



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2LK5 / pdb_00002lk5
BMRB ID : 17979
Title : Solution structure of the Zn(II) form of Desulforedoxin
Authors : Goodfellow, B.J.; Tavares, P.; Romao, M.J.; Czaja, C.; Rusnak, F.; Legall, J.;
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Deposited on : 2011-10-06

This is a wwPDB NMR Structure Validation Summary 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	:	FAILED
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 27%.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.

2 Ensemble composition and analysis

This entry contains 29 models. Model 29 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:3-A:36, B:4-B:36 (67)	0.39	29

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 4 clusters and 2 single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1016 atoms, of which 494 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Desulforedoxin.

Mol	Chain	Residues	Atoms						Trace
1	A	36	Total	C	H	N	O	S	0
			507	158	247	42	55	5	
1	B	36	Total	C	H	N	O	S	0
			507	158	247	42	55	5	

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

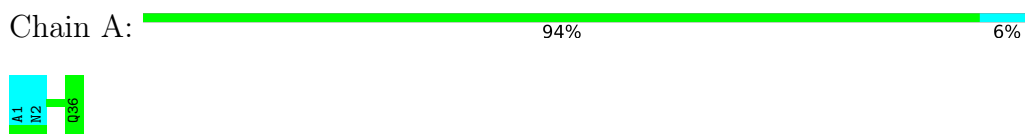
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1
2	B	1	Total	Zn
			1	1

4 Residue-property plots [i](#)

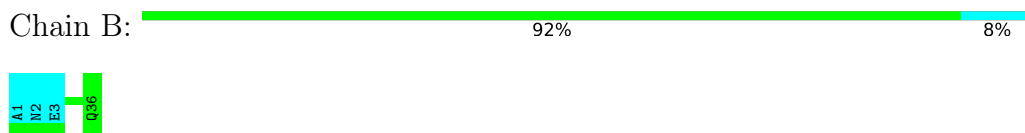
4.1 Average score per residue in the NMR ensemble

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: Desulforedoxin



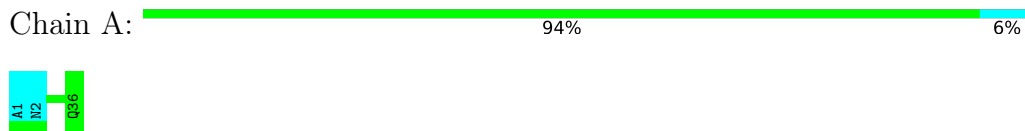
- Molecule 1: Desulforedoxin



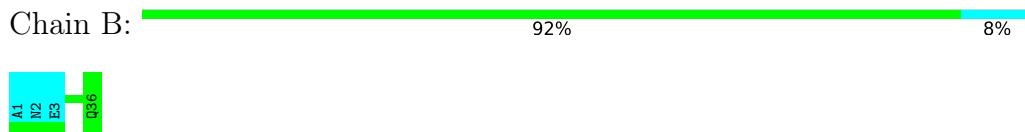
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 29. Colouring as in section 4.1 above.

- Molecule 1: Desulforedoxin



- Molecule 1: Desulforedoxin



5 Refinement protocol and experimental data overview

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

Of the 300 calculated structures, 29 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
DIANA	structure solution	2.8
DIANA	refinement	2.8

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	231
Number of shifts mapped to atoms	231
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	27%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts [i](#)

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6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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6.3.2 Protein sidechains [i](#)

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6.3.3 RNA [i](#)

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

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6.5 Carbohydrates [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.6 Ligand geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.7 Other polymers [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.8 Polymer linkage issues

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 27% for the well-defined parts and 26% 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	231
Number of shifts mapped to atoms	231
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing [i](#)

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

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 27%, i.e. 223 atoms were assigned a chemical shift out of a possible 822. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	74/347 (21%)	74/146 (51%)	0/134 (0%)	0/67 (0%)
Sidechain	147/457 (32%)	147/296 (50%)	0/151 (0%)	0/10 (0%)
Aromatic	2/18 (11%)	2/8 (25%)	0/10 (0%)	0/0 (—%)
Overall	223/822 (27%)	223/450 (50%)	0/295 (0%)	0/77 (0%)

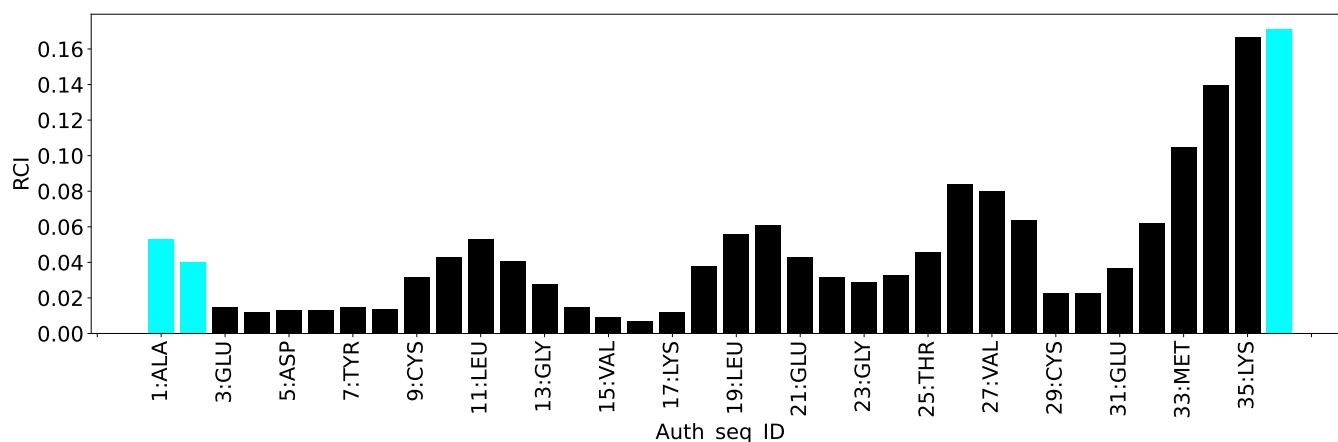
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis [i](#)

8.1 Conformationally restricting restraints [i](#)

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

Description	Value
Total distance restraints	670
Intra-residue ($ i-j =0$)	138
Sequential ($ i-j =1$)	172
Medium range ($ i-j >1$ and $ i-j <5$)	70
Long range ($ i-j \geq 5$)	176
Inter-chain	26
Hydrogen bond restraints	60
Disulfide bond restraints	10
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	9.1
Number of long range restraints per residue ¹	2.9

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

8.2 Residual restraint violations [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)	25.5	0.2
0.2-0.5 (Medium)	11.0	0.5
>0.5 (Large)	33.1	4.11

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 ⓘ

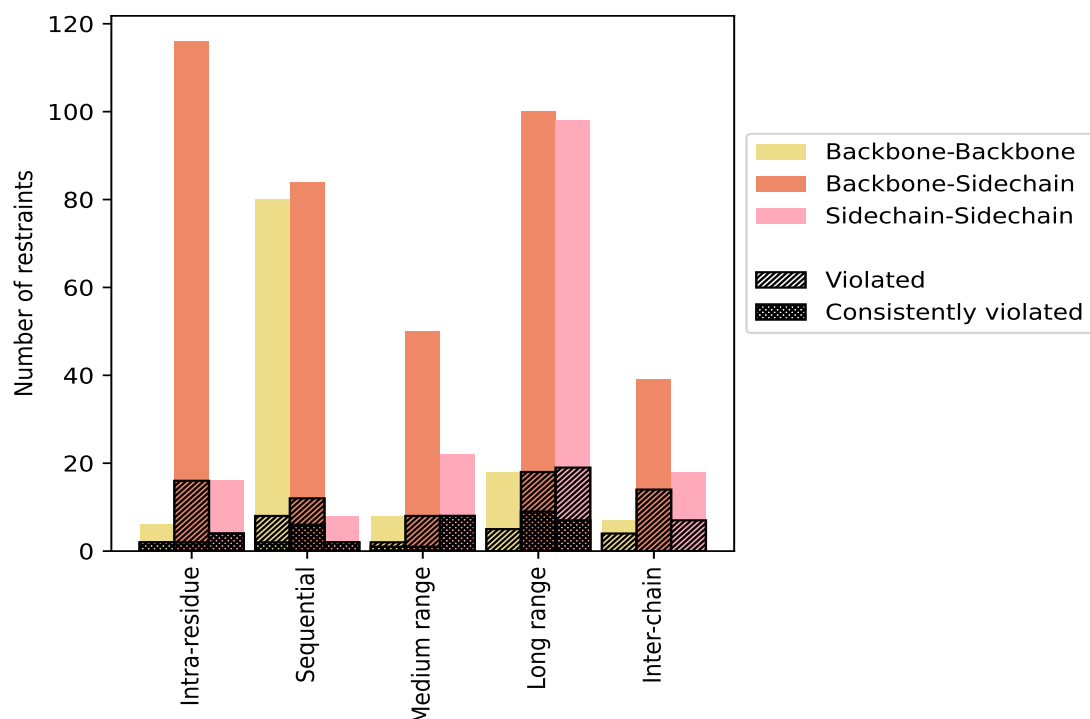
9.1 Summary of distance violations ⓘ

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.

Restraints type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue (i-j =0)	138	20.6	22	15.9	3.3	8	5.8	1.2
Backbone-Backbone	6	0.9	2	33.3	0.3	2	33.3	0.3
Backbone-Sidechain	116	17.3	16	13.8	2.4	2	1.7	0.3
Sidechain-Sidechain	16	2.4	4	25.0	0.6	4	25.0	0.6
Sequential (i-j =1)	172	25.7	22	12.8	3.3	10	5.8	1.5
Backbone-Backbone	80	11.9	8	10.0	1.2	2	2.5	0.3
Backbone-Sidechain	84	12.5	12	14.3	1.8	6	7.1	0.9
Sidechain-Sidechain	8	1.2	2	25.0	0.3	2	25.0	0.3
Medium range (i-j >1 & i-j <5)	70	10.4	17	24.3	2.5	10	14.3	1.5
Backbone-Backbone	8	1.2	2	25.0	0.3	1	12.5	0.1
Backbone-Sidechain	42	6.3	7	16.7	1.0	1	2.4	0.1
Sidechain-Sidechain	20	3.0	8	40.0	1.2	8	40.0	1.2
Long range (i-j ≥5)	176	26.3	32	18.2	4.8	16	9.1	2.4
Backbone-Backbone	18	2.7	5	27.8	0.7	0	0.0	0.0
Backbone-Sidechain	68	10.1	12	17.6	1.8	9	13.2	1.3
Sidechain-Sidechain	90	13.4	15	16.7	2.2	7	7.8	1.0
Inter-chain	26	3.9	5	19.2	0.7	0	0.0	0.0
Backbone-Backbone	7	1.0	4	57.1	0.6	0	0.0	0.0
Backbone-Sidechain	13	1.9	1	7.7	0.1	0	0.0	0.0
Sidechain-Sidechain	6	0.9	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	60	9.0	16	26.7	2.4	0	0.0	0.0
Disulfide bond	10	1.5	4	40.0	0.6	0	0.0	0.0
Total	670	100.0	129	19.3	19.3	44	6.6	6.6
Backbone-Backbone	119	17.8	21	17.6	3.1	5	4.2	0.7
Backbone-Sidechain	389	58.1	68	17.5	10.1	18	4.6	2.7
Sidechain-Sidechain	162	24.2	40	24.7	6.0	21	13.0	3.1

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 disulfid 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	12	12	13	28	8	73	1.05	3.64	1.16	0.34
2	13	15	12	22	6	68	1.08	3.79	1.1	0.48
3	16	12	13	23	10	74	1.02	3.76	1.14	0.31
4	13	14	13	27	8	75	1.02	3.83	1.12	0.31
5	14	13	13	24	10	74	1.06	4.03	1.17	0.35
6	10	12	12	24	9	67	1.11	4.08	1.18	0.55
7	14	12	12	26	9	73	1.06	3.88	1.17	0.35
8	11	15	12	25	13	76	1.02	3.71	1.12	0.37
9	11	13	13	23	11	71	1.07	4.0	1.14	0.36
10	13	11	12	25	5	66	1.12	3.74	1.15	0.52

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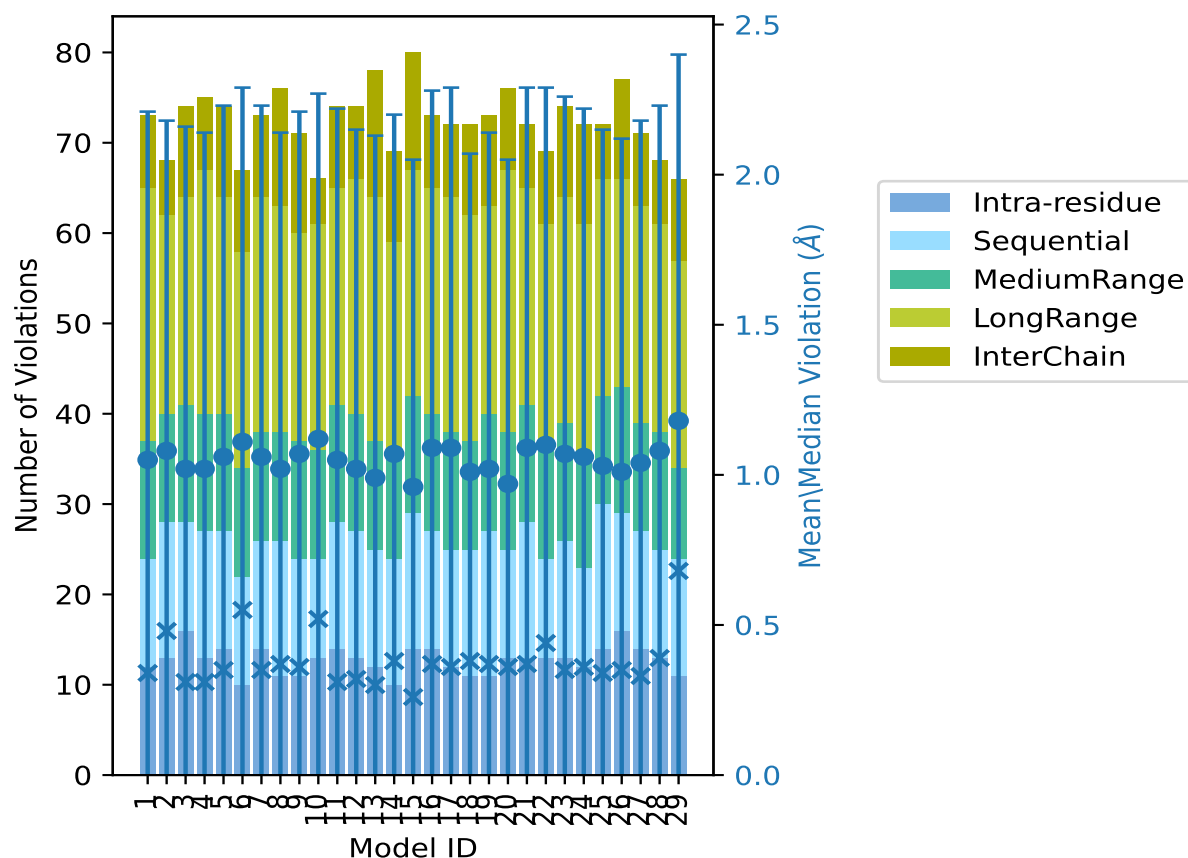
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	14	14	13	24	9	74	1.05	3.6	1.17	0.31
12	13	14	13	26	8	74	1.02	3.63	1.13	0.32
13	12	13	12	27	14	78	0.99	3.73	1.14	0.3
14	10	14	12	23	10	69	1.07	3.65	1.13	0.38
15	14	15	13	25	13	80	0.96	3.63	1.09	0.26
16	14	13	13	25	8	73	1.09	3.83	1.19	0.37
17	12	13	13	26	8	72	1.09	4.11	1.2	0.36
18	11	14	12	25	10	72	1.01	3.47	1.06	0.38
19	11	16	13	23	10	73	1.02	3.57	1.12	0.37
20	13	12	13	29	9	76	0.97	3.55	1.08	0.36
21	13	15	13	24	7	72	1.09	4.04	1.2	0.37
22	13	11	12	25	8	69	1.1	4.1	1.19	0.44
23	13	13	13	25	10	74	1.07	3.89	1.19	0.35
24	12	11	12	26	11	72	1.06	3.87	1.16	0.36
25	14	16	12	24	6	72	1.03	3.59	1.12	0.34
26	16	13	14	23	11	77	1.01	3.61	1.11	0.35
27	14	13	12	24	8	71	1.04	3.69	1.14	0.33
28	13	12	13	23	7	68	1.08	3.64	1.15	0.39
29	11	13	10	23	9	66	1.18	3.93	1.22	0.68

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, 484(IR:116, SQ:150, MR:53, LR:144, IC:21) 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	%
4	2	2	4	1	13	1	3.4
0	1	1	0	1	3	2	6.9
0	1	1	1	0	3	3	10.3
0	0	0	0	0	0	4	13.8
1	1	0	2	0	4	5	17.2
1	1	0	0	0	2	6	20.7

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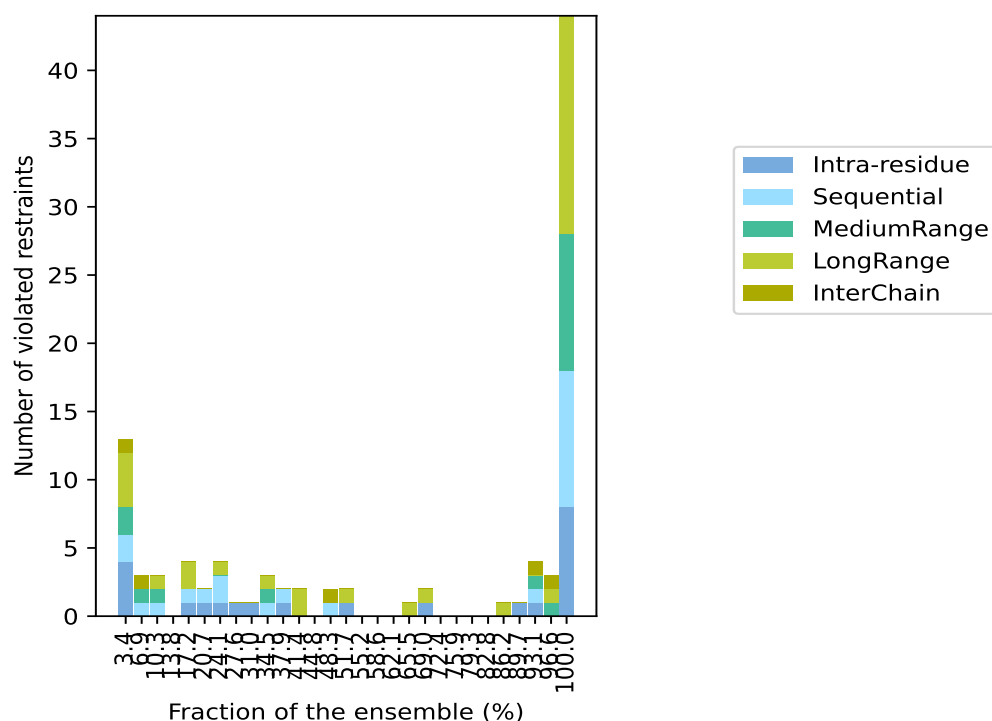
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
1	2	0	1	0	4	7	24.1
1	0	0	0	0	1	8	27.6
1	0	0	0	0	1	9	31.0
0	1	1	1	0	3	10	34.5
1	1	0	0	0	2	11	37.9
0	0	0	2	0	2	12	41.4
0	0	0	0	0	0	13	44.8
0	1	0	0	1	2	14	48.3
1	0	0	1	0	2	15	51.7
0	0	0	0	0	0	16	55.2
0	0	0	0	0	0	17	58.6
0	0	0	0	0	0	18	62.1
0	0	0	1	0	1	19	65.5
1	0	0	1	0	2	20	69.0
0	0	0	0	0	0	21	72.4
0	0	0	0	0	0	22	75.9
0	0	0	0	0	0	23	79.3
0	0	0	0	0	0	24	82.8
0	0	0	1	0	1	25	86.2
1	0	0	0	0	1	26	89.7
1	1	1	0	1	4	27	93.1
0	0	1	1	1	3	28	96.6
8	10	10	16	0	44	29	100.0

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

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

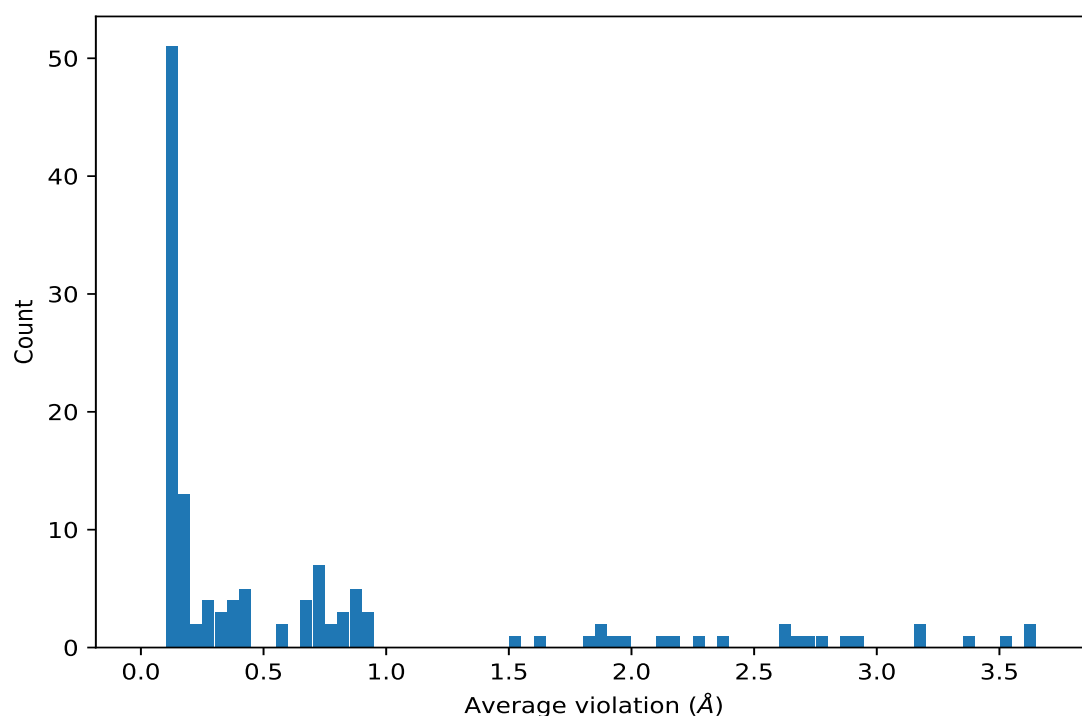
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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 violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation 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.

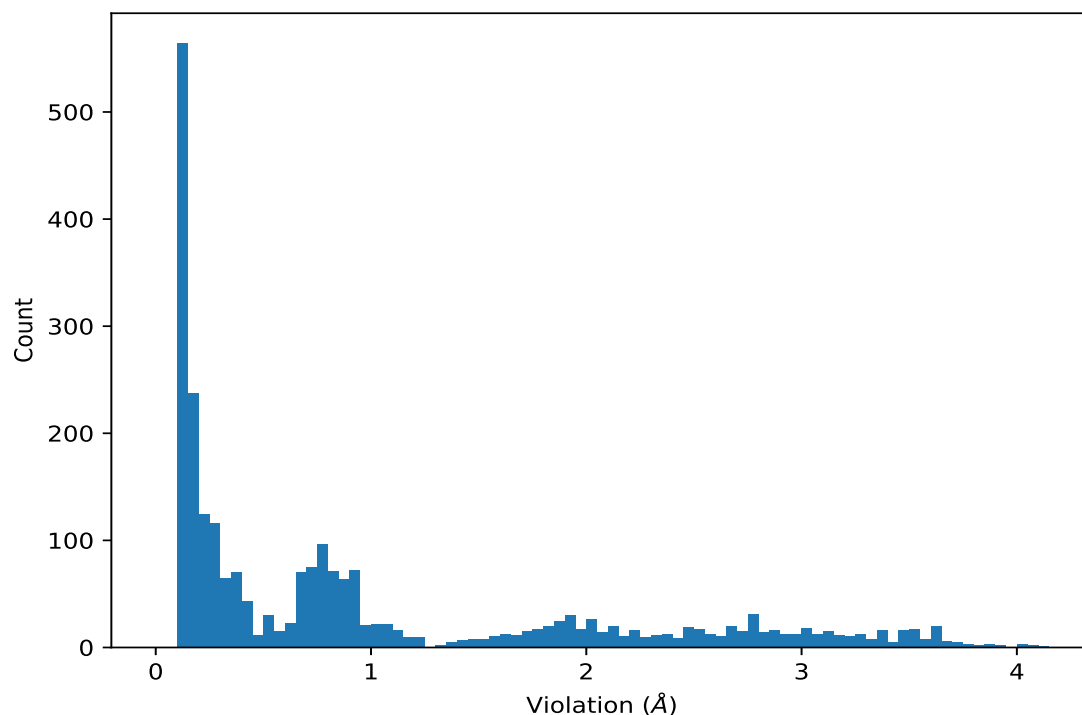
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,257)	1:6:B:VAL:HB	1:7:B:TYR:HD2	29	3.62	0.07	3.63
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	29	3.61	0.4	3.7
(2,30)	1:6:A:VAL:HB	1:7:A:TYR:HD2	29	3.51	0.07	3.51
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	29	3.35	0.29	3.31
(2,26)	1:6:A:VAL:H	1:7:A:TYR:HE2	29	3.19	0.2	3.22
(2,253)	1:6:B:VAL:H	1:7:B:TYR:HE2	29	3.16	0.14	3.16
(2,246)	1:5:B:ASP:HB2	1:7:B:TYR:HD2	29	2.94	0.38	2.95
(2,249)	1:5:B:ASP:HB3	1:7:B:TYR:HE2	29	2.88	0.2	2.89
(2,19)	1:5:A:ASP:HB2	1:7:A:TYR:HD2	29	2.79	0.27	2.76
(2,22)	1:5:A:ASP:HB3	1:7:A:TYR:HE2	29	2.74	0.23	2.78

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 provides the 10 worst performing restraints, sorted by the violation 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)
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	17	4.11
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	22	4.1
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	6	4.08
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	21	4.04
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	5	4.03
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	9	4.0
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	29	3.93
(2,18)	1:5:A:ASP:HB2	1:7:A:TYR:HE2	29	3.92
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	23	3.89
(2,245)	1:5:B:ASP:HB2	1:7:B:TYR:HE2	7	3.88

10 Dihedral-angle violation analysis

No dihedral-angle restraints found