



Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 02:51 AM EST

PDB ID : 2W9U
BMRB ID : 16150
Title : Solution structure of jerdostatin mutant R24K from Trimeresurus jerdonii
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 : 4.02b-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

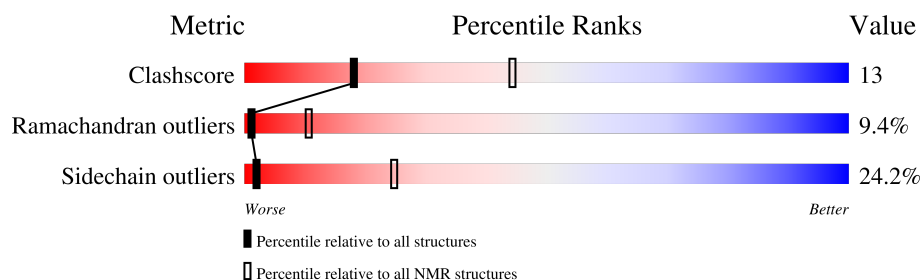
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 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	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	46	

2 Ensemble composition and analysis

This entry contains 42 models. Model 24 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:6-A:43 (38)	0.75	24

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 6 clusters and 4 single-model clusters were found.

Cluster number	Models
1	1, 3, 5, 10, 15, 20, 24, 25, 26, 27, 28, 29, 31, 32, 34, 36, 37, 39
2	9, 12, 16, 17, 19, 21, 30, 33, 35, 42
3	2, 4, 11, 13
4	22, 38
5	8, 41
6	7, 18
Single-model clusters	6; 14; 23; 40

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 641 atoms, of which 308 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SHORT DISINTEGRIN JERDOSTATIN.

Mol	Chain	Residues	Atoms							Trace
1	A	46	Total	C	H	N	O	S		0
			641	198	308	60	66	9		

There is a discrepancy between the modelled and reference sequences:

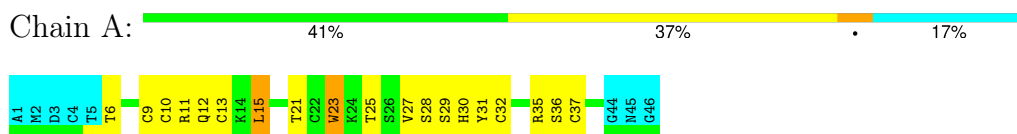
Chain	Residue	Modelled	Actual	Comment	Reference
A	24	LYS	ARG	engineered mutation	UNP Q7ZZM2

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

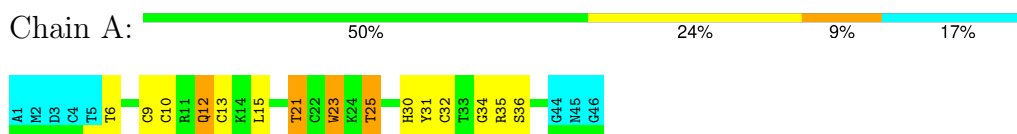


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

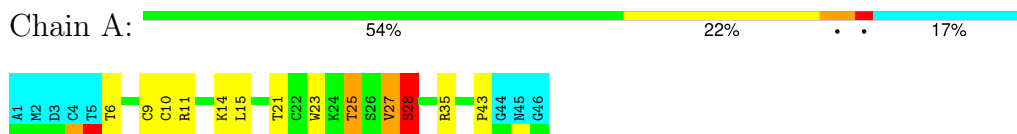
4.2.1 Score per residue for model 1

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



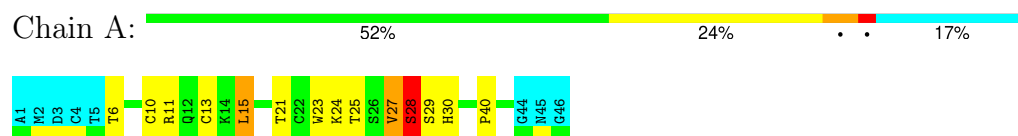
4.2.2 Score per residue for model 2

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



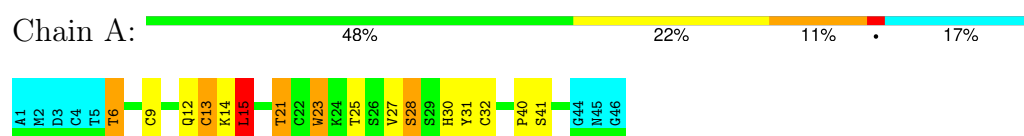
4.2.3 Score per residue for model 3

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



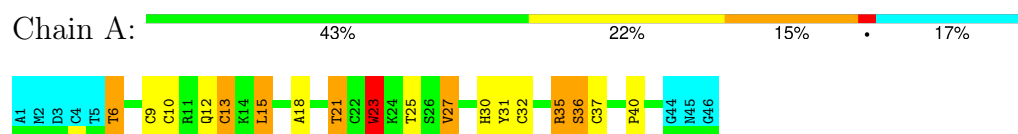
4.2.4 Score per residue for model 4

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



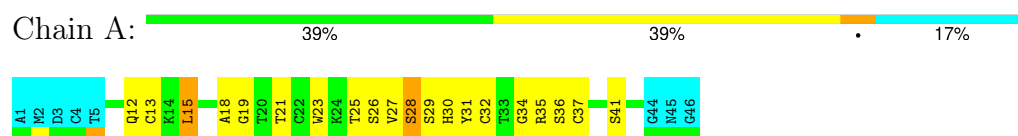
4.2.5 Score per residue for model 5

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



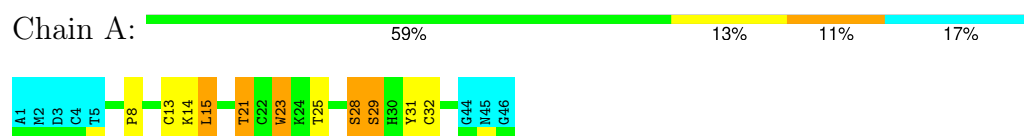
4.2.6 Score per residue for model 6

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



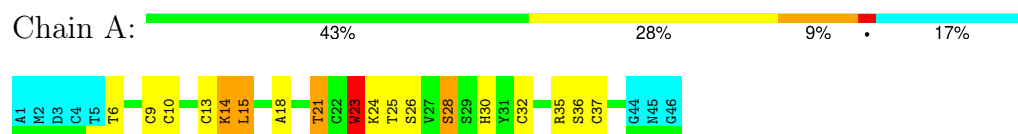
4.2.7 Score per residue for model 7

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



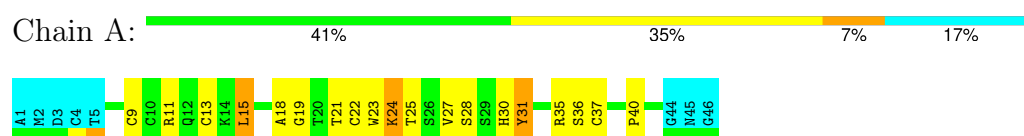
4.2.8 Score per residue for model 8

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



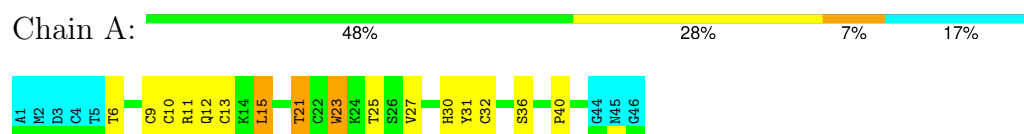
4.2.9 Score per residue for model 9

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



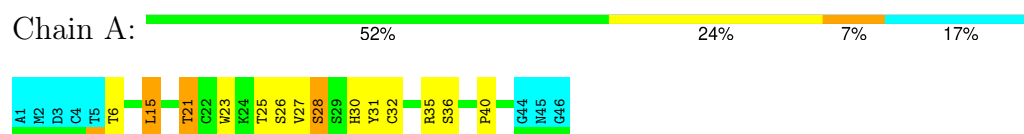
4.2.10 Score per residue for model 10

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



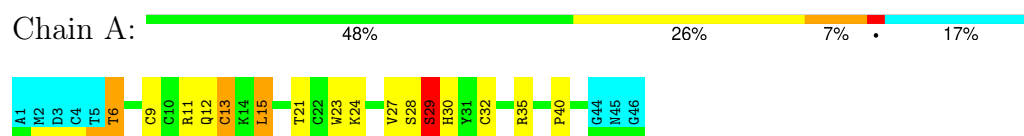
4.2.11 Score per residue for model 11

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



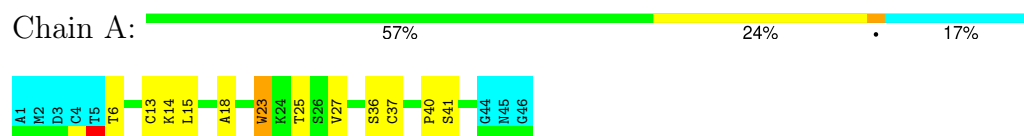
4.2.12 Score per residue for model 12

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



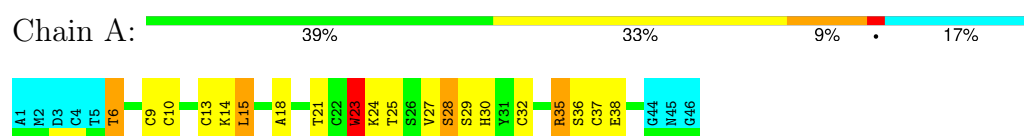
4.2.13 Score per residue for model 13

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



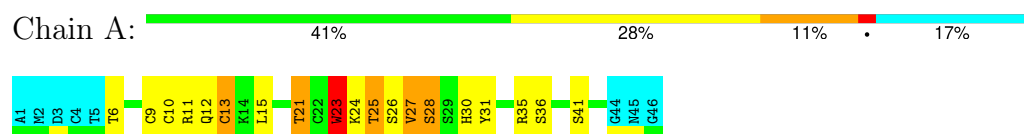
4.2.14 Score per residue for model 14

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



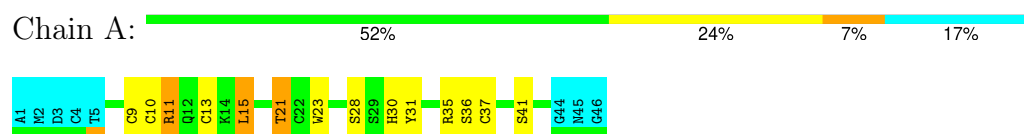
4.2.15 Score per residue for model 15

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



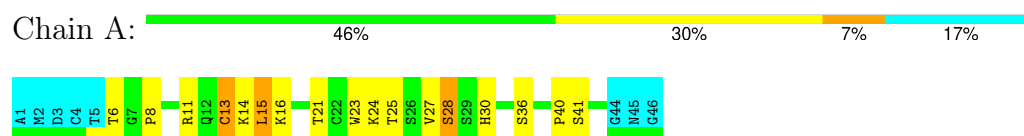
4.2.16 Score per residue for model 16

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



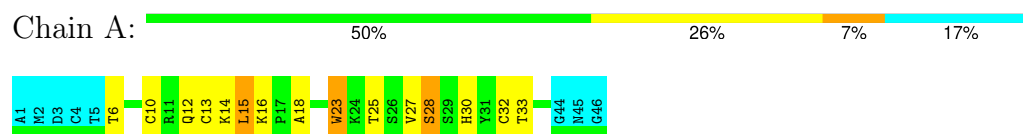
4.2.17 Score per residue for model 17

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



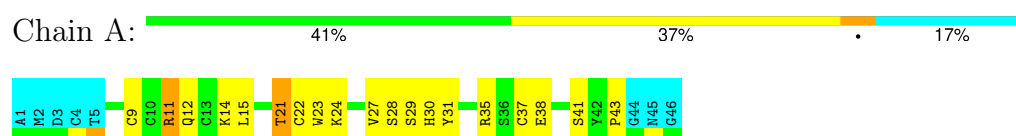
4.2.18 Score per residue for model 18

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



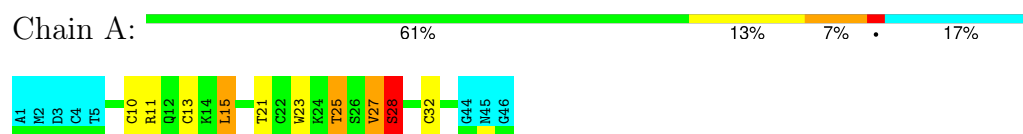
4.2.19 Score per residue for model 19

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



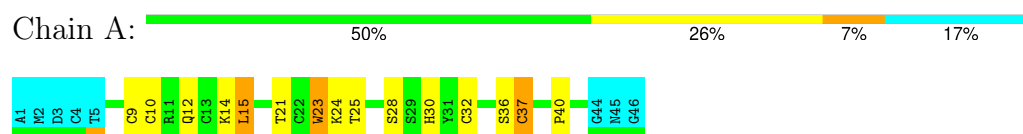
4.2.20 Score per residue for model 20

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



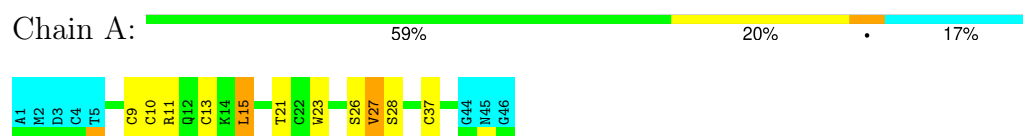
4.2.21 Score per residue for model 21

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



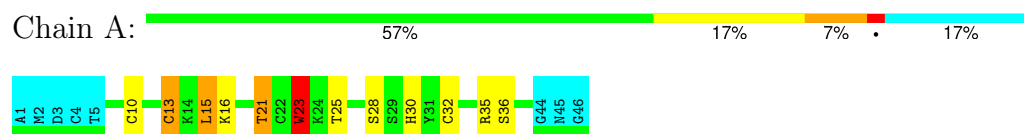
4.2.22 Score per residue for model 22

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



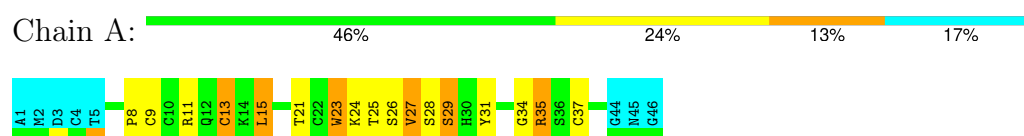
4.2.23 Score per residue for model 23

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



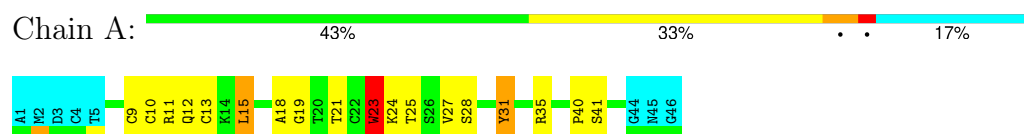
4.2.24 Score per residue for model 24 (medoid)

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



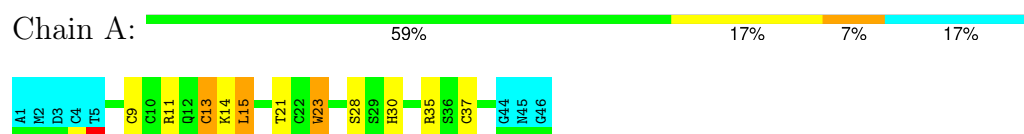
4.2.25 Score per residue for model 25

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



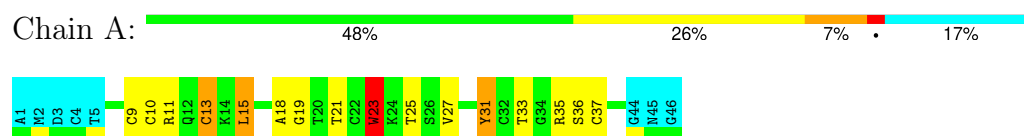
4.2.26 Score per residue for model 26

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



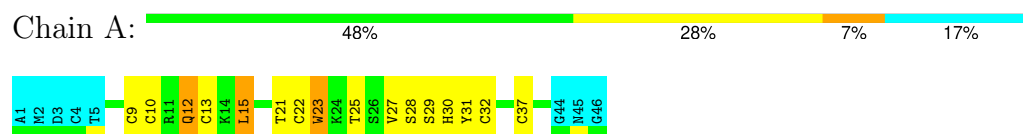
4.2.27 Score per residue for model 27

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



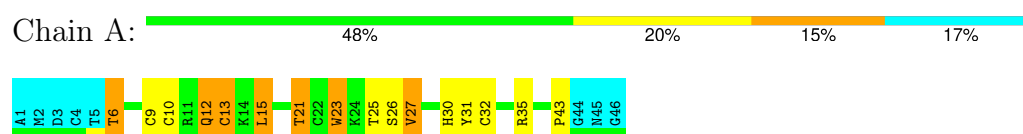
4.2.28 Score per residue for model 28

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



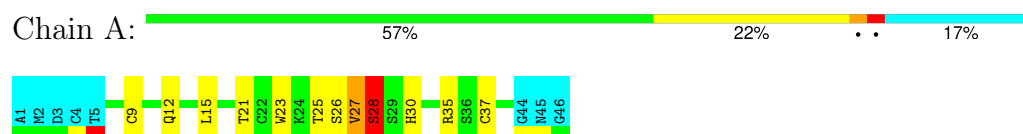
4.2.29 Score per residue for model 29

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



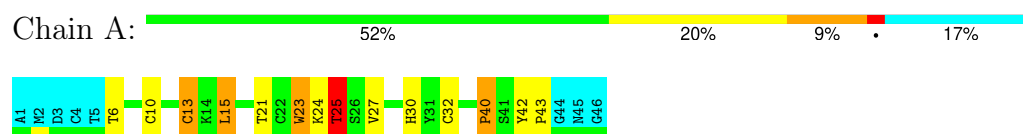
4.2.30 Score per residue for model 30

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



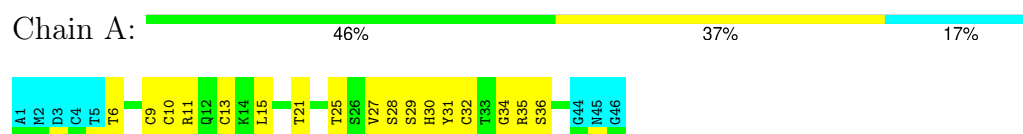
4.2.31 Score per residue for model 31

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



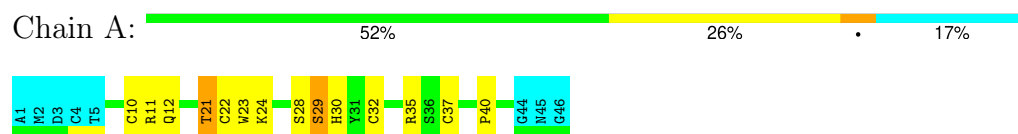
4.2.32 Score per residue for model 32

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



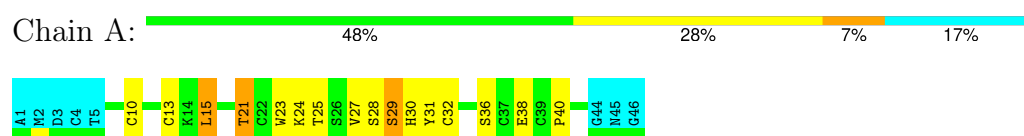
4.2.33 Score per residue for model 33

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



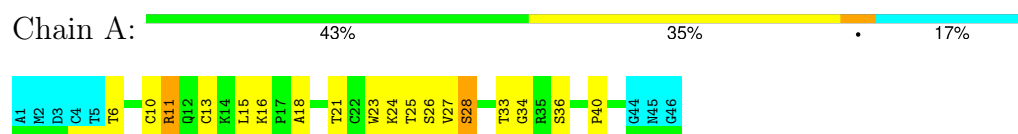
4.2.34 Score per residue for model 34

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



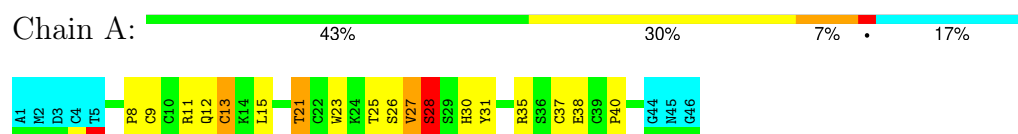
4.2.35 Score per residue for model 35

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



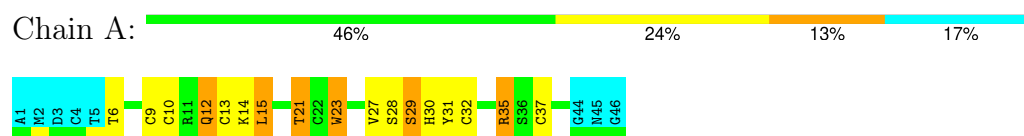
4.2.36 Score per residue for model 36

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



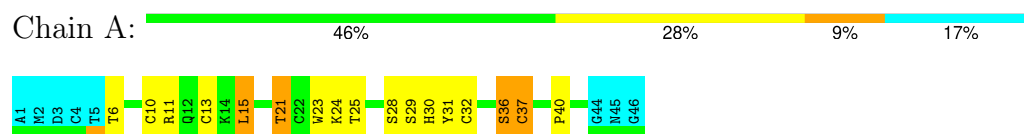
4.2.37 Score per residue for model 37

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



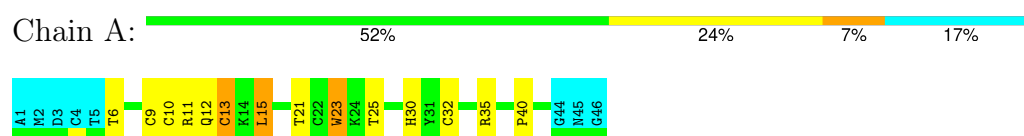
4.2.38 Score per residue for model 38

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



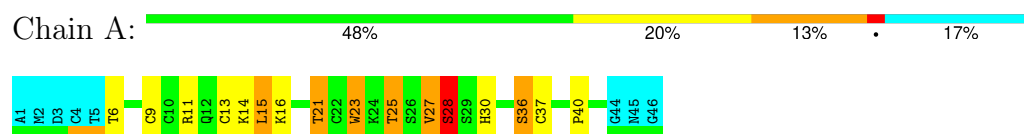
4.2.39 Score per residue for model 39

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



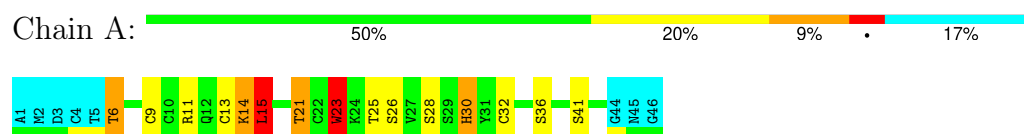
4.2.40 Score per residue for model 40

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



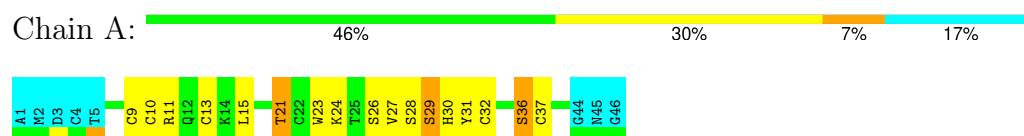
4.2.41 Score per residue for model 41

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



4.2.42 Score per residue for model 42

- Molecule 1: SHORT DISINTEGRIN JERDOSTATIN



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 42 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	437
Number of shifts mapped to atoms	437
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	282	265	264	7±2
All	All	11844	11130	11088	298

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 13.

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	0.87	2.04	38	8
1:A:25:THR:HG22	1:A:28:SER:O	0.82	1.75	36	8
1:A:15:LEU:HD13	1:A:36:SER:N	0.81	1.91	5	2
1:A:15:LEU:HD11	1:A:36:SER:N	0.77	1.95	15	4
1:A:15:LEU:HD11	1:A:36:SER:HA	0.76	1.55	23	3
1:A:21:THR:HG23	1:A:31:TYR:CE1	0.75	2.17	34	5
1:A:15:LEU:HD11	1:A:36:SER:O	0.74	1.81	38	2
1:A:15:LEU:HD11	1:A:35:ARG:C	0.74	2.02	1	3
1:A:15:LEU:HD21	1:A:36:SER:C	0.69	2.07	13	2
1:A:15:LEU:HD23	1:A:37:CYS:SG	0.69	2.28	14	3
1:A:15:LEU:HD21	1:A:36:SER:N	0.69	2.03	16	4
1:A:15:LEU:HD21	1:A:36:SER:HA	0.69	1.63	41	3
1:A:15:LEU:O	1:A:15:LEU:HD13	0.68	1.88	17	1
1:A:15:LEU:HD22	1:A:35:ARG:O	0.67	1.89	24	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:LEU:HD12	1:A:37:CYS:SG	0.66	2.31	27	1
1:A:15:LEU:HD12	1:A:16:LYS:O	0.63	1.93	35	1
1:A:25:THR:HG23	1:A:28:SER:H	0.62	1.52	15	6
1:A:15:LEU:HD21	1:A:35:ARG:C	0.62	2.15	19	2
1:A:15:LEU:HD13	1:A:35:ARG:C	0.61	2.16	37	7
1:A:15:LEU:HD13	1:A:15:LEU:H	0.61	1.54	6	12
1:A:15:LEU:HD21	1:A:36:SER:CA	0.60	2.27	27	4
1:A:15:LEU:N	1:A:15:LEU:HD13	0.59	2.12	22	1
1:A:21:THR:HG21	1:A:24:LYS:HD3	0.57	1.76	9	3
1:A:15:LEU:C	1:A:15:LEU:HD22	0.57	2.20	17	1
1:A:21:THR:O	1:A:21:THR:HG23	0.57	2.00	33	4
1:A:15:LEU:HD21	1:A:37:CYS:N	0.57	2.15	38	1
1:A:27:VAL:O	1:A:27:VAL:HG22	0.56	1.99	14	5
1:A:15:LEU:HD13	1:A:35:ARG:N	0.55	2.16	24	1
1:A:25:THR:HG23	1:A:27:VAL:H	0.55	1.61	36	2
1:A:15:LEU:HD22	1:A:35:ARG:C	0.55	2.22	9	2
1:A:15:LEU:HD22	1:A:36:SER:HA	0.54	1.80	35	3
1:A:26:SER:O	1:A:27:VAL:HG13	0.54	2.03	36	1
1:A:30:HIS:CD2	1:A:30:HIS:N	0.53	2.76	41	28
1:A:21:THR:HA	1:A:31:TYR:HA	0.53	1.79	24	6
1:A:15:LEU:HD13	1:A:35:ARG:O	0.53	2.04	37	3
1:A:25:THR:HG22	1:A:27:VAL:HG12	0.53	1.80	25	6
1:A:25:THR:HG23	1:A:28:SER:N	0.52	2.19	17	5
1:A:27:VAL:O	1:A:27:VAL:HG12	0.52	2.04	11	6
1:A:12:GLN:O	1:A:13:CYS:HB2	0.52	2.03	5	1
1:A:15:LEU:HD22	1:A:34:GLY:HA2	0.51	1.81	32	2
1:A:15:LEU:HD21	1:A:36:SER:O	0.51	2.04	13	2
1:A:23:TRP:CE3	1:A:28:SER:HB3	0.51	2.41	41	1
1:A:15:LEU:HD11	1:A:36:SER:CA	0.50	2.33	23	1
1:A:15:LEU:HD22	1:A:15:LEU:N	0.50	2.21	6	11
1:A:21:THR:HG22	1:A:30:HIS:O	0.50	2.06	40	4
1:A:14:LYS:O	1:A:15:LEU:C	0.50	2.49	4	1
1:A:25:THR:HG22	1:A:25:THR:O	0.50	2.05	7	2
1:A:21:THR:HG23	1:A:31:TYR:CZ	0.50	2.41	1	4
1:A:21:THR:HG23	1:A:31:TYR:HE2	0.48	1.61	4	1
1:A:15:LEU:HD22	1:A:36:SER:N	0.48	2.23	9	2
1:A:15:LEU:HD22	1:A:36:SER:C	0.48	2.28	14	1
1:A:14:LYS:O	1:A:15:LEU:O	0.48	2.31	14	3
1:A:15:LEU:HD13	1:A:34:GLY:C	0.48	2.29	24	1
1:A:15:LEU:HD13	1:A:15:LEU:N	0.48	2.24	4	1
1:A:15:LEU:HD22	1:A:16:LYS:O	0.47	2.10	17	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:THR:HG21	1:A:24:LYS:HG3	0.47	1.87	33	1
1:A:15:LEU:O	1:A:15:LEU:CD2	0.46	2.63	18	10
1:A:23:TRP:CZ3	1:A:28:SER:HB3	0.46	2.45	41	1
1:A:23:TRP:CZ3	1:A:28:SER:HB2	0.46	2.45	8	2
1:A:15:LEU:HD11	1:A:34:GLY:C	0.46	2.31	35	1
1:A:40:PRO:CB	1:A:42:TYR:CE2	0.46	2.99	31	1
1:A:23:TRP:CD1	1:A:25:THR:OG1	0.45	2.69	27	10
1:A:15:LEU:HD11	1:A:36:SER:C	0.45	2.32	41	1
1:A:25:THR:HG22	1:A:27:VAL:H	0.45	1.71	14	1
1:A:21:THR:N	1:A:31:TYR:CD1	0.45	2.85	32	1
1:A:27:VAL:HG13	1:A:28:SER:N	0.45	2.25	17	4
1:A:11:ARG:O	1:A:12:GLN:CB	0.44	2.65	15	1
1:A:21:THR:N	1:A:31:TYR:CE1	0.44	2.85	1	1
1:A:29:SER:C	1:A:30:HIS:CD2	0.44	2.91	33	10
1:A:22:CYS:N	1:A:30:HIS:O	0.44	2.51	19	3
1:A:25:THR:CG2	1:A:27:VAL:HG12	0.44	2.43	14	2
1:A:18:ALA:HB2	1:A:33:THR:C	0.44	2.33	35	3
1:A:15:LEU:HD22	1:A:36:SER:CA	0.44	2.43	42	2
1:A:23:TRP:O	1:A:25:THR:N	0.43	2.51	4	1
1:A:21:THR:N	1:A:31:TYR:CE2	0.43	2.86	10	1
1:A:26:SER:O	1:A:27:VAL:HB	0.43	2.14	24	4
1:A:15:LEU:O	1:A:15:LEU:HD23	0.43	2.13	18	2
1:A:23:TRP:CE3	1:A:30:HIS:NE2	0.43	2.87	41	1
1:A:18:ALA:HB2	1:A:34:GLY:N	0.43	2.29	6	1
1:A:25:THR:HG22	1:A:28:SER:C	0.43	2.34	40	4
1:A:25:THR:CG2	1:A:28:SER:CB	0.43	2.97	4	3
1:A:25:THR:HG22	1:A:28:SER:HB3	0.43	1.89	11	2
1:A:23:TRP:CE3	1:A:30:HIS:CD2	0.42	3.06	28	2
1:A:12:GLN:O	1:A:13:CYS:CB	0.42	2.68	39	2
1:A:21:THR:N	1:A:31:TYR:CD2	0.42	2.88	24	2
1:A:9:CYS:O	1:A:9:CYS:SG	0.42	2.77	15	1
1:A:9:CYS:HB3	1:A:37:CYS:HA	0.42	1.92	21	1
1:A:23:TRP:O	1:A:24:LYS:CG	0.41	2.67	38	3
1:A:24:LYS:HA	1:A:29:SER:HA	0.41	1.92	34	1
1:A:27:VAL:CG1	1:A:28:SER:N	0.41	2.83	18	2
1:A:28:SER:O	1:A:29:SER:O	0.41	2.38	7	1
1:A:21:THR:HG23	1:A:31:TYR:CD2	0.41	2.49	42	1
1:A:19:GLY:O	1:A:31:TYR:CE1	0.41	2.74	9	3
1:A:15:LEU:CD2	1:A:36:SER:CA	0.41	2.99	9	1
1:A:21:THR:O	1:A:21:THR:CG2	0.41	2.70	33	1
1:A:19:GLY:O	1:A:31:TYR:CD1	0.40	2.74	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:LEU:N	1:A:15:LEU:HD22	0.40	2.32	4	1
1:A:10:CYS:SG	1:A:15:LEU:HD22	0.40	2.56	38	1
1:A:21:THR:HG21	1:A:24:LYS:CD	0.40	2.46	9	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	38/46 (83%)	28±3 (72±7%)	7±2 (18±6%)	4±1 (9±4%)	1	10
All	All	1596/1932 (83%)	1156 (72%)	290 (18%)	150 (9%)	1	10

All 16 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	27
1	A	40	PRO	19
1	A	27	VAL	18
1	A	11	ARG	17
1	A	23	TRP	15
1	A	12	GLN	9
1	A	28	SER	7
1	A	29	SER	7
1	A	18	ALA	6
1	A	25	THR	5
1	A	15	LEU	5
1	A	43	PRO	4
1	A	8	PRO	4
1	A	6	THR	3
1	A	21	THR	3
1	A	35	ARG	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	34/39 (87%)	26±2 (76±5%)	8±2 (24±5%)	2	25
All	All	1428/1638 (87%)	1082 (76%)	346 (24%)	2	25

All 25 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	23	TRP	39
1	A	15	LEU	31
1	A	21	THR	30
1	A	28	SER	28
1	A	9	CYS	26
1	A	32	CYS	25
1	A	10	CYS	24
1	A	6	THR	23
1	A	13	CYS	16
1	A	35	ARG	13
1	A	14	LYS	12
1	A	24	LYS	10
1	A	12	GLN	9
1	A	11	ARG	9
1	A	41	SER	9
1	A	25	THR	8
1	A	36	SER	7
1	A	26	SER	7
1	A	31	TYR	4
1	A	29	SER	4
1	A	38	GLU	4
1	A	37	CYS	3
1	A	16	LYS	3
1	A	22	CYS	1
1	A	30	HIS	1

6.3.3 RNA ⓘ

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 [i](#)

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 [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	437
Number of shifts mapped to atoms	437
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 [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	44	0.40 ± 0.24	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	39	-0.07 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	41	0.65 ± 0.95	None needed (imprecise)

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 82%, i.e. 374 atoms were assigned a chemical shift out of a possible 456. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	145/185 (78%)	75/75 (100%)	36/76 (47%)	34/34 (100%)
Sidechain	212/233 (91%)	143/151 (95%)	66/72 (92%)	3/10 (30%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	17/38 (45%)	16/18 (89%)	0/17 (0%)	1/3 (33%)
Overall	374/456 (82%)	234/244 (96%)	102/165 (62%)	38/47 (81%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 437 atoms were assigned a chemical shift out of a possible 532. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	177/227 (78%)	92/93 (99%)	44/92 (48%)	41/42 (98%)
Sidechain	243/267 (91%)	164/173 (95%)	75/83 (90%)	4/11 (36%)
Aromatic	17/38 (45%)	16/18 (89%)	0/17 (0%)	1/3 (33%)
Overall	437/532 (82%)	272/284 (96%)	119/192 (62%)	46/56 (82%)

7.1.4 Statistically unusual chemical shifts ⓘ

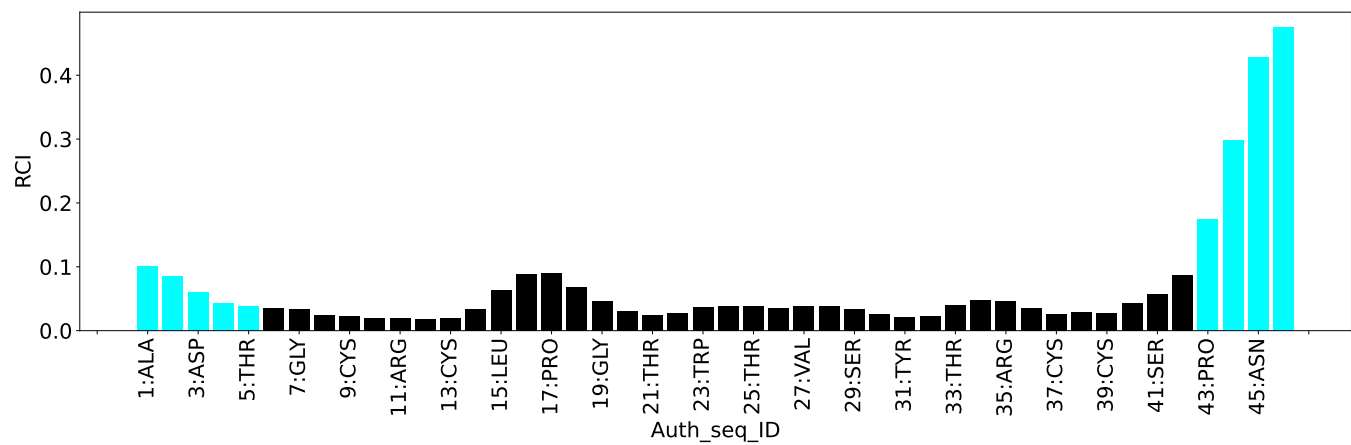
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

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	109.40	76.53 – 92.65	15.4

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 [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	615
Intra-residue ($ i-j =0$)	102
Sequential ($ i-j =1$)	197
Medium range ($ i-j >1$ and $ i-j <5$)	94
Long range ($ i-j \geq 5$)	216
Inter-chain	0
Hydrogen bond restraints	6
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	13.4
Number of long range restraints per residue ¹	4.8

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

8.2 Residual restraint violations [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)	1.7	0.2
0.2-0.5 (Medium)	1.7	0.5
>0.5 (Large)	1.3	1.27

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 ⓘ

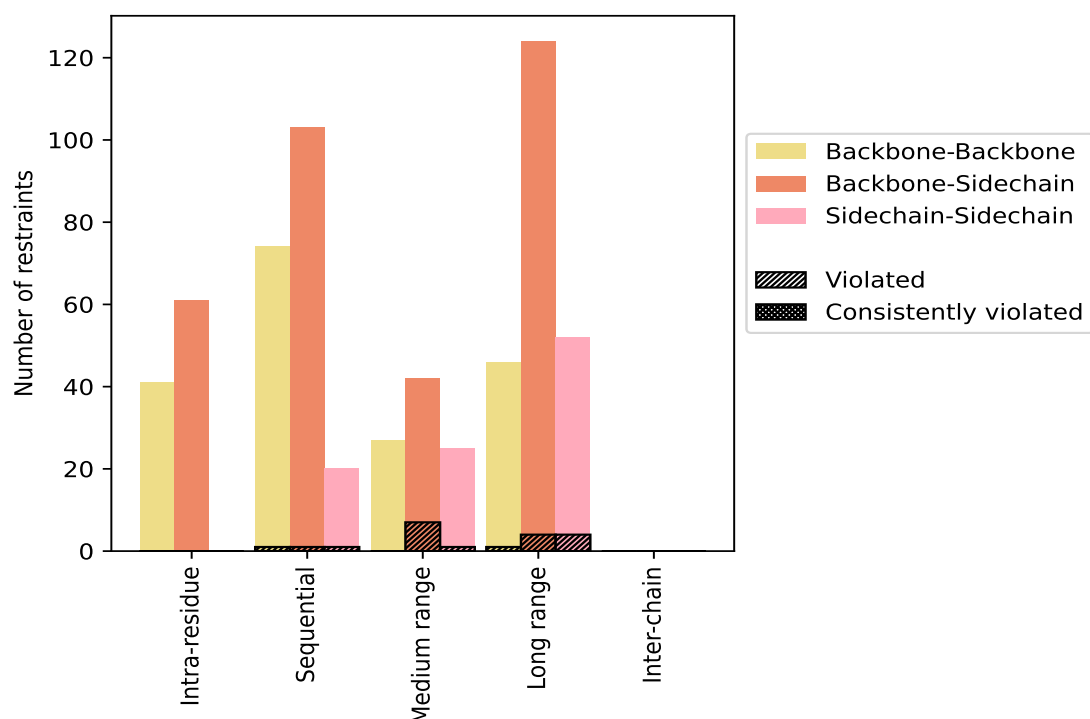
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	102	16.6	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	41	6.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	61	9.9	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 ($i-j =1$)	197	32.0	3	1.5	0.5	0	0.0	0.0
Backbone-Backbone	74	12.0	1	1.4	0.2	0	0.0	0.0
Backbone-Sidechain	103	16.7	1	1.0	0.2	0	0.0	0.0
Sidechain-Sidechain	20	3.3	1	5.0	0.2	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	94	15.3	8	8.5	1.3	0	0.0	0.0
Backbone-Backbone	27	4.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	42	6.8	7	16.7	1.1	0	0.0	0.0
Sidechain-Sidechain	25	4.1	1	4.0	0.2	0	0.0	0.0
Long range ($i-j \geq 5$)	216	35.1	9	4.2	1.5	0	0.0	0.0
Backbone-Backbone	46	7.5	1	2.2	0.2	0	0.0	0.0
Backbone-Sidechain	118	19.2	4	3.4	0.7	0	0.0	0.0
Sidechain-Sidechain	52	8.5	4	7.7	0.7	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	6	1.0	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	615	100.0	20	3.3	3.3	0	0.0	0.0
Backbone-Backbone	188	30.6	2	1.1	0.3	0	0.0	0.0
Backbone-Sidechain	330	53.7	12	3.6	2.0	0	0.0	0.0
Sidechain-Sidechain	97	15.8	6	6.2	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	0	3	2	0	5	0.38	0.6	0.18	0.37
2	0	0	3	3	0	6	0.28	0.58	0.17	0.2
3	0	0	3	3	0	6	0.4	0.71	0.19	0.35
4	0	0	3	3	0	6	0.48	1.19	0.37	0.32
5	0	0	2	3	0	5	0.38	0.79	0.24	0.35
6	0	0	5	2	0	7	0.31	0.5	0.11	0.31
7	0	0	1	3	0	4	0.39	0.73	0.24	0.36
8	0	0	7	1	0	8	0.37	0.73	0.25	0.22
9	0	0	2	2	0	4	0.37	0.6	0.16	0.37
10	0	0	3	1	0	4	0.45	0.67	0.2	0.48

Continued on next page...

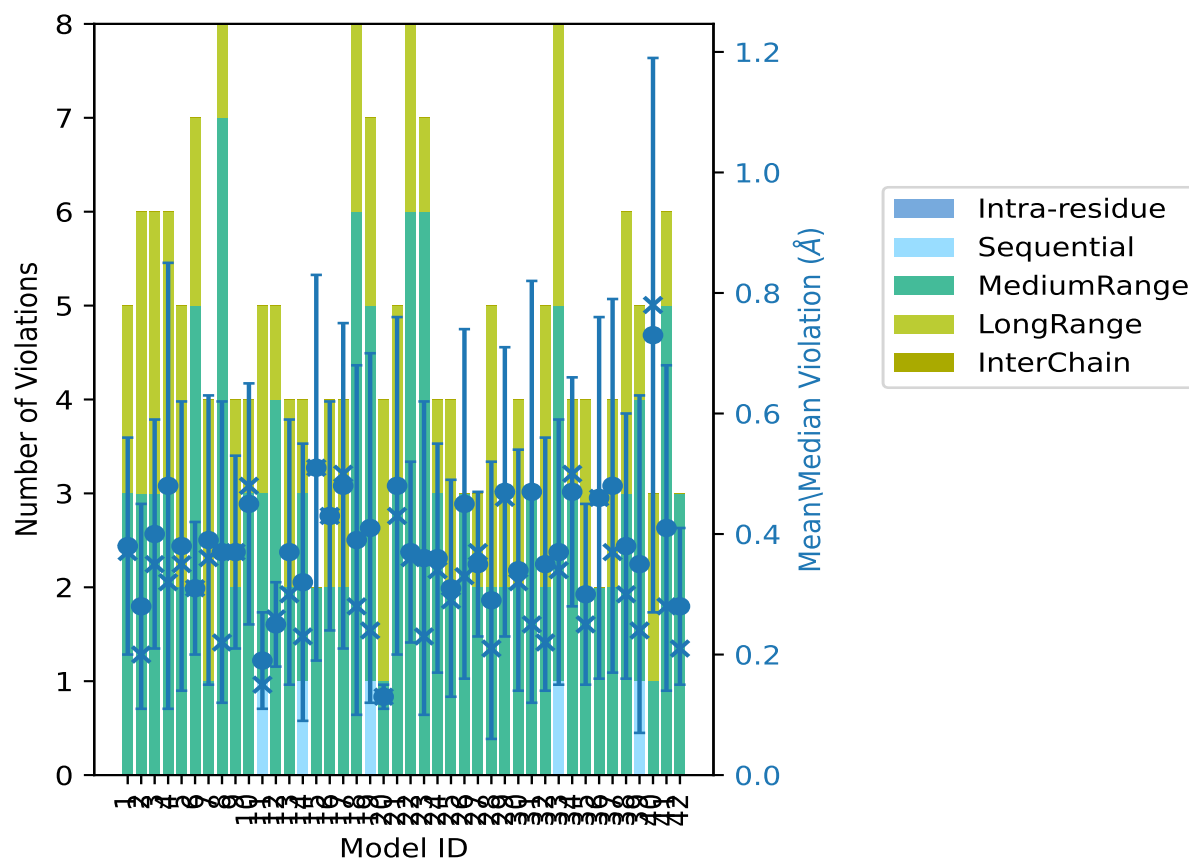
Continued from previous page...

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	1	2	2	0	5	0.19	0.29	0.08	0.15
12	0	0	4	1	0	5	0.25	0.33	0.07	0.26
13	0	0	2	2	0	4	0.37	0.73	0.22	0.3
14	0	1	2	1	0	4	0.32	0.71	0.23	0.23
15	0	0	2	0	0	2	0.51	0.83	0.32	0.51
16	0	0	2	2	0	4	0.43	0.7	0.19	0.43
17	0	0	2	2	0	4	0.48	0.78	0.27	0.5
18	0	0	6	2	0	8	0.39	0.89	0.29	0.28
19	0	1	4	2	0	7	0.41	0.87	0.29	0.24
20	0	0	1	3	0	4	0.13	0.15	0.02	0.13
21	0	0	3	2	0	5	0.48	0.97	0.28	0.43
22	0	0	6	2	0	8	0.37	0.65	0.15	0.36
23	0	0	6	1	0	7	0.36	0.81	0.26	0.23
24	0	0	3	1	0	4	0.36	0.63	0.19	0.34
25	0	0	2	2	0	4	0.31	0.57	0.18	0.29
26	0	0	3	0	0	3	0.45	0.85	0.29	0.33
27	0	0	2	1	0	3	0.35	0.49	0.12	0.37
28	0	0	2	3	0	5	0.29	0.74	0.23	0.21
29	0	0	2	1	0	3	0.47	0.76	0.24	0.46
30	0	0	2	2	0	4	0.34	0.59	0.2	0.32
31	0	0	3	0	0	3	0.47	0.96	0.35	0.25
32	0	0	2	3	0	5	0.35	0.71	0.21	0.22
33	0	1	4	3	0	8	0.37	0.82	0.22	0.34
34	0	0	3	1	0	4	0.47	0.67	0.19	0.5
35	0	0	2	2	0	4	0.3	0.56	0.15	0.25
36	0	0	2	0	0	2	0.46	0.76	0.3	0.46
37	0	0	2	2	0	4	0.48	1.0	0.31	0.37
38	0	0	3	3	0	6	0.38	0.7	0.22	0.3
39	0	1	3	1	0	5	0.35	0.89	0.28	0.24
40	0	0	1	2	0	3	0.73	1.27	0.46	0.78
41	0	0	5	1	0	6	0.41	0.95	0.27	0.28
42	0	0	3	0	0	3	0.28	0.46	0.13	0.21

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, 589(IR:102, SQ:194, MR:86, LR:207, 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	1	1	4	0	6	1	2.4
0	0	0	1	0	1	2	4.8
0	0	0	1	0	1	3	7.1
0	1	1	0	0	2	4	9.5
0	0	0	1	0	1	5	11.9
0	1	2	0	0	3	6	14.3

Continued on next page...

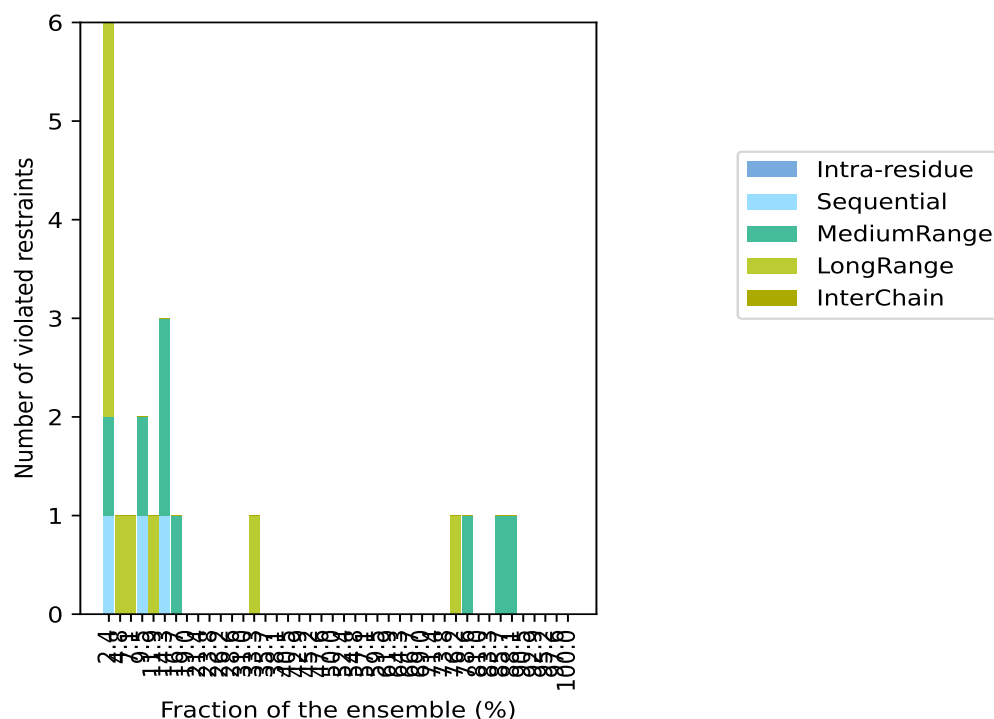
Continued from previous page...

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	16.7
0	0	0	0	0	0	8	19.0
0	0	0	0	0	0	9	21.4
0	0	0	0	0	0	10	23.8
0	0	0	0	0	0	11	26.2
0	0	0	0	0	0	12	28.6
0	0	0	0	0	0	13	31.0
0	0	0	1	0	1	14	33.3
0	0	0	0	0	0	15	35.7
0	0	0	0	0	0	16	38.1
0	0	0	0	0	0	17	40.5
0	0	0	0	0	0	18	42.9
0	0	0	0	0	0	19	45.2
0	0	0	0	0	0	20	47.6
0	0	0	0	0	0	21	50.0
0	0	0	0	0	0	22	52.4
0	0	0	0	0	0	23	54.8
0	0	0	0	0	0	24	57.1
0	0	0	0	0	0	25	59.5
0	0	0	0	0	0	26	61.9
0	0	0	0	0	0	27	64.3
0	0	0	0	0	0	28	66.7
0	0	0	0	0	0	29	69.0
0	0	0	0	0	0	30	71.4
0	0	0	0	0	0	31	73.8
0	0	0	1	0	1	32	76.2
0	0	1	0	0	1	33	78.6
0	0	0	0	0	0	34	81.0
0	0	0	0	0	0	35	83.3
0	0	1	0	0	1	36	85.7
0	0	1	0	0	1	37	88.1
0	0	0	0	0	0	38	90.5
0	0	0	0	0	0	39	92.9
0	0	0	0	0	0	40	95.2
0	0	0	0	0	0	41	97.6
0	0	0	0	0	0	42	100.0

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

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

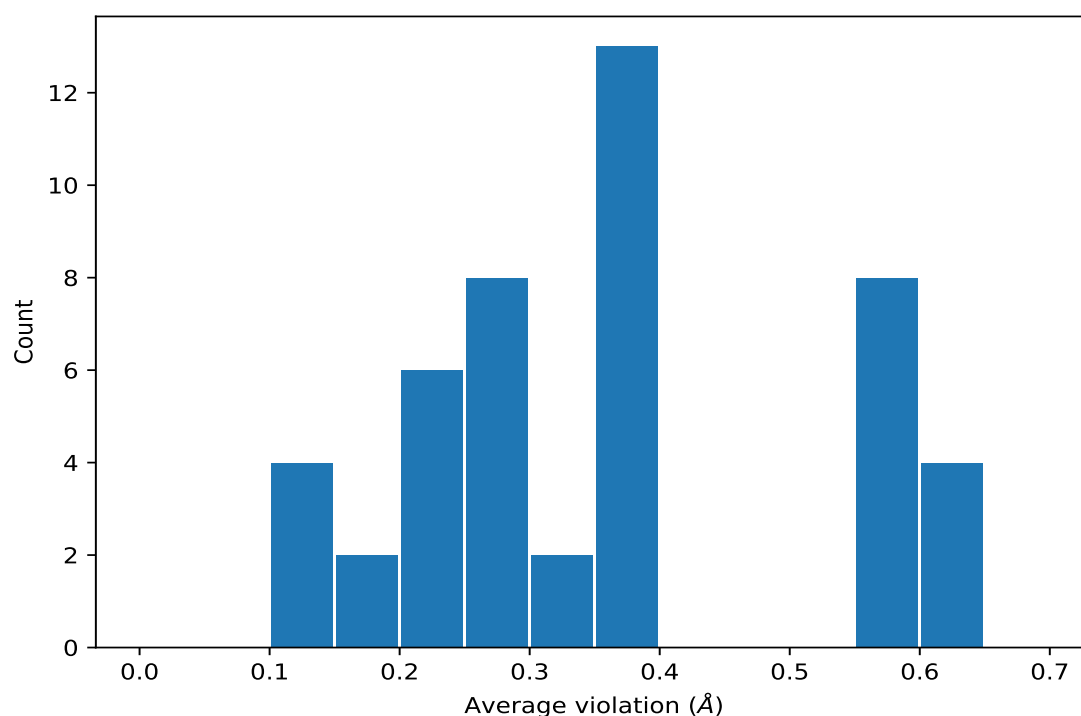
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	37	0.17	0.03	0.16
(2,205)	1:33:A:THR:HG23	1:31:A:TYR:HD1	36	0.57	0.26	0.59
(2,205)	1:33:A:THR:HG23	1:31:A:TYR:HD2	36	0.57	0.26	0.59
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD1	36	0.57	0.26	0.59
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD2	36	0.57	0.26	0.59
(2,205)	1:33:A:THR:HG23	1:42:A:TYR:HD1	36	0.57	0.26	0.59
(2,205)	1:33:A:THR:HG23	1:42:A:TYR:HD2	36	0.57	0.26	0.59
(2,205)	1:33:A:THR:HG22	1:42:A:TYR:HD1	36	0.57	0.26	0.59
(2,205)	1:33:A:THR:HG22	1:42:A:TYR:HD2	36	0.57	0.26	0.59
(2,203)	1:31:A:TYR:HE2	1:45:A:ASN:H	33	0.61	0.23	0.59
(2,203)	1:31:A:TYR:HE1	1:45:A:ASN:H	33	0.61	0.23	0.59
(2,203)	1:31:A:TYR:HE2	1:29:A:SER:H	33	0.61	0.23	0.59
(2,203)	1:31:A:TYR:HE1	1:29:A:SER:H	33	0.61	0.23	0.59
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG11	32	0.37	0.16	0.35
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG12	32	0.37	0.16	0.35
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG13	32	0.37	0.16	0.35

Continued on next page...

Continued from previous page...

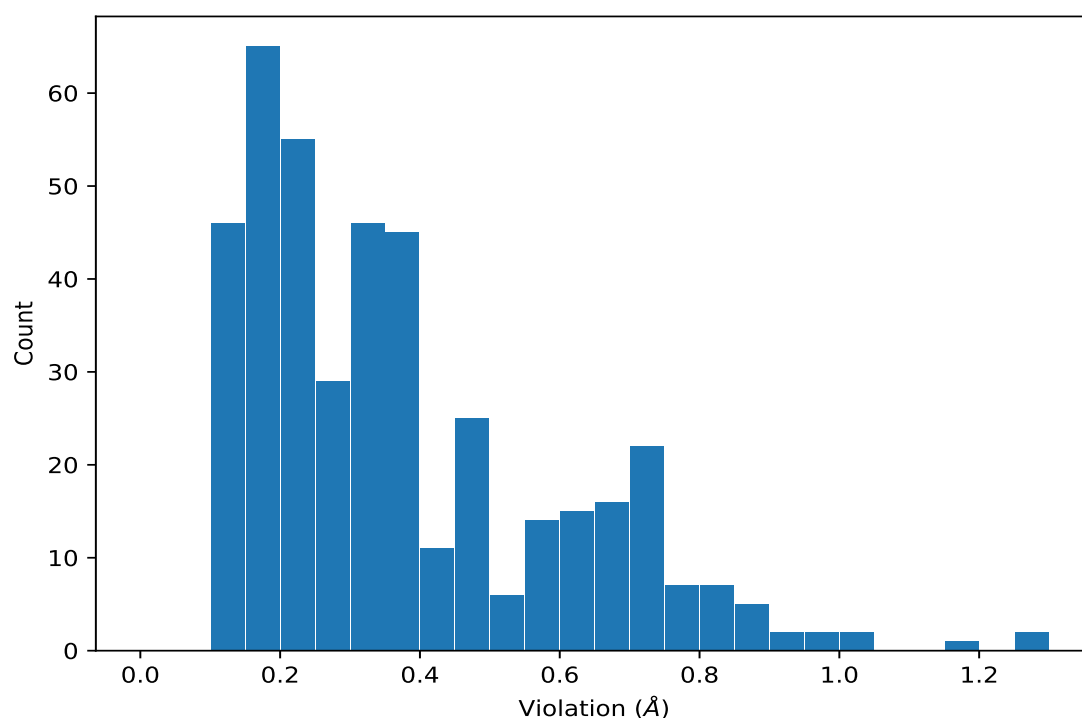
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG21	32	0.37	0.16	0.35
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG22	32	0.37	0.16	0.35
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG23	32	0.37	0.16	0.35
(2,201)	1:30:A:HIS:HE1	1:25:A:THR:HG21	32	0.37	0.16	0.35
(2,201)	1:30:A:HIS:HE1	1:25:A:THR:HG22	32	0.37	0.16	0.35
(2,201)	1:30:A:HIS:HE1	1:25:A:THR:HG23	32	0.37	0.16	0.35
(2,193)	1:23:A:TRP:HH2	1:8:A:PRO:HG2	14	0.38	0.24	0.32
(2,193)	1:23:A:TRP:HH2	1:8:A:PRO:HG3	14	0.38	0.24	0.32
(2,193)	1:23:A:TRP:HH2	1:27:A:VAL:HB	14	0.38	0.24	0.32
(2,190)	1:23:A:TRP:HZ2	1:25:A:THR:HB	7	0.19	0.04	0.2
(2,191)	1:23:A:TRP:HE1	1:25:A:THR:HB	6	0.36	0.09	0.36
(2,189)	1:23:A:TRP:HD1	1:25:A:THR:HB	6	0.27	0.07	0.27
(2,189)	1:23:A:TRP:HD1	1:25:A:THR:HA	6	0.27	0.07	0.27
(2,192)	1:23:A:TRP:HE1	1:39:A:CYS:HB2	6	0.14	0.02	0.14
(2,192)	1:23:A:TRP:HE1	1:39:A:CYS:HB3	6	0.14	0.02	0.14
(2,207)	1:40:A:PRO:HB3	1:32:A:CYS:HA	5	0.34	0.22	0.18
(2,207)	1:40:A:PRO:HB2	1:30:A:HIS:HA	5	0.34	0.22	0.18
(1,394)	1:11:A:ARG:H	1:16:A:LYS:HD2	4	0.26	0.06	0.26
(1,394)	1:11:A:ARG:H	1:16:A:LYS:HD3	4	0.26	0.06	0.26
(1,394)	1:11:A:ARG:H	1:14:A:LYS:HB2	4	0.26	0.06	0.26
(1,394)	1:11:A:ARG:H	1:14:A:LYS:HB3	4	0.26	0.06	0.26
(1,100)	1:12:A:GLN:HB2	1:13:A:CYS:H	4	0.13	0.03	0.12
(1,100)	1:12:A:GLN:HB3	1:13:A:CYS:H	4	0.13	0.03	0.12
(1,400)	1:40:A:PRO:HG2	1:30:A:HIS:HA	3	0.29	0.04	0.29
(1,400)	1:40:A:PRO:HG2	1:32:A:CYS:HA	3	0.29	0.04	0.29
(2,202)	1:30:A:HIS:HD2	1:27:A:VAL:HG11	2	0.2	0.02	0.2
(2,202)	1:30:A:HIS:HD2	1:27:A:VAL:HG12	2	0.2	0.02	0.2
(2,202)	1:30:A:HIS:HD2	1:27:A:VAL:HG13	2	0.2	0.02	0.2
(2,202)	1:30:A:HIS:HD2	1:27:A:VAL:HG21	2	0.2	0.02	0.2
(2,202)	1:30:A:HIS:HD2	1:27:A:VAL:HG22	2	0.2	0.02	0.2
(2,202)	1:30:A:HIS:HD2	1:27:A:VAL:HG23	2	0.2	0.02	0.2

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)
(2,205)	1:33:A:THR:HG23	1:42:A:TYR:HD1	40	1.27
(2,205)	1:33:A:THR:HG23	1:42:A:TYR:HD2	40	1.27
(2,203)	1:31:A:TYR:HE1	1:45:A:ASN:H	4	1.19
(2,205)	1:33:A:THR:HG23	1:42:A:TYR:HD1	37	1.0
(2,205)	1:33:A:THR:HG23	1:42:A:TYR:HD2	37	1.0
(2,203)	1:31:A:TYR:HE2	1:45:A:ASN:H	21	0.97
(2,203)	1:31:A:TYR:HE2	1:29:A:SER:H	31	0.96
(2,193)	1:23:A:TRP:HH2	1:8:A:PRO:HG2	41	0.95
(2,193)	1:23:A:TRP:HH2	1:8:A:PRO:HG3	41	0.95
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD1	18	0.89
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD2	18	0.89
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD1	39	0.89
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD2	39	0.89
(2,203)	1:31:A:TYR:HE1	1:29:A:SER:H	19	0.87
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD1	26	0.85
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD2	26	0.85

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,203)	1:31:A:TYR:HE2	1:29:A:SER:H	15	0.83
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD1	33	0.82
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD2	33	0.82
(2,203)	1:31:A:TYR:HE2	1:45:A:ASN:H	18	0.82
(2,193)	1:23:A:TRP:HH2	1:27:A:VAL:HB	23	0.81
(2,203)	1:31:A:TYR:HE2	1:45:A:ASN:H	5	0.79
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD1	17	0.78
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD2	17	0.78
(2,203)	1:31:A:TYR:HE1	1:45:A:ASN:H	40	0.78
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD1	36	0.76
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD2	36	0.76
(2,203)	1:31:A:TYR:HE1	1:45:A:ASN:H	29	0.76
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD1	4	0.74
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD2	4	0.74
(2,203)	1:31:A:TYR:HE2	1:45:A:ASN:H	28	0.74
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD1	8	0.73
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD2	8	0.73
(2,203)	1:31:A:TYR:HE1	1:45:A:ASN:H	13	0.73
(2,201)	1:30:A:HIS:HE1	1:25:A:THR:HG21	7	0.73
(2,201)	1:30:A:HIS:HE1	1:25:A:THR:HG22	7	0.73
(2,201)	1:30:A:HIS:HE1	1:25:A:THR:HG23	7	0.73
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD1	23	0.72
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD2	23	0.72
(2,203)	1:31:A:TYR:HE1	1:45:A:ASN:H	17	0.72
(2,207)	1:40:A:PRO:HB3	1:32:A:CYS:HA	32	0.71
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD1	3	0.71
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD2	3	0.71
(2,203)	1:31:A:TYR:HE1	1:45:A:ASN:H	8	0.71
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG11	14	0.71
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG12	14	0.71
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG13	14	0.71
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG21	14	0.71
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG22	14	0.71
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG23	14	0.71
(2,205)	1:33:A:THR:HG23	1:42:A:TYR:HD1	16	0.7
(2,205)	1:33:A:THR:HG23	1:42:A:TYR:HD2	16	0.7
(2,205)	1:33:A:THR:HG23	1:42:A:TYR:HD1	38	0.7
(2,205)	1:33:A:THR:HG23	1:42:A:TYR:HD2	38	0.7
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD1	19	0.69
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD2	19	0.69
(2,203)	1:31:A:TYR:HE1	1:45:A:ASN:H	10	0.67
(2,203)	1:31:A:TYR:HE2	1:45:A:ASN:H	34	0.67

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD1	22	0.65
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD2	22	0.65
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG11	38	0.65
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG12	38	0.65
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG13	38	0.65
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG21	38	0.65
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG22	38	0.65
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG23	38	0.65
(2,205)	1:33:A:THR:HG23	1:31:A:TYR:HD1	34	0.64
(2,205)	1:33:A:THR:HG23	1:31:A:TYR:HD2	34	0.64
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG11	19	0.64
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG12	19	0.64
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG13	19	0.64
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG21	19	0.64
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG22	19	0.64
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG23	19	0.64
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG11	24	0.63
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG12	24	0.63
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG13	24	0.63
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG21	24	0.63
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG22	24	0.63
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG23	24	0.63
(2,193)	1:23:A:TRP:HH2	1:27:A:VAL:HB	8	0.61
(2,205)	1:33:A:THR:HG23	1:31:A:TYR:HD1	1	0.6
(2,205)	1:33:A:THR:HG23	1:31:A:TYR:HD2	1	0.6
(2,203)	1:31:A:TYR:HE1	1:45:A:ASN:H	9	0.6
(2,203)	1:31:A:TYR:HE1	1:45:A:ASN:H	30	0.59
(2,203)	1:31:A:TYR:HE2	1:45:A:ASN:H	33	0.59
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD1	10	0.58
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD2	10	0.58
(2,203)	1:31:A:TYR:HE1	1:45:A:ASN:H	2	0.58
(2,203)	1:31:A:TYR:HE2	1:45:A:ASN:H	3	0.58
(2,203)	1:31:A:TYR:HE2	1:45:A:ASN:H	1	0.57
(2,203)	1:31:A:TYR:HE1	1:45:A:ASN:H	25	0.57
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD1	41	0.56
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD2	41	0.56
(2,203)	1:31:A:TYR:HE1	1:45:A:ASN:H	35	0.56
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD1	21	0.52
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD2	21	0.52
(2,203)	1:31:A:TYR:HE2	1:45:A:ASN:H	7	0.51
(2,191)	1:23:A:TRP:HE1	1:25:A:THR:HB	22	0.51
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD1	6	0.5

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD2	6	0.5
(2,207)	1:40:A:PRO:HB3	1:32:A:CYS:HA	27	0.49
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD1	30	0.49
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD2	30	0.49
(2,203)	1:31:A:TYR:HE2	1:45:A:ASN:H	16	0.48
(2,203)	1:31:A:TYR:HE2	1:45:A:ASN:H	32	0.47
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD1	42	0.46
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD2	42	0.46
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG11	5	0.46
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG12	5	0.46
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG13	5	0.46
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG21	5	0.46
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG22	5	0.46
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG23	5	0.46
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG11	29	0.46
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG12	29	0.46
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG13	29	0.46
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG21	29	0.46
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG22	29	0.46
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG23	29	0.46
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD1	2	0.45
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD2	2	0.45
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD1	24	0.45
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD2	24	0.45
(2,193)	1:23:A:TRP:HH2	1:8:A:PRO:HG2	22	0.45
(2,193)	1:23:A:TRP:HH2	1:8:A:PRO:HG3	22	0.45
(2,193)	1:23:A:TRP:HH2	1:8:A:PRO:HG2	21	0.43
(2,193)	1:23:A:TRP:HH2	1:8:A:PRO:HG3	21	0.43
(2,203)	1:31:A:TYR:HE1	1:45:A:ASN:H	37	0.41
(2,201)	1:30:A:HIS:HE1	1:25:A:THR:HG21	9	0.41
(2,201)	1:30:A:HIS:HE1	1:25:A:THR:HG22	9	0.41
(2,201)	1:30:A:HIS:HE1	1:25:A:THR:HG23	9	0.41
(2,201)	1:30:A:HIS:HE1	1:25:A:THR:HG21	4	0.4
(2,201)	1:30:A:HIS:HE1	1:25:A:THR:HG22	4	0.4
(2,201)	1:30:A:HIS:HE1	1:25:A:THR:HG23	4	0.4
(2,191)	1:23:A:TRP:HE1	1:25:A:THR:HB	6	0.4
(2,191)	1:23:A:TRP:HE1	1:25:A:THR:HB	18	0.4
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG11	13	0.39
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG12	13	0.39
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG13	13	0.39
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG21	13	0.39
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG22	13	0.39

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG23	13	0.39
(2,203)	1:31:A:TYR:HE1	1:45:A:ASN:H	22	0.38
(2,203)	1:31:A:TYR:HE2	1:29:A:SER:H	38	0.38
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG11	10	0.38
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG12	10	0.38
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG13	10	0.38
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG21	10	0.38
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG22	10	0.38
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG23	10	0.38
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG11	16	0.38
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG12	16	0.38
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG13	16	0.38
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG21	16	0.38
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG22	16	0.38
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG23	16	0.38
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG11	25	0.38
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG12	25	0.38
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG13	25	0.38
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG21	25	0.38
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG22	25	0.38
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG23	25	0.38
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG11	1	0.37
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG12	1	0.37
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG13	1	0.37
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG21	1	0.37
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG22	1	0.37
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG23	1	0.37
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG11	27	0.37
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG12	27	0.37
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG13	27	0.37
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG21	27	0.37
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG22	27	0.37
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG23	27	0.37
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG11	34	0.36
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG12	34	0.36
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG13	34	0.36
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG21	34	0.36
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG22	34	0.36
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG23	34	0.36
(2,189)	1:23:A:TRP:HD1	1:25:A:THR:HB	18	0.36
(2,205)	1:33:A:THR:HG23	1:42:A:TYR:HD1	5	0.35
(2,205)	1:33:A:THR:HG23	1:42:A:TYR:HD2	5	0.35

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,193)	1:23:A:TRP:HH2	1:8:A:PRO:HG2	3	0.35
(2,193)	1:23:A:TRP:HH2	1:8:A:PRO:HG3	3	0.35
(2,187)	1:13:A:CYS:H	1:11:A:ARG:HG2	33	0.35
(2,187)	1:13:A:CYS:H	1:11:A:ARG:HG3	33	0.35
(1,400)	1:40:A:PRO:HG2	1:30:A:HIS:HA	33	0.35
(1,394)	1:11:A:ARG:H	1:14:A:LYS:HB2	3	0.35
(1,394)	1:11:A:ARG:H	1:14:A:LYS:HB3	3	0.35
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG11	33	0.34
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG12	33	0.34
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG13	33	0.34
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG21	33	0.34
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG22	33	0.34
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG23	33	0.34
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG11	39	0.34
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG12	39	0.34
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG13	39	0.34
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG21	39	0.34
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG22	39	0.34
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG23	39	0.34
(2,193)	1:23:A:TRP:HH2	1:8:A:PRO:HG2	6	0.34
(2,193)	1:23:A:TRP:HH2	1:8:A:PRO:HG3	6	0.34
(2,189)	1:23:A:TRP:HD1	1:25:A:THR:HA	22	0.34
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD1	9	0.33
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD2	9	0.33
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG11	12	0.33
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG12	12	0.33
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG13	12	0.33
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG21	12	0.33
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG22	12	0.33
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG23	12	0.33
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG11	26	0.33
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG12	26	0.33
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG13	26	0.33
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG21	26	0.33
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG22	26	0.33
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG23	26	0.33
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG11	37	0.33
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG12	37	0.33
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG13	37	0.33
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG21	37	0.33
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG22	37	0.33
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG23	37	0.33

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,191)	1:23:A:TRP:HE1	1:25:A:THR:HB	41	0.32
(2,189)	1:23:A:TRP:HD1	1:25:A:THR:HB	6	0.31
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD1	12	0.3
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD2	12	0.3
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG11	21	0.3
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG12	21	0.3
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG13	21	0.3
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG21	21	0.3
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG22	21	0.3
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG23	21	0.3
(2,203)	1:31:A:TYR:HE2	1:45:A:ASN:H	6	0.29
(2,193)	1:23:A:TRP:HH2	1:8:A:PRO:HG2	35	0.29
(2,193)	1:23:A:TRP:HH2	1:8:A:PRO:HG3	35	0.29
(1,400)	1:40:A:PRO:HG2	1:30:A:HIS:HA	17	0.29
(1,394)	1:11:A:ARG:H	1:16:A:LYS:HD2	11	0.29
(1,394)	1:11:A:ARG:H	1:16:A:LYS:HD3	11	0.29
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD1	11	0.28
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD2	11	0.28
(2,205)	1:33:A:THR:HG23	1:42:A:TYR:HD1	14	0.28
(2,205)	1:33:A:THR:HG23	1:42:A:TYR:HD2	14	0.28
(2,191)	1:23:A:TRP:HE1	1:25:A:THR:HB	23	0.26
(2,190)	1:23:A:TRP:HZ2	1:25:A:THR:HB	12	0.26
(2,201)	1:30:A:HIS:HE1	1:25:A:THR:HG21	3	0.25
(2,201)	1:30:A:HIS:HE1	1:25:A:THR:HG22	3	0.25
(2,201)	1:30:A:HIS:HE1	1:25:A:THR:HG23	3	0.25
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG11	31	0.25
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG12	31	0.25
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG13	31	0.25
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG21	31	0.25
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG22	31	0.25
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG23	31	0.25
(2,193)	1:23:A:TRP:HH2	1:8:A:PRO:HG2	19	0.24
(2,193)	1:23:A:TRP:HH2	1:8:A:PRO:HG3	19	0.24
(2,191)	1:23:A:TRP:HE1	1:25:A:THR:HB	8	0.24
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	19	0.24
(1,400)	1:40:A:PRO:HG2	1:32:A:CYS:HA	39	0.24
(2,203)	1:31:A:TYR:HE1	1:45:A:ASN:H	23	0.23
(2,189)	1:23:A:TRP:HD1	1:25:A:THR:HB	41	0.23
(1,401)	1:44:A:GLY:H	1:31:A:TYR:HD1	38	0.23
(1,401)	1:44:A:GLY:H	1:31:A:TYR:HD2	38	0.23
(1,394)	1:11:A:ARG:H	1:14:A:LYS:HB2	4	0.23
(1,394)	1:11:A:ARG:H	1:14:A:LYS:HB3	4	0.23

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD1	32	0.22
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD2	32	0.22
(2,202)	1:30:A:HIS:HD2	1:27:A:VAL:HG11	22	0.22
(2,202)	1:30:A:HIS:HD2	1:27:A:VAL:HG12	22	0.22
(2,202)	1:30:A:HIS:HD2	1:27:A:VAL:HG13	22	0.22
(2,202)	1:30:A:HIS:HD2	1:27:A:VAL:HG21	22	0.22
(2,202)	1:30:A:HIS:HD2	1:27:A:VAL:HG22	22	0.22
(2,202)	1:30:A:HIS:HD2	1:27:A:VAL:HG23	22	0.22
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	24	0.22
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	34	0.22
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD1	28	0.21
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD2	28	0.21
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD1	35	0.21
(2,205)	1:33:A:THR:HG21	1:31:A:TYR:HD2	35	0.21
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG11	18	0.21
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG12	18	0.21
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG13	18	0.21
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG21	18	0.21
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG22	18	0.21
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG23	18	0.21
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG11	42	0.21
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG12	42	0.21
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG13	42	0.21
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG21	42	0.21
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG22	42	0.21
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG23	42	0.21
(2,189)	1:23:A:TRP:HD1	1:25:A:THR:HB	8	0.21
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	28	0.21
(2,201)	1:30:A:HIS:HE1	1:25:A:THR:HG21	2	0.2
(2,201)	1:30:A:HIS:HE1	1:25:A:THR:HG22	2	0.2
(2,201)	1:30:A:HIS:HE1	1:25:A:THR:HG23	2	0.2
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG11	22	0.2
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG12	22	0.2
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG13	22	0.2
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG21	22	0.2
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG22	22	0.2
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG23	22	0.2
(2,193)	1:23:A:TRP:HH2	1:8:A:PRO:HG2	13	0.2
(2,193)	1:23:A:TRP:HH2	1:8:A:PRO:HG3	13	0.2
(2,190)	1:23:A:TRP:HZ2	1:25:A:THR:HB	6	0.2
(2,190)	1:23:A:TRP:HZ2	1:25:A:THR:HB	22	0.2
(2,190)	1:23:A:TRP:HZ2	1:25:A:THR:HB	41	0.2

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	7	0.2
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	31	0.2
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG11	41	0.19
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG12	41	0.19
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG13	41	0.19
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG21	41	0.19
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG22	41	0.19
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG23	41	0.19
(2,193)	1:23:A:TRP:HH2	1:8:A:PRO:HG2	12	0.19
(2,193)	1:23:A:TRP:HH2	1:8:A:PRO:HG3	12	0.19
(2,190)	1:23:A:TRP:HZ2	1:25:A:THR:HB	23	0.19
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	5	0.19
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	15	0.19
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	25	0.19
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	27	0.19
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	32	0.19
(1,394)	1:11:A:ARG:H	1:14:A:LYS:HB2	2	0.19
(1,394)	1:11:A:ARG:H	1:14:A:LYS:HB3	2	0.19
(2,207)	1:40:A:PRO:HB3	1:32:A:CYS:HA	1	0.18
(2,207)	1:40:A:PRO:HB2	1:30:A:HIS:HA	28	0.18
(2,190)	1:23:A:TRP:HZ2	1:25:A:THR:HB	8	0.18
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	1	0.18
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	29	0.18
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	37	0.18
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	38	0.18
(1,100)	1:12:A:GLN:HB2	1:13:A:CYS:H	33	0.18
(1,100)	1:12:A:GLN:HB3	1:13:A:CYS:H	33	0.18
(2,202)	1:30:A:HIS:HD2	1:27:A:VAL:HG11	18	0.17
(2,202)	1:30:A:HIS:HD2	1:27:A:VAL:HG12	18	0.17
(2,202)	1:30:A:HIS:HD2	1:27:A:VAL:HG13	18	0.17
(2,202)	1:30:A:HIS:HD2	1:27:A:VAL:HG21	18	0.17
(2,202)	1:30:A:HIS:HD2	1:27:A:VAL:HG22	18	0.17
(2,202)	1:30:A:HIS:HD2	1:27:A:VAL:HG23	18	0.17
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG11	23	0.17
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG12	23	0.17
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG13	23	0.17
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG21	23	0.17
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG22	23	0.17
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG23	23	0.17
(2,193)	1:23:A:TRP:HH2	1:8:A:PRO:HG2	4	0.17
(2,193)	1:23:A:TRP:HH2	1:8:A:PRO:HG3	4	0.17
(2,192)	1:23:A:TRP:HE1	1:39:A:CYS:HB2	38	0.17

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,192)	1:23:A:TRP:HE1	1:39:A:CYS:HB3	38	0.17
(2,189)	1:23:A:TRP:HD1	1:25:A:THR:HB	23	0.17
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	13	0.17
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	14	0.17
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	42	0.17
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG11	6	0.16
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG12	6	0.16
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG13	6	0.16
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG21	6	0.16
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG22	6	0.16
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG23	6	0.16
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG11	8	0.16
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG12	8	0.16
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG13	8	0.16
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG21	8	0.16
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG22	8	0.16
(2,201)	1:30:A:HIS:HE1	1:27:A:VAL:HG23	8	0.16
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	4	0.16
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	16	0.16
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	21	0.16
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	26	0.16
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	30	0.16
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	33	0.16
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	35	0.16
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	39	0.16
(2,207)	1:40:A:PRO:HB2	1:30:A:HIS:HA	24	0.15
(2,203)	1:31:A:TYR:HE1	1:45:A:ASN:H	11	0.15
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	3	0.15
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	9	0.15
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	10	0.15
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	12	0.15
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	17	0.15
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	20	0.15
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	36	0.15
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	40	0.15
(2,193)	1:23:A:TRP:HH2	1:8:A:PRO:HG2	18	0.14
(2,193)	1:23:A:TRP:HH2	1:8:A:PRO:HG3	18	0.14
(2,193)	1:23:A:TRP:HH2	1:8:A:PRO:HG2	20	0.14
(2,193)	1:23:A:TRP:HH2	1:8:A:PRO:HG3	20	0.14
(2,192)	1:23:A:TRP:HE1	1:39:A:CYS:HB2	32	0.14
(2,192)	1:23:A:TRP:HE1	1:39:A:CYS:HB3	32	0.14
(2,192)	1:23:A:TRP:HE1	1:39:A:CYS:HB2	33	0.14

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,192)	1:23:A:TRP:HE1	1:39:A:CYS:HB3	33	0.14
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	2	0.14
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	11	0.14
(2,205)	1:33:A:THR:HG22	1:42:A:TYR:HD1	7	0.13
(2,205)	1:33:A:THR:HG22	1:42:A:TYR:HD2	7	0.13
(2,192)	1:23:A:TRP:HE1	1:39:A:CYS:HB2	2	0.13
(2,192)	1:23:A:TRP:HE1	1:39:A:CYS:HB3	2	0.13
(1,112)	1:14:A:LYS:HA	1:15:A:LEU:H	14	0.13
(2,203)	1:31:A:TYR:HE2	1:45:A:ASN:H	20	0.12
(2,192)	1:23:A:TRP:HE1	1:39:A:CYS:HB2	30	0.12
(2,192)	1:23:A:TRP:HE1	1:39:A:CYS:HB3	30	0.12
(2,190)	1:23:A:TRP:HZ2	1:25:A:THR:HB	18	0.12
(2,188)	1:23:A:TRP:HH2	1:25:A:THR:HB	8	0.12
(1,396)	1:23:A:TRP:HZ2	1:8:A:PRO:HB2	28	0.12
(1,396)	1:23:A:TRP:HZ2	1:8:A:PRO:HB3	28	0.12
(1,100)	1:12:A:GLN:HB2	1:13:A:CYS:H	19	0.12
(1,100)	1:12:A:GLN:HB3	1:13:A:CYS:H	19	0.12
(1,100)	1:12:A:GLN:HB2	1:13:A:CYS:H	39	0.12
(1,100)	1:12:A:GLN:HB3	1:13:A:CYS:H	39	0.12
(2,205)	1:33:A:THR:HG23	1:42:A:TYR:HD1	25	0.11
(2,205)	1:33:A:THR:HG23	1:42:A:TYR:HD2	25	0.11
(2,192)	1:23:A:TRP:HE1	1:39:A:CYS:HB2	20	0.11
(2,192)	1:23:A:TRP:HE1	1:39:A:CYS:HB3	20	0.11
(1,100)	1:12:A:GLN:HB2	1:13:A:CYS:H	11	0.11
(1,100)	1:12:A:GLN:HB3	1:13:A:CYS:H	11	0.11
(2,3)	1:4:A:CYS:HA	1:13:A:CYS:H	5	0.1
(1,214)	1:21:A:THR:HG21	1:32:A:CYS:H	19	0.1
(1,214)	1:21:A:THR:HG22	1:32:A:CYS:H	19	0.1
(1,214)	1:21:A:THR:HG23	1:32:A:CYS:H	19	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found