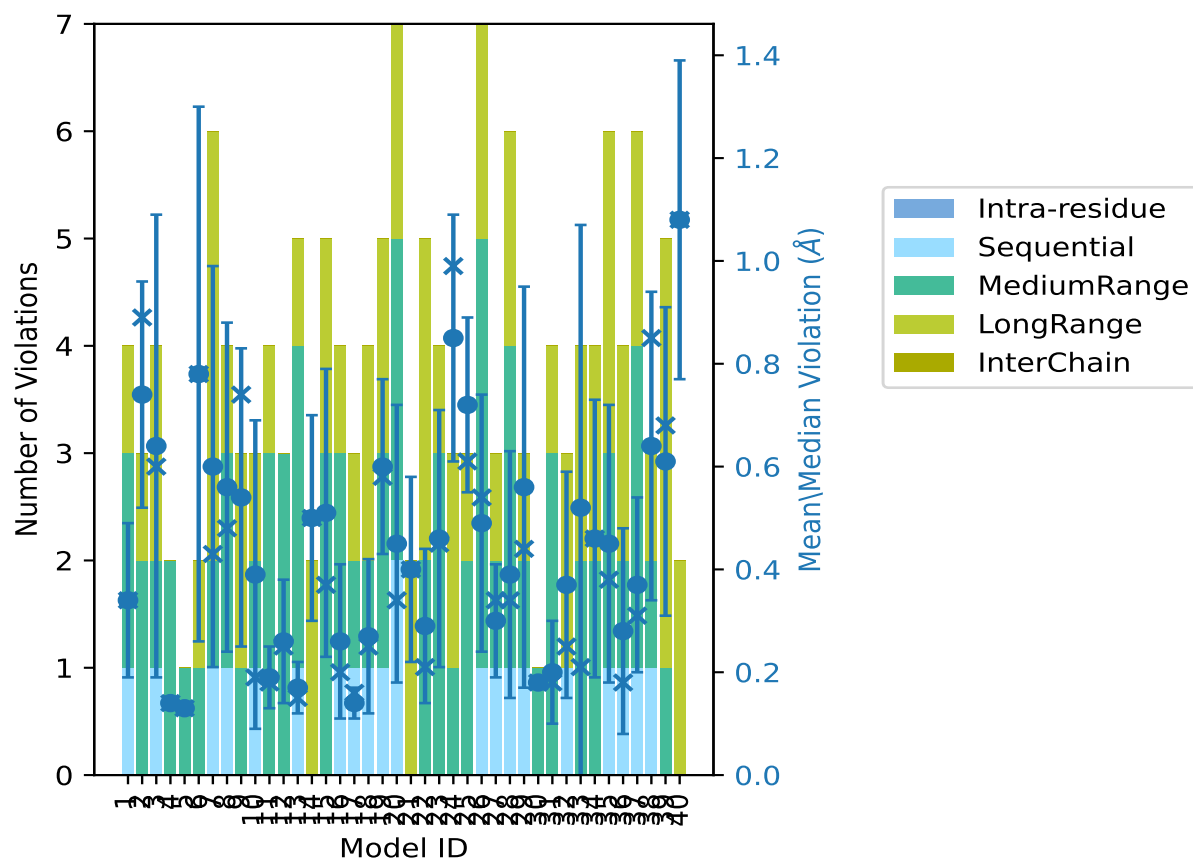
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	0	3	1	0	4	0.19	0.28	0.06	0.18
12	0	0	3	0	0	3	0.26	0.41	0.12	0.25
13	0	1	3	1	0	5	0.17	0.27	0.05	0.15
14	0	0	0	2	0	2	0.5	0.7	0.2	0.5
15	0	0	3	2	0	5	0.51	0.98	0.28	0.37
16	0	1	2	1	0	4	0.26	0.52	0.15	0.2
17	0	1	1	1	0	3	0.14	0.17	0.03	0.16
18	0	1	1	2	0	4	0.27	0.45	0.15	0.25
19	0	1	2	2	0	5	0.6	0.9	0.17	0.58
20	0	2	3	2	0	7	0.45	0.84	0.27	0.34
21	0	0	0	2	0	2	0.4	0.59	0.18	0.4
22	0	0	2	3	0	5	0.29	0.49	0.15	0.21
23	0	0	3	1	0	4	0.46	0.73	0.25	0.45
24	0	0	1	2	0	3	0.85	1.05	0.24	0.99
25	0	0	2	1	0	3	0.72	0.95	0.17	0.61
26	0	1	4	2	0	7	0.49	0.82	0.25	0.54
27	0	1	1	1	0	3	0.3	0.42	0.11	0.34
28	0	1	3	2	0	6	0.39	0.82	0.24	0.34
29	0	1	1	1	0	3	0.56	1.09	0.39	0.44
30	0	0	1	0	0	1	0.18	0.18	0.0	0.18
31	0	0	3	1	0	4	0.2	0.35	0.1	0.18
32	0	1	0	2	0	3	0.37	0.68	0.22	0.25
33	0	0	2	2	0	4	0.52	1.47	0.55	0.21
34	0	0	2	2	0	4	0.46	0.79	0.27	0.46
35	0	1	2	3	0	6	0.45	0.98	0.27	0.38
36	0	1	1	2	0	4	0.28	0.62	0.2	0.18
37	0	1	3	2	0	6	0.37	0.67	0.17	0.31
38	0	1	1	1	0	3	0.64	0.86	0.3	0.85
39	0	0	1	4	0	5	0.61	0.93	0.3	0.68
40	0	0	0	2	0	2	1.08	1.39	0.31	1.08

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, 498(IR:96, SQ:169, MR:62, LR:171, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	1	0	0	1	1	2.5
0	2	1	0	0	3	2	5.0
0	0	1	0	0	1	3	7.5
0	0	2	0	0	2	4	10.0
0	0	1	0	0	1	5	12.5
0	1	1	0	0	2	6	15.0

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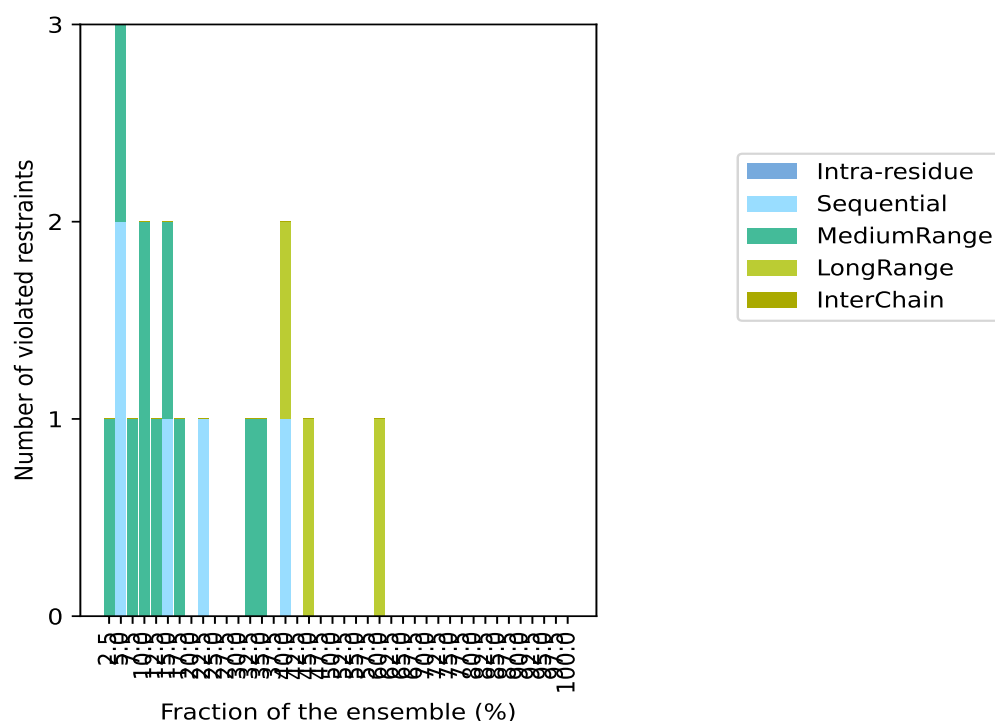
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	1	0	0	1	7	17.5
0	0	0	0	0	0	8	20.0
0	1	0	0	0	1	9	22.5
0	0	0	0	0	0	10	25.0
0	0	0	0	0	0	11	27.5
0	0	0	0	0	0	12	30.0
0	0	1	0	0	1	13	32.5
0	0	1	0	0	1	14	35.0
0	0	0	0	0	0	15	37.5
0	1	0	1	0	2	16	40.0
0	0	0	0	0	0	17	42.5
0	0	0	1	0	1	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	1	0	1	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	0	0	0	0	0	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	0	0	0	0	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	0	0	0	0	0	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

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

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

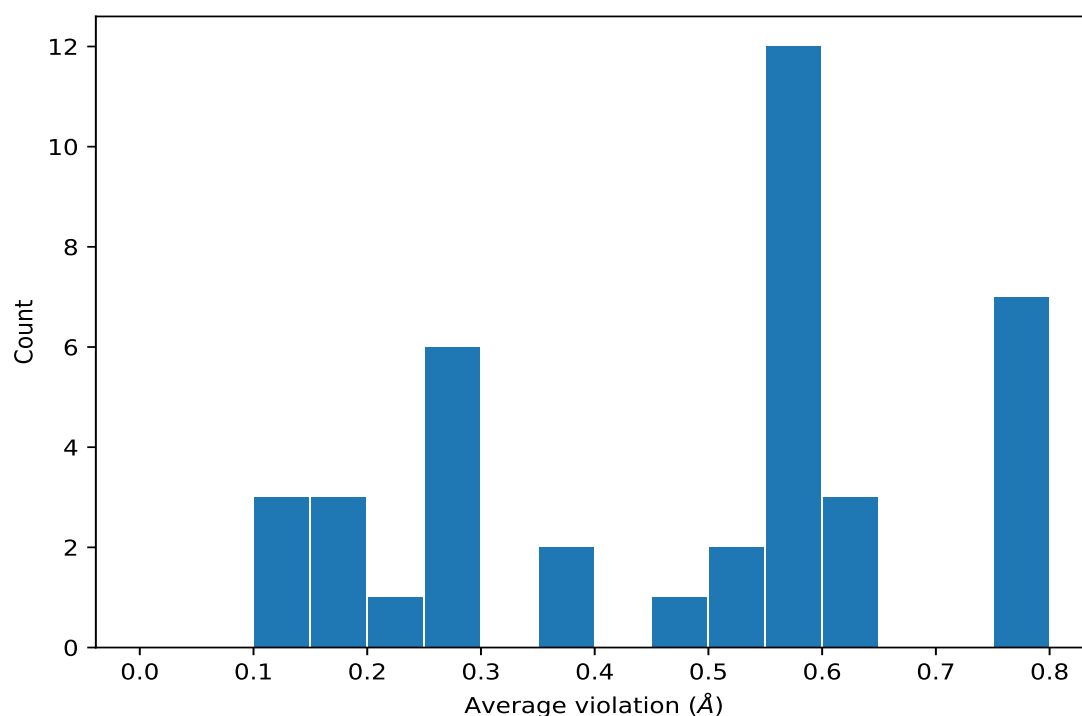
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(2,138)	1:30:A:HIS:HD2	1:27:A:VAL:HG21	24	0.75	0.44	0.82
(2,138)	1:30:A:HIS:HD2	1:27:A:VAL:HG12	24	0.75	0.44	0.82
(2,138)	1:30:A:HIS:HD2	1:27:A:VAL:HG13	24	0.75	0.44	0.82
(2,138)	1:30:A:HIS:HD2	1:25:A:THR:HG22	24	0.75	0.44	0.82
(2,138)	1:30:A:HIS:HD2	1:27:A:VAL:HG22	24	0.75	0.44	0.82
(2,138)	1:30:A:HIS:HD2	1:25:A:THR:HG23	24	0.75	0.44	0.82
(2,138)	1:30:A:HIS:HD2	1:25:A:THR:HG21	24	0.75	0.44	0.82
(1,374)	1:30:A:HIS:HD2	1:43:A:PRO:HB3	18	0.29	0.1	0.29
(1,375)	1:44:A:GLY:HA3	1:31:A:TYR:HE1	16	0.55	0.26	0.56
(1,375)	1:44:A:GLY:HA3	1:42:A:TYR:HE2	16	0.55	0.26	0.56
(1,375)	1:44:A:GLY:HA2	1:31:A:TYR:HE1	16	0.55	0.26	0.56
(1,375)	1:44:A:GLY:HA2	1:31:A:TYR:HE2	16	0.55	0.26	0.56
(1,375)	1:44:A:GLY:HA3	1:31:A:TYR:HE2	16	0.55	0.26	0.56
(1,375)	1:44:A:GLY:HA3	1:42:A:TYR:HE1	16	0.55	0.26	0.56
(2,134)	1:23:A:TRP:HE3	1:39:A:CYS:HB3	16	0.53	0.25	0.5
(2,134)	1:23:A:TRP:HE3	1:39:A:CYS:HB2	16	0.53	0.25	0.5

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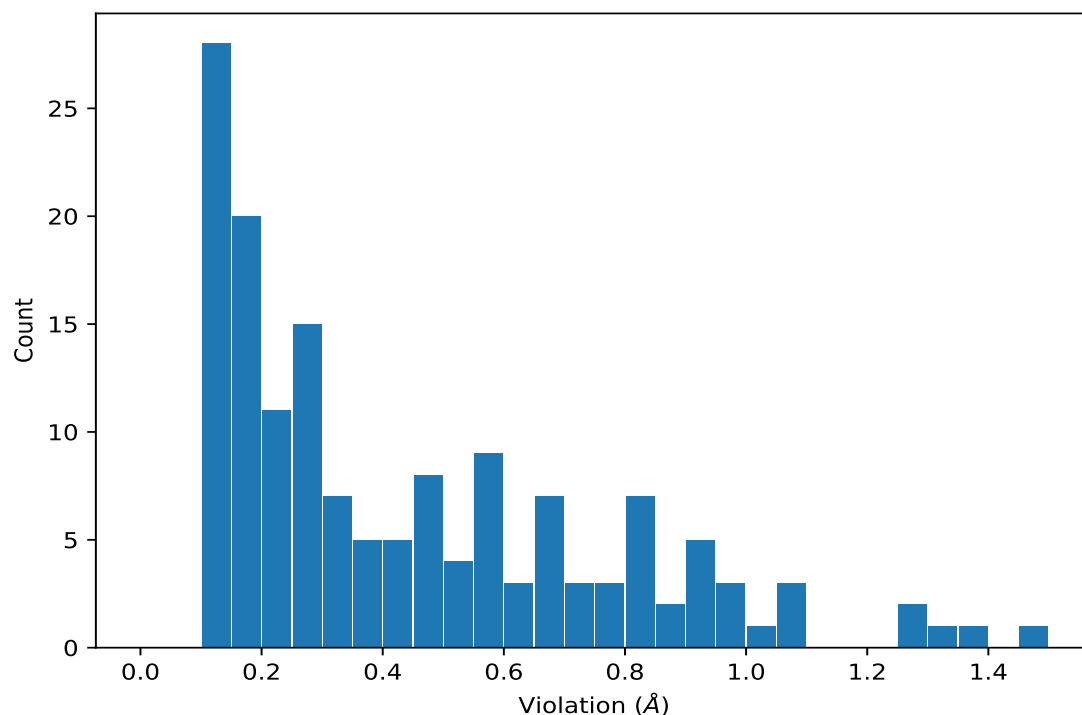
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,141)	1:31:A:TYR:HE1	1:29:A:SER:H	14	0.16	0.09	0.13
(2,141)	1:31:A:TYR:HE2	1:29:A:SER:H	14	0.16	0.09	0.13
(2,131)	1:23:A:TRP:HD1	1:25:A:THR:HA	13	0.37	0.18	0.33
(2,131)	1:23:A:TRP:HD1	1:25:A:THR:HB	13	0.37	0.18	0.33
(1,368)	1:12:A:GLN:HG3	1:11:A:ARG:HG2	9	0.57	0.31	0.57
(1,368)	1:12:A:GLN:HG3	1:11:A:ARG:HG3	9	0.57	0.31	0.57
(1,368)	1:12:A:GLN:HG2	1:11:A:ARG:HG3	9	0.57	0.31	0.57
(2,130)	1:23:A:TRP:HH2	1:25:A:THR:HB	7	0.24	0.18	0.18
(1,369)	1:13:A:CYS:H	1:11:A:ARG:HG3	6	0.59	0.3	0.68
(1,369)	1:13:A:CYS:H	1:14:A:LYS:HG3	6	0.59	0.3	0.68
(1,369)	1:13:A:CYS:H	1:11:A:ARG:HG2	6	0.59	0.3	0.68
(2,139)	1:30:A:HIS:H	1:31:A:TYR:HE1	6	0.3	0.16	0.24
(2,139)	1:30:A:HIS:H	1:31:A:TYR:HE2	6	0.3	0.16	0.24
(1,373)	1:28:A:SER:H	1:25:A:THR:HB	5	0.29	0.1	0.27
(1,373)	1:28:A:SER:H	1:25:A:THR:HA	5	0.29	0.1	0.27
(2,140)	1:31:A:TYR:HD1	1:44:A:GLY:HA3	4	0.61	0.14	0.6
(2,140)	1:31:A:TYR:HD2	1:44:A:GLY:HA2	4	0.61	0.14	0.6
(2,140)	1:31:A:TYR:HD1	1:44:A:GLY:HA2	4	0.61	0.14	0.6
(1,367)	1:11:A:ARG:H	1:14:A:LYS:HB2	4	0.49	0.23	0.5
(2,133)	1:23:A:TRP:HE1	1:25:A:THR:HB	3	0.28	0.1	0.34
(1,371)	1:26:A:SER:HB2	1:25:A:THR:HA	2	0.18	0.02	0.18
(2,137)	1:30:A:HIS:HD2	1:43:A:PRO:HA	2	0.14	0.03	0.14
(1,94)	1:12:A:GLN:HB2	1:13:A:CYS:H	2	0.11	0.01	0.11
(1,94)	1:12:A:GLN:HB3	1:13:A:CYS:H	2	0.11	0.01	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,138)	1:30:A:HIS:HD2	1:27:A:VAL:HG22	33	1.47
(2,138)	1:30:A:HIS:HD2	1:25:A:THR:HG22	40	1.39
(2,138)	1:30:A:HIS:HD2	1:27:A:VAL:HG13	6	1.31
(2,138)	1:30:A:HIS:HD2	1:27:A:VAL:HG13	3	1.27
(2,138)	1:30:A:HIS:HD2	1:25:A:THR:HG22	7	1.26
(1,368)	1:12:A:GLN:HG3	1:11:A:ARG:HG3	29	1.09
(2,138)	1:30:A:HIS:HD2	1:27:A:VAL:HG22	8	1.08
(2,138)	1:30:A:HIS:HD2	1:25:A:THR:HG22	24	1.05
(1,375)	1:44:A:GLY:HA3	1:31:A:TYR:HE2	7	1.02
(1,369)	1:13:A:CYS:H	1:11:A:ARG:HG3	24	0.99
(2,138)	1:30:A:HIS:HD2	1:27:A:VAL:HG12	15	0.98
(2,138)	1:30:A:HIS:HD2	1:25:A:THR:HG22	35	0.98
(2,138)	1:30:A:HIS:HD2	1:27:A:VAL:HG12	25	0.95
(2,138)	1:30:A:HIS:HD2	1:25:A:THR:HG21	39	0.93
(1,375)	1:44:A:GLY:HA3	1:31:A:TYR:HE1	39	0.91
(1,375)	1:44:A:GLY:HA3	1:42:A:TYR:HE2	2	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,368)	1:12:A:GLN:HG3	1:11:A:ARG:HG3	19	0.9
(2,138)	1:30:A:HIS:HD2	1:27:A:VAL:HG12	2	0.89
(2,134)	1:23:A:TRP:HE3	1:39:A:CYS:HB3	38	0.86
(2,134)	1:23:A:TRP:HE3	1:39:A:CYS:HB3	3	0.85
(1,368)	1:12:A:GLN:HG2	1:11:A:ARG:HG3	38	0.85
(2,134)	1:23:A:TRP:HE3	1:39:A:CYS:HB3	20	0.84
(2,140)	1:31:A:TYR:HD1	1:44:A:GLY:HA2	28	0.82
(2,134)	1:23:A:TRP:HE3	1:39:A:CYS:HB3	26	0.82
(1,369)	1:13:A:CYS:H	1:14:A:LYS:HG3	20	0.81
(1,367)	1:11:A:ARG:H	1:14:A:LYS:HB2	10	0.81
(2,134)	1:23:A:TRP:HE3	1:39:A:CYS:HB3	34	0.79
(1,375)	1:44:A:GLY:HA2	1:31:A:TYR:HE1	40	0.77
(1,375)	1:44:A:GLY:HA2	1:31:A:TYR:HE1	9	0.75
(2,138)	1:30:A:HIS:HD2	1:25:A:THR:HG23	9	0.74
(2,138)	1:30:A:HIS:HD2	1:27:A:VAL:HG12	23	0.73
(2,131)	1:23:A:TRP:HD1	1:25:A:THR:HB	26	0.71
(2,134)	1:23:A:TRP:HE3	1:39:A:CYS:HB3	14	0.7
(2,131)	1:23:A:TRP:HD1	1:25:A:THR:HA	15	0.69
(1,369)	1:13:A:CYS:H	1:11:A:ARG:HG2	23	0.69
(2,134)	1:23:A:TRP:HE3	1:39:A:CYS:HB3	32	0.68
(2,130)	1:23:A:TRP:HH2	1:25:A:THR:HB	39	0.68
(2,138)	1:30:A:HIS:HD2	1:25:A:THR:HG22	37	0.67
(1,369)	1:13:A:CYS:H	1:11:A:ARG:HG3	34	0.66
(2,138)	1:30:A:HIS:HD2	1:25:A:THR:HG22	26	0.62
(1,368)	1:12:A:GLN:HG3	1:11:A:ARG:HG3	36	0.62
(2,140)	1:31:A:TYR:HD1	1:44:A:GLY:HA3	25	0.61
(2,138)	1:30:A:HIS:HD2	1:25:A:THR:HG21	19	0.59
(1,375)	1:44:A:GLY:HA2	1:31:A:TYR:HE1	21	0.59
(1,375)	1:44:A:GLY:HA3	1:42:A:TYR:HE2	25	0.59
(2,140)	1:31:A:TYR:HD2	1:44:A:GLY:HA2	19	0.58
(1,368)	1:12:A:GLN:HG3	1:11:A:ARG:HG2	28	0.57
(1,375)	1:44:A:GLY:HA3	1:42:A:TYR:HE2	19	0.56
(1,375)	1:44:A:GLY:HA2	1:31:A:TYR:HE1	35	0.56
(2,131)	1:23:A:TRP:HD1	1:25:A:THR:HB	20	0.55
(1,367)	1:11:A:ARG:H	1:14:A:LYS:HB2	1	0.55
(2,139)	1:30:A:HIS:H	1:31:A:TYR:HE2	26	0.54
(2,134)	1:23:A:TRP:HE3	1:39:A:CYS:HB2	16	0.52
(1,374)	1:30:A:HIS:HD2	1:43:A:PRO:HB3	24	0.52
(1,375)	1:44:A:GLY:HA3	1:31:A:TYR:HE2	37	0.51
(2,139)	1:30:A:HIS:H	1:31:A:TYR:HE2	8	0.49
(2,134)	1:23:A:TRP:HE3	1:39:A:CYS:HB3	22	0.49
(2,141)	1:31:A:TYR:HE1	1:29:A:SER:H	26	0.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,134)	1:23:A:TRP:HE3	1:39:A:CYS:HB3	7	0.46
(1,374)	1:30:A:HIS:HD2	1:43:A:PRO:HB3	8	0.46
(1,368)	1:12:A:GLN:HG3	1:11:A:ARG:HG2	35	0.46
(1,373)	1:28:A:SER:H	1:25:A:THR:HA	22	0.45
(1,367)	1:11:A:ARG:H	1:14:A:LYS:HB2	18	0.45
(1,375)	1:44:A:GLY:HA2	1:31:A:TYR:HE1	29	0.44
(2,140)	1:31:A:TYR:HD1	1:44:A:GLY:HA3	2	0.43
(2,134)	1:23:A:TRP:HE3	1:39:A:CYS:HB2	27	0.42
(2,131)	1:23:A:TRP:HD1	1:25:A:THR:HB	12	0.41
(1,375)	1:44:A:GLY:HA3	1:42:A:TYR:HE1	28	0.41
(2,131)	1:23:A:TRP:HD1	1:25:A:THR:HA	7	0.39
(2,131)	1:23:A:TRP:HD1	1:25:A:THR:HA	19	0.38
(2,133)	1:23:A:TRP:HE1	1:25:A:THR:HB	15	0.37
(1,374)	1:30:A:HIS:HD2	1:43:A:PRO:HB3	18	0.37
(1,368)	1:12:A:GLN:HG3	1:11:A:ARG:HG2	1	0.36
(1,374)	1:30:A:HIS:HD2	1:43:A:PRO:HB3	3	0.35
(1,374)	1:30:A:HIS:HD2	1:43:A:PRO:HB3	31	0.35
(1,374)	1:30:A:HIS:HD2	1:43:A:PRO:HB3	39	0.35
(2,133)	1:23:A:TRP:HE1	1:25:A:THR:HB	20	0.34
(1,373)	1:28:A:SER:H	1:25:A:THR:HA	27	0.34
(2,131)	1:23:A:TRP:HD1	1:25:A:THR:HA	37	0.33
(1,374)	1:30:A:HIS:HD2	1:43:A:PRO:HB3	1	0.32
(2,134)	1:23:A:TRP:HE3	1:39:A:CYS:HB2	35	0.3
(1,374)	1:30:A:HIS:HD2	1:43:A:PRO:HB3	14	0.3
(1,374)	1:30:A:HIS:HD2	1:43:A:PRO:HB3	15	0.3
(1,369)	1:13:A:CYS:H	1:14:A:LYS:HG3	7	0.3
(2,139)	1:30:A:HIS:H	1:31:A:TYR:HE2	37	0.28
(2,131)	1:23:A:TRP:HD1	1:25:A:THR:HA	35	0.28
(1,375)	1:44:A:GLY:HA3	1:31:A:TYR:HE1	20	0.28
(1,374)	1:30:A:HIS:HD2	1:43:A:PRO:HB3	11	0.28
(2,138)	1:30:A:HIS:HD2	1:27:A:VAL:HG12	28	0.27
(1,374)	1:30:A:HIS:HD2	1:43:A:PRO:HB3	34	0.27
(1,373)	1:28:A:SER:H	1:25:A:THR:HB	13	0.27
(1,374)	1:30:A:HIS:HD2	1:43:A:PRO:HB3	6	0.26
(1,372)	1:27:A:VAL:H	1:25:A:THR:HA	37	0.26
(1,375)	1:44:A:GLY:HA3	1:31:A:TYR:HE1	32	0.25
(1,373)	1:28:A:SER:H	1:25:A:THR:HB	12	0.25
(2,131)	1:23:A:TRP:HD1	1:25:A:THR:HA	33	0.24
(2,134)	1:23:A:TRP:HE3	1:39:A:CYS:HB3	15	0.22
(2,134)	1:23:A:TRP:HE3	1:39:A:CYS:HB3	21	0.22
(2,131)	1:23:A:TRP:HD1	1:25:A:THR:HA	31	0.22
(2,131)	1:23:A:TRP:HD1	1:25:A:THR:HA	38	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,130)	1:23:A:TRP:HH2	1:25:A:THR:HB	23	0.22
(2,138)	1:30:A:HIS:HD2	1:27:A:VAL:HG12	20	0.21
(2,130)	1:23:A:TRP:HH2	1:25:A:THR:HB	22	0.21
(2,141)	1:31:A:TYR:HE2	1:29:A:SER:H	8	0.2
(2,131)	1:23:A:TRP:HD1	1:25:A:THR:HB	16	0.2
(1,374)	1:30:A:HIS:HD2	1:43:A:PRO:HB3	7	0.2
(2,139)	1:30:A:HIS:H	1:31:A:TYR:HE1	32	0.19
(2,138)	1:30:A:HIS:HD2	1:27:A:VAL:HG12	11	0.19
(2,134)	1:23:A:TRP:HE3	1:39:A:CYS:HB2	10	0.19
(1,374)	1:30:A:HIS:HD2	1:43:A:PRO:HB3	22	0.19
(1,374)	1:30:A:HIS:HD2	1:43:A:PRO:HB3	23	0.19
(1,374)	1:30:A:HIS:HD2	1:43:A:PRO:HB3	36	0.19
(1,371)	1:26:A:SER:HB2	1:25:A:THR:HA	16	0.19
(2,130)	1:23:A:TRP:HH2	1:25:A:THR:HB	30	0.18
(1,374)	1:30:A:HIS:HD2	1:43:A:PRO:HB3	33	0.18
(2,137)	1:30:A:HIS:HD2	1:43:A:PRO:HA	28	0.17
(2,134)	1:23:A:TRP:HE3	1:39:A:CYS:HB2	39	0.17
(1,375)	1:44:A:GLY:HA3	1:31:A:TYR:HE1	33	0.17
(1,374)	1:30:A:HIS:HD2	1:43:A:PRO:HB3	17	0.17
(1,368)	1:12:A:GLN:HG3	1:11:A:ARG:HG3	10	0.17
(2,141)	1:31:A:TYR:HE2	1:29:A:SER:H	37	0.16
(2,130)	1:23:A:TRP:HH2	1:25:A:THR:HB	11	0.16
(1,375)	1:44:A:GLY:HA2	1:31:A:TYR:HE2	36	0.16
(1,373)	1:28:A:SER:H	1:25:A:THR:HB	29	0.16
(1,371)	1:26:A:SER:HB2	1:25:A:THR:HA	17	0.16
(1,367)	1:11:A:ARG:H	1:14:A:LYS:HB2	13	0.16
(2,139)	1:30:A:HIS:H	1:31:A:TYR:HE1	13	0.15
(2,138)	1:30:A:HIS:HD2	1:27:A:VAL:HG21	4	0.15
(1,368)	1:12:A:GLN:HG2	1:11:A:ARG:HG3	27	0.15
(2,141)	1:31:A:TYR:HE1	1:29:A:SER:H	13	0.14
(2,138)	1:30:A:HIS:HD2	1:25:A:THR:HG23	13	0.14
(2,133)	1:23:A:TRP:HE1	1:25:A:THR:HB	26	0.14
(2,131)	1:23:A:TRP:HD1	1:25:A:THR:HA	36	0.14
(2,130)	1:23:A:TRP:HH2	1:25:A:THR:HB	26	0.14
(2,141)	1:31:A:TYR:HE2	1:29:A:SER:H	4	0.13
(2,141)	1:31:A:TYR:HE2	1:29:A:SER:H	5	0.13
(2,141)	1:31:A:TYR:HE1	1:29:A:SER:H	16	0.13
(2,141)	1:31:A:TYR:HE1	1:29:A:SER:H	31	0.13
(2,141)	1:31:A:TYR:HE1	1:29:A:SER:H	34	0.13
(2,141)	1:31:A:TYR:HE1	1:29:A:SER:H	35	0.13
(2,139)	1:30:A:HIS:H	1:31:A:TYR:HE2	18	0.13
(2,138)	1:30:A:HIS:HD2	1:27:A:VAL:HG21	1	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,141)	1:31:A:TYR:HE2	1:29:A:SER:H	9	0.12
(2,141)	1:31:A:TYR:HE1	1:29:A:SER:H	11	0.12
(2,141)	1:31:A:TYR:HE2	1:29:A:SER:H	12	0.12
(2,138)	1:30:A:HIS:HD2	1:25:A:THR:HG21	18	0.12
(1,94)	1:12:A:GLN:HB2	1:13:A:CYS:H	20	0.12
(1,94)	1:12:A:GLN:HB3	1:13:A:CYS:H	20	0.12
(2,137)	1:30:A:HIS:HD2	1:43:A:PRO:HA	22	0.11
(2,130)	1:23:A:TRP:HH2	1:25:A:THR:HB	28	0.11
(2,141)	1:31:A:TYR:HE2	1:29:A:SER:H	17	0.1
(1,369)	1:13:A:CYS:H	1:11:A:ARG:HG3	31	0.1
(1,94)	1:12:A:GLN:HB2	1:13:A:CYS:H	3	0.1
(1,94)	1:12:A:GLN:HB3	1:13:A:CYS:H	3	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found