



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 02:48 AM UTC

PDB ID : 5O57 / pdb_00005o57
BMRB ID : 34146
Title : Solution Structure of the N-terminal Region of Dkk4
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Holdsworth, G.; Carr, M.D.
Deposited on : 2017-06-01

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

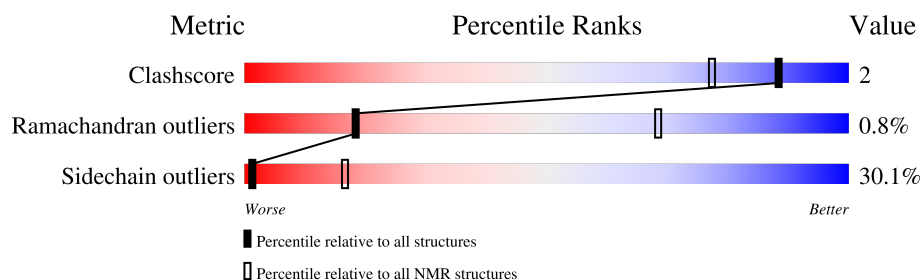
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 85%.

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	95	44% 15% 41%

2 Ensemble composition and analysis

This entry contains 70 models. Model 13 is the overall representative, medoid model (most similar to other models).

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:41-A:96 (56)	1.15	13

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 9 clusters and 5 single-model clusters were found.

Cluster number	Models
1	1, 2, 4, 9, 12, 15, 21, 23, 24, 26, 28, 33, 49, 53, 59, 65, 70
2	3, 5, 7, 13, 18, 20, 22, 25, 29, 36, 39, 42, 46, 48, 57, 58, 64
3	6, 14, 43, 45, 56, 61, 62, 66
4	17, 19, 31, 35, 37, 38, 69
5	27, 40, 50, 67
6	30, 44, 52, 60
7	8, 32, 41
8	10, 11, 47
9	16, 63
Single-model clusters	34; 51; 54; 55; 68

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1477 atoms, of which 723 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Dickkopf-related protein 4.

Mol	Chain	Residues	Atoms						Trace
1	A	95	Total	C	H	N	O	S	0
			1477	452	723	148	141	13	

There are 16 discrepancies between the modelled and reference sequences:

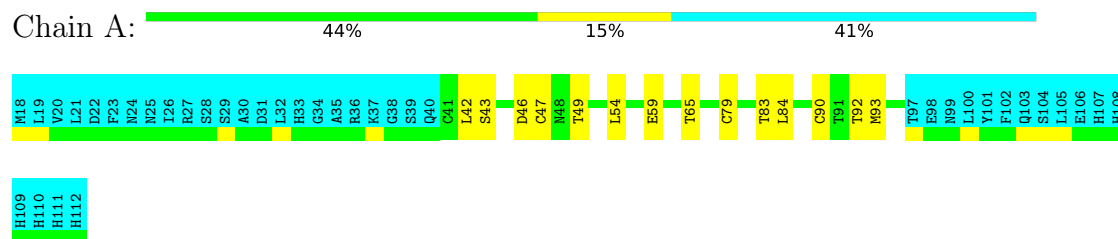
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	initiating methionine	UNP Q9UBT3
A	98	GLU	-	expression tag	UNP Q9UBT3
A	99	ASN	-	expression tag	UNP Q9UBT3
A	100	LEU	-	expression tag	UNP Q9UBT3
A	101	TYR	-	expression tag	UNP Q9UBT3
A	102	PHE	-	expression tag	UNP Q9UBT3
A	103	GLN	-	expression tag	UNP Q9UBT3
A	104	SER	-	expression tag	UNP Q9UBT3
A	105	LEU	-	expression tag	UNP Q9UBT3
A	106	GLU	-	expression tag	UNP Q9UBT3
A	107	HIS	-	expression tag	UNP Q9UBT3
A	108	HIS	-	expression tag	UNP Q9UBT3
A	109	HIS	-	expression tag	UNP Q9UBT3
A	110	HIS	-	expression tag	UNP Q9UBT3
A	111	HIS	-	expression tag	UNP Q9UBT3
A	112	HIS	-	expression tag	UNP Q9UBT3

4 Residue-property plots

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: Dickkopf-related protein 4

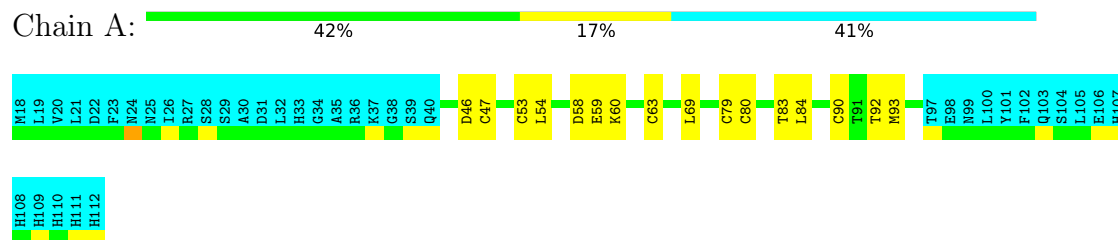


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

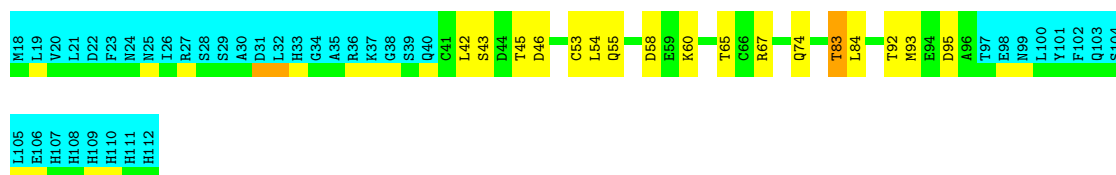
- Molecule 1: Dickkopf-related protein 4



4.2.2 Score per residue for model 2

- Molecule 1: Dickkopf-related protein 4

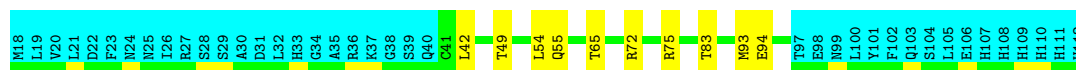




4.2.3 Score per residue for model 3

- Molecule 1: Dickkopf-related protein 4

Chain A: 48% 11% 41%



4.2.4 Score per residue for model 4

- Molecule 1: Dickkopf-related protein 4

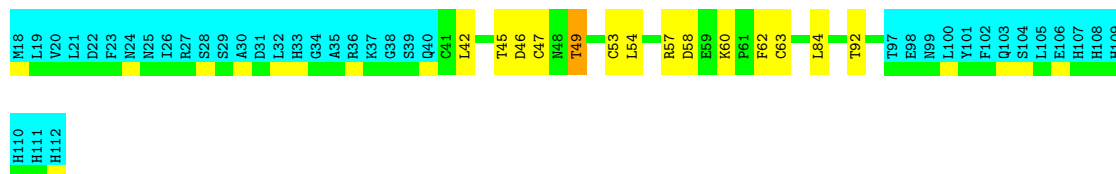
Chain A: 40% 18% 41%



4.2.5 Score per residue for model 5

- Molecule 1: Dickkopf-related protein 4

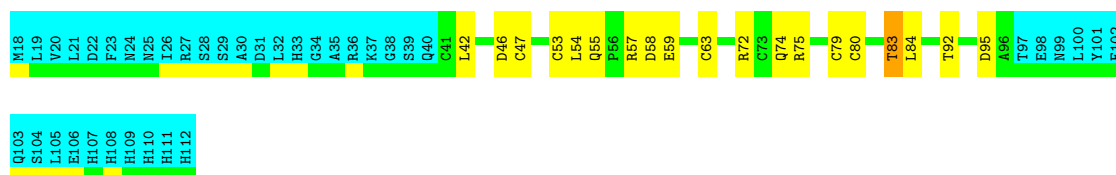
Chain A: 44% 14% 41%



4.2.6 Score per residue for model 6

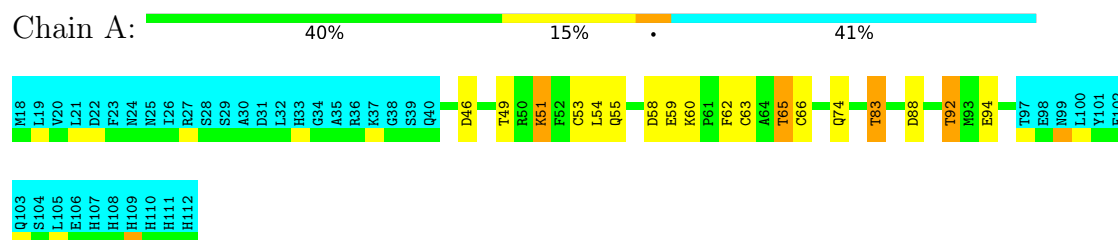
- Molecule 1: Dickkopf-related protein 4

Chain A: 39% 19% 41%



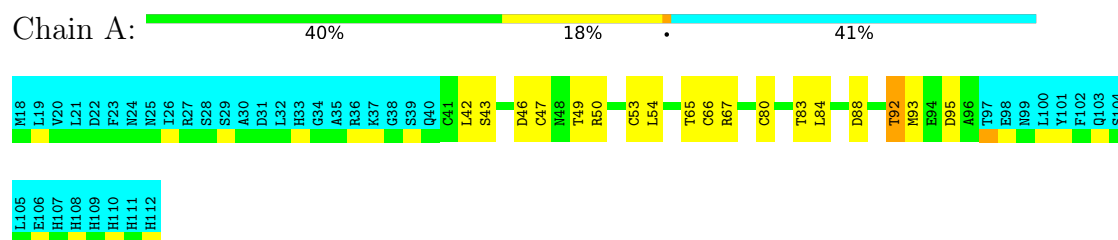
4.2.7 Score per residue for model 7

- Molecule 1: Dickkopf-related protein 4



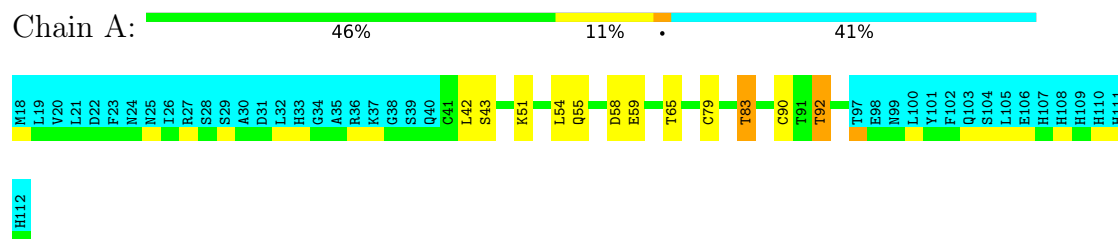
4.2.8 Score per residue for model 8

- Molecule 1: Dickkopf-related protein 4



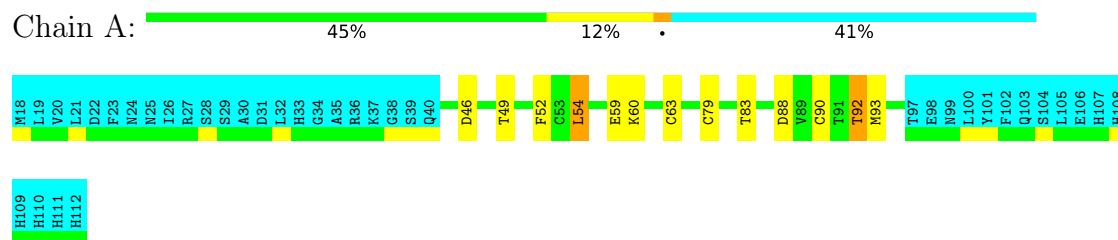
4.2.9 Score per residue for model 9

- Molecule 1: Dickkopf-related protein 4



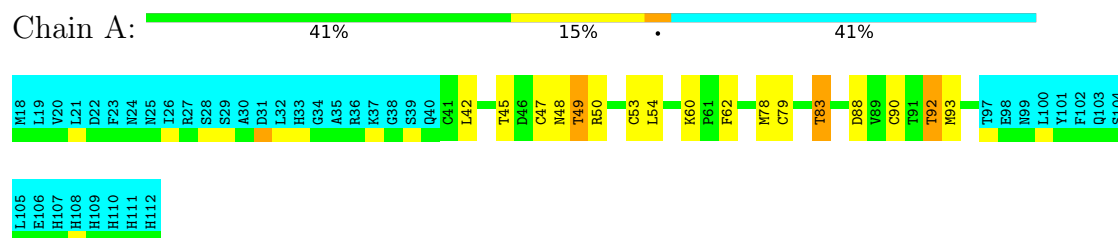
4.2.10 Score per residue for model 10

- Molecule 1: Dickkopf-related protein 4



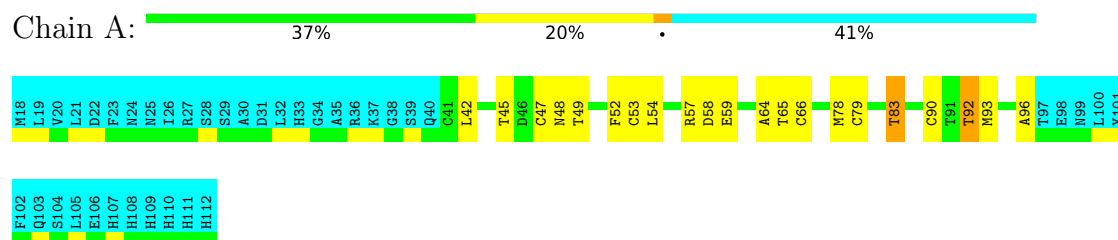
4.2.11 Score per residue for model 11

- Molecule 1: Dickkopf-related protein 4



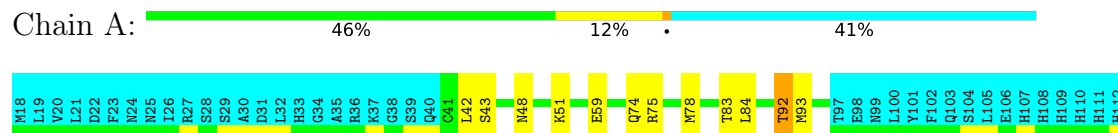
4.2.12 Score per residue for model 12

- Molecule 1: Dickkopf-related protein 4



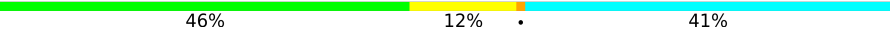
4.2.13 Score per residue for model 13 (medoid)

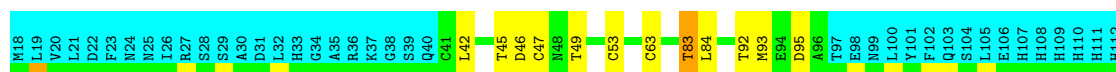
- Molecule 1: Dickkopf-related protein 4



4.2.14 Score per residue for model 14

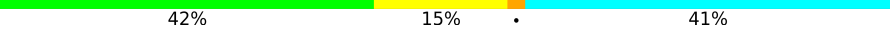
- Molecule 1: Dickkopf-related protein 4

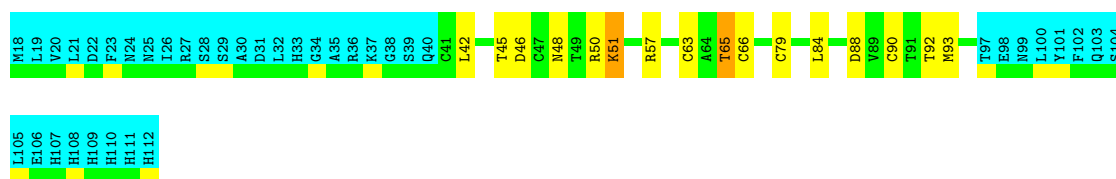
Chain A:  46% 12% 41%



4.2.15 Score per residue for model 15

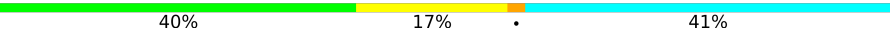
- Molecule 1: Dickkopf-related protein 4

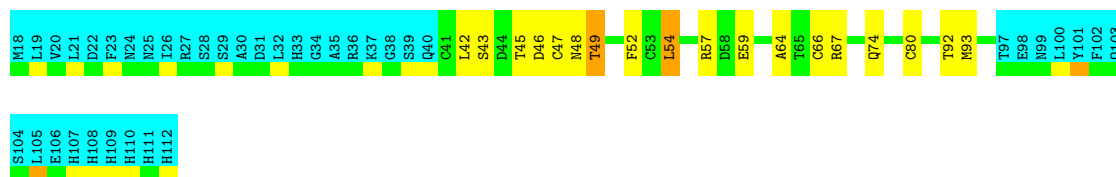
Chain A:  42% 15% 41%



4.2.16 Score per residue for model 16

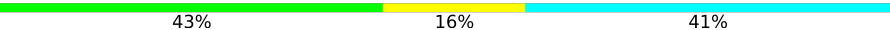
- Molecule 1: Dickkopf-related protein 4

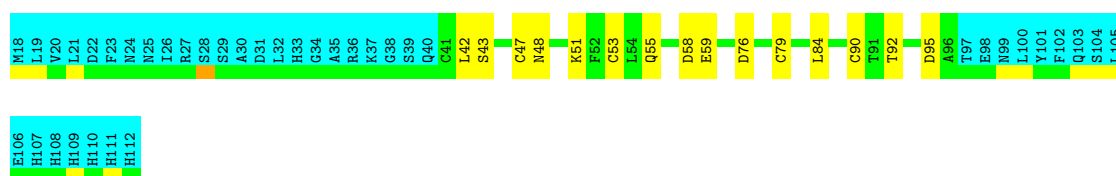
Chain A:  40% 17% 41%



4.2.17 Score per residue for model 17

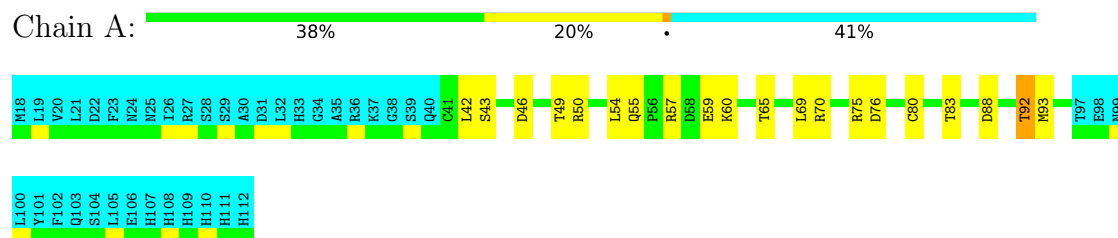
- Molecule 1: Dickkopf-related protein 4

Chain A:  43% 16% 41%



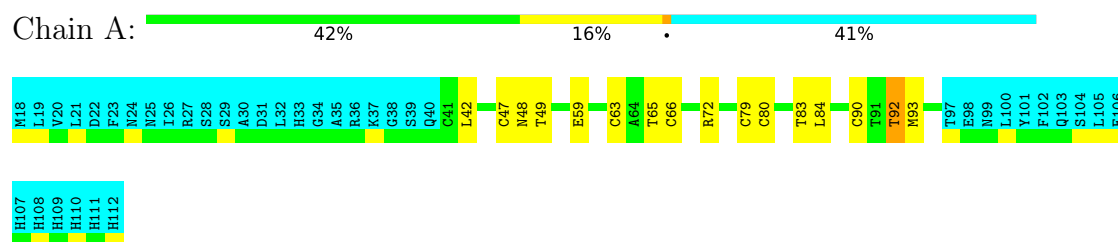
4.2.18 Score per residue for model 18

- Molecule 1: Dickkopf-related protein 4



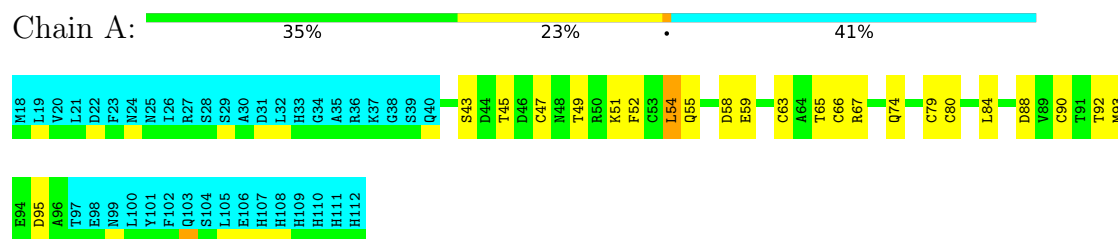
4.2.19 Score per residue for model 19

- Molecule 1: Dickkopf-related protein 4



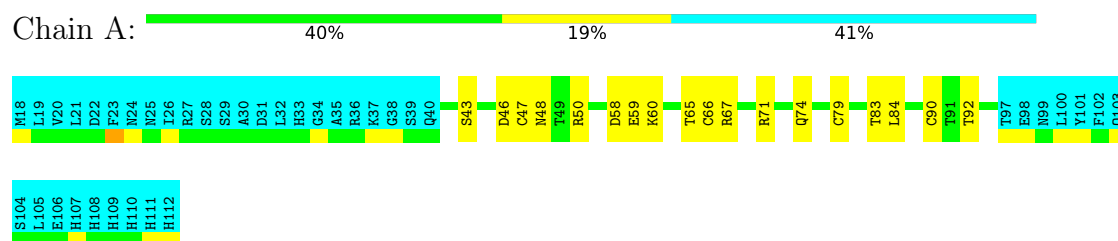
4.2.20 Score per residue for model 20

- Molecule 1: Dickkopf-related protein 4



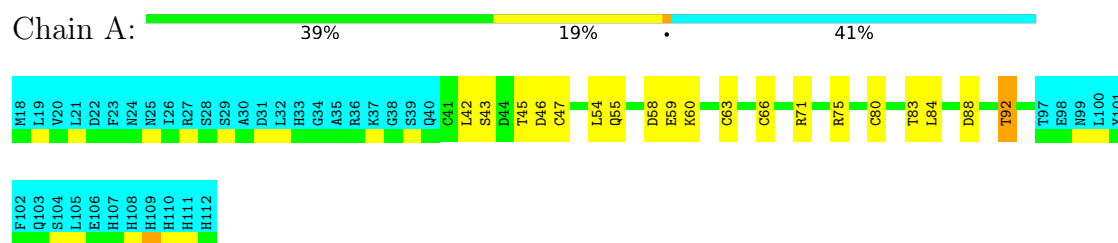
4.2.21 Score per residue for model 21

- Molecule 1: Dickkopf-related protein 4



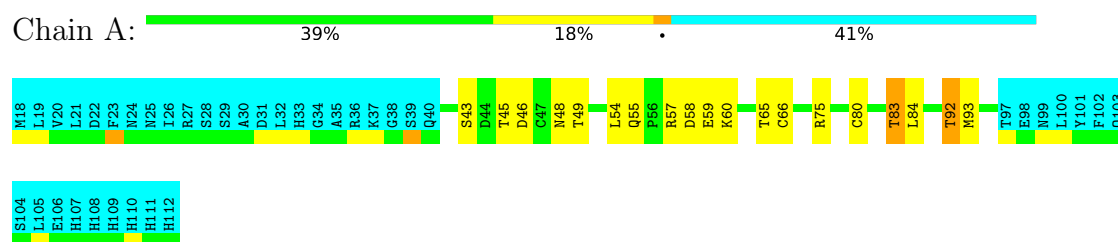
4.2.22 Score per residue for model 22

- Molecule 1: Dickkopf-related protein 4



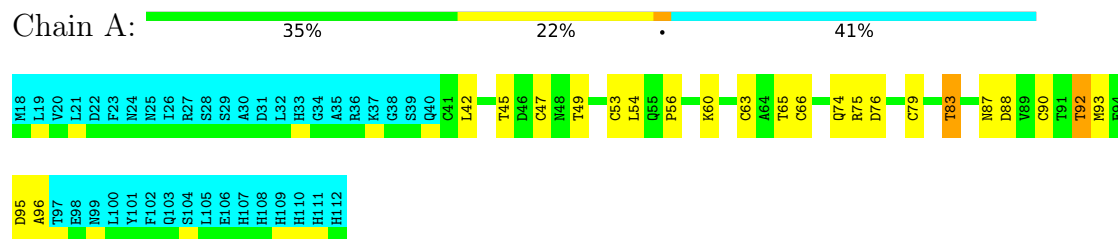
4.2.23 Score per residue for model 23

- Molecule 1: Dickkopf-related protein 4



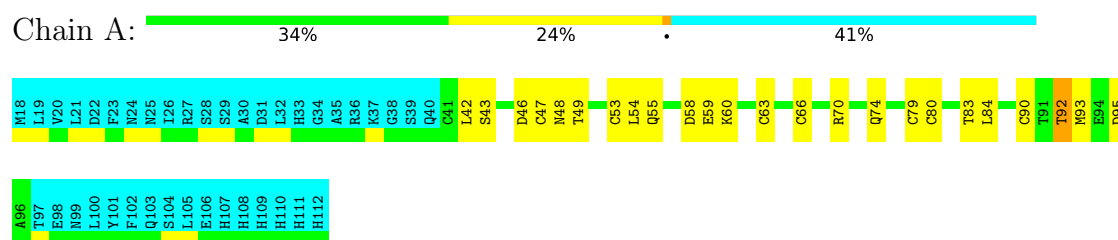
4.2.24 Score per residue for model 24

- Molecule 1: Dickkopf-related protein 4



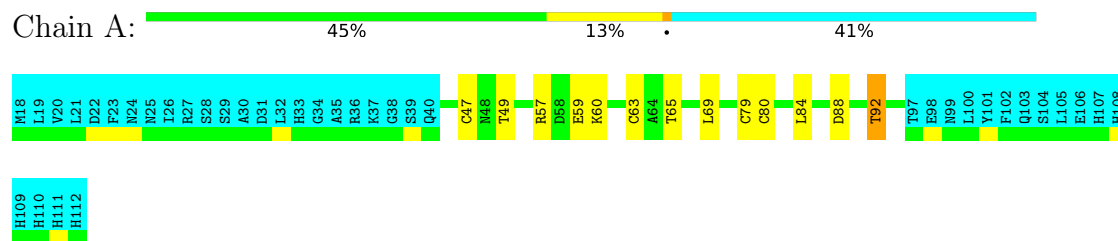
4.2.25 Score per residue for model 25

- Molecule 1: Dickkopf-related protein 4



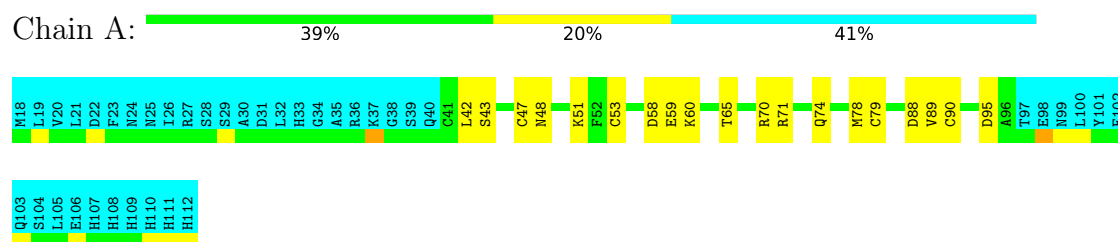
4.2.30 Score per residue for model 30

- Molecule 1: Dickkopf-related protein 4



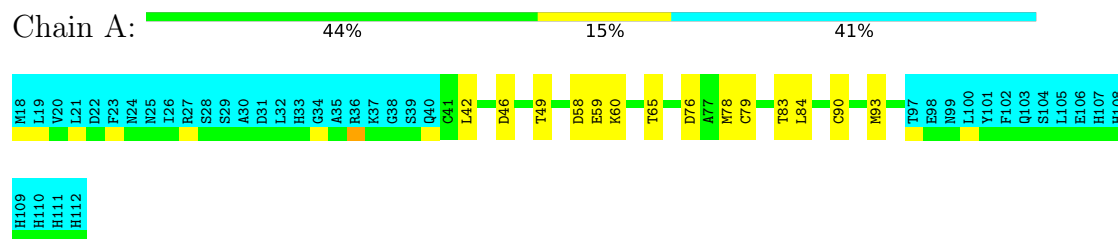
4.2.31 Score per residue for model 31

- Molecule 1: Dickkopf-related protein 4



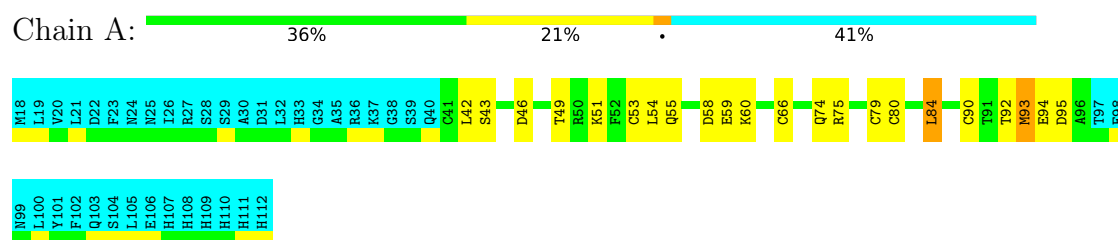
4.2.32 Score per residue for model 32

- Molecule 1: Dickkopf-related protein 4



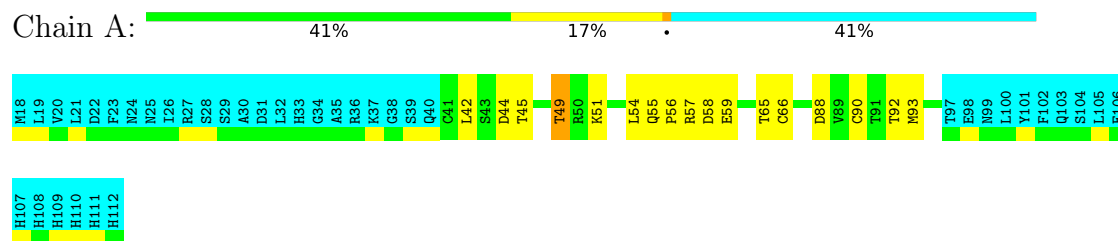
4.2.33 Score per residue for model 33

- Molecule 1: Dickkopf-related protein 4



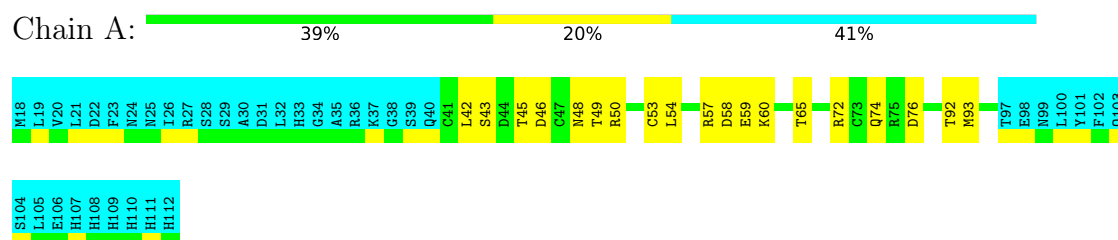
4.2.34 Score per residue for model 34

- Molecule 1: Dickkopf-related protein 4



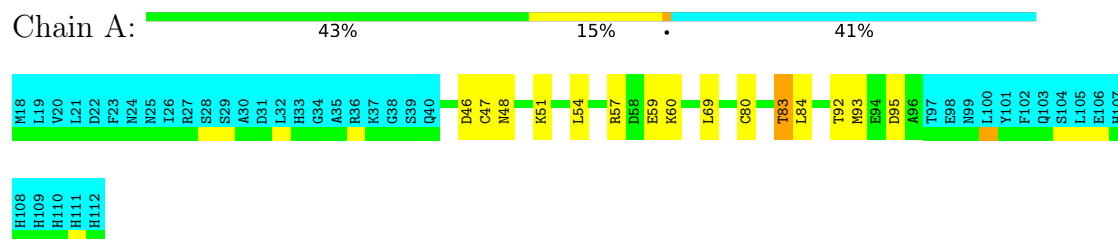
4.2.35 Score per residue for model 35

- Molecule 1: Dickkopf-related protein 4



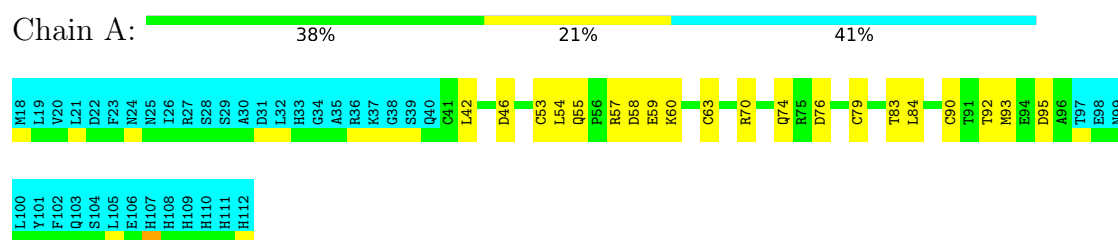
4.2.36 Score per residue for model 36

- Molecule 1: Dickkopf-related protein 4



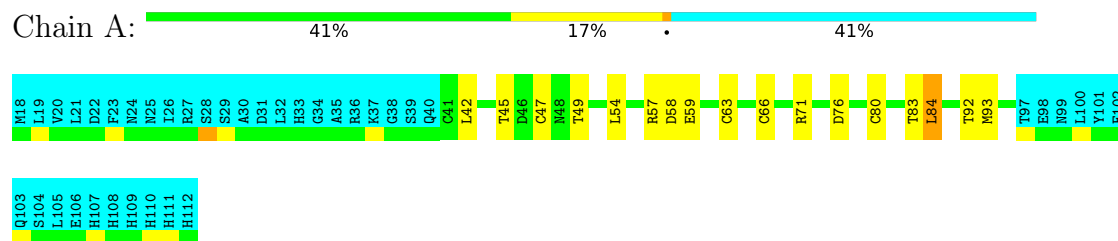
4.2.37 Score per residue for model 37

- Molecule 1: Dickkopf-related protein 4



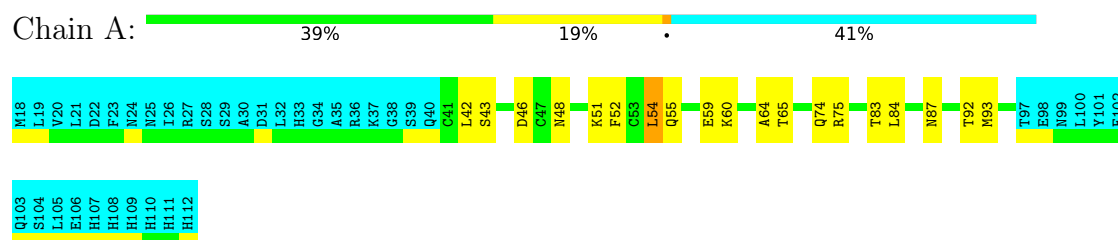
4.2.38 Score per residue for model 38

- Molecule 1: Dickkopf-related protein 4



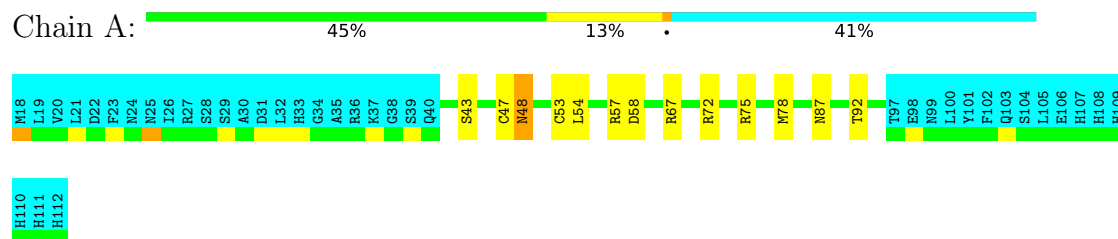
4.2.39 Score per residue for model 39

- Molecule 1: Dickkopf-related protein 4



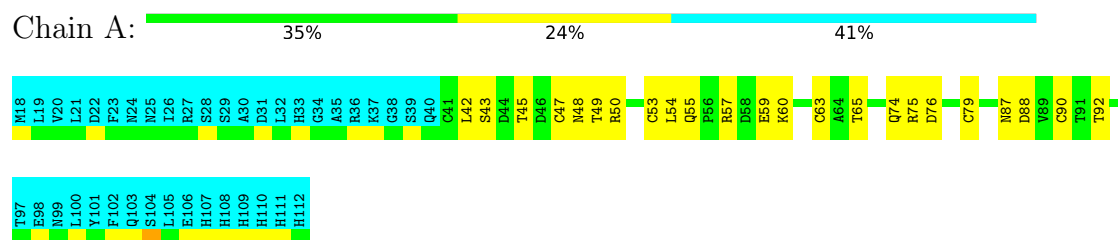
4.2.40 Score per residue for model 40

- Molecule 1: Dickkopf-related protein 4



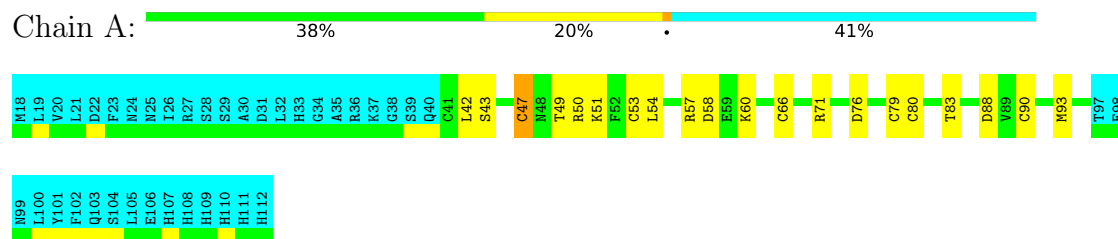
4.2.41 Score per residue for model 41

- Molecule 1: Dickkopf-related protein 4



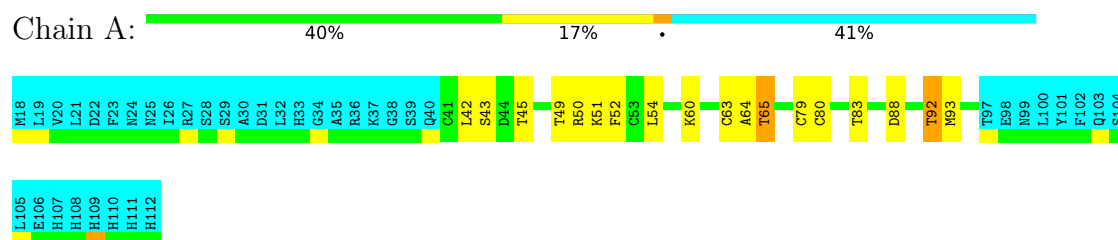
4.2.42 Score per residue for model 42

- Molecule 1: Dickkopf-related protein 4



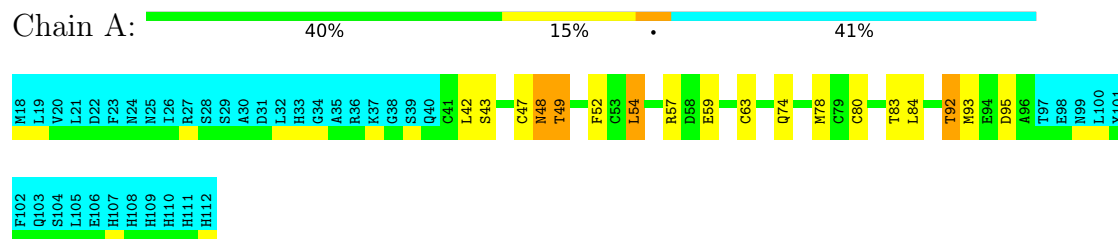
4.2.43 Score per residue for model 43

- Molecule 1: Dickkopf-related protein 4



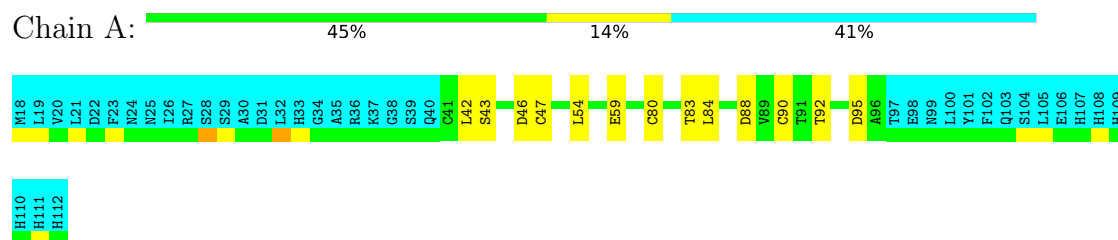
4.2.44 Score per residue for model 44

- Molecule 1: Dickkopf-related protein 4



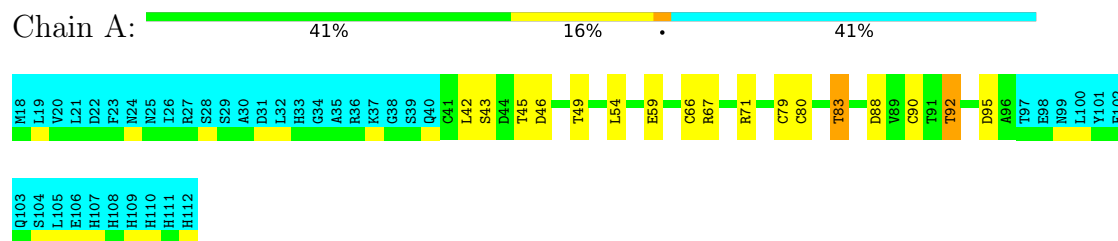
4.2.45 Score per residue for model 45

- Molecule 1: Dickkopf-related protein 4



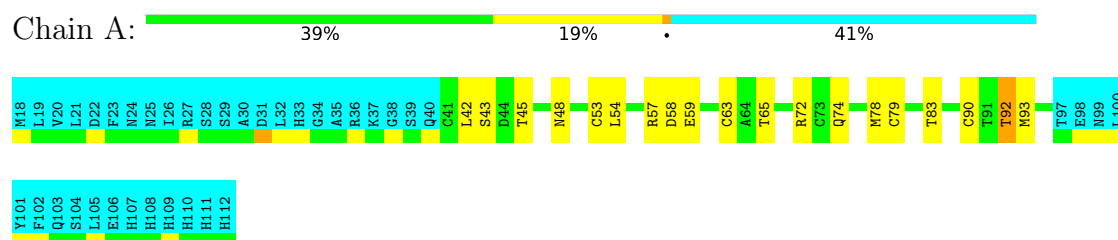
4.2.46 Score per residue for model 46

- Molecule 1: Dickkopf-related protein 4



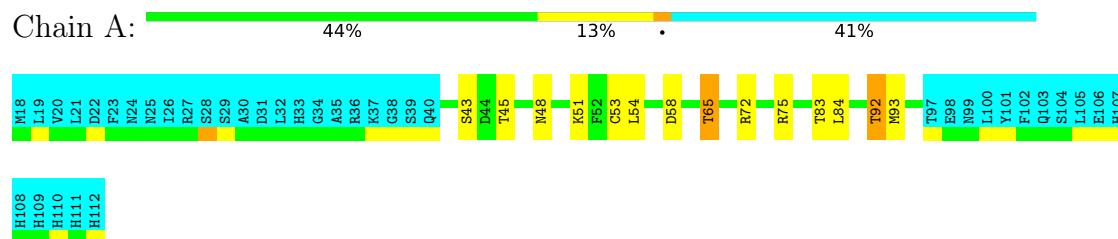
4.2.47 Score per residue for model 47

- Molecule 1: Dickkopf-related protein 4



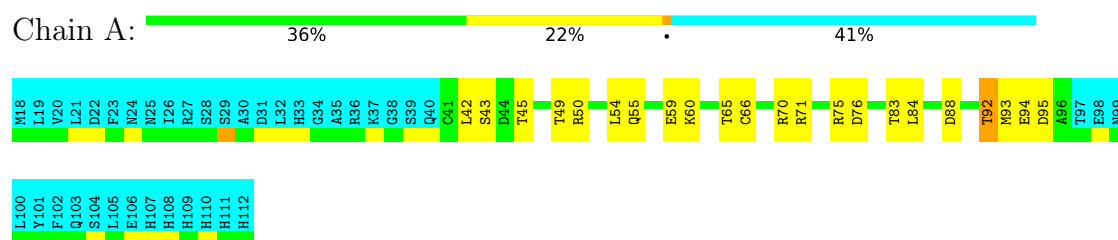
4.2.48 Score per residue for model 48

- Molecule 1: Dickkopf-related protein 4



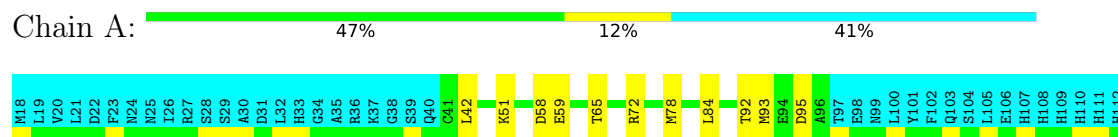
4.2.49 Score per residue for model 49

- Molecule 1: Dickkopf-related protein 4



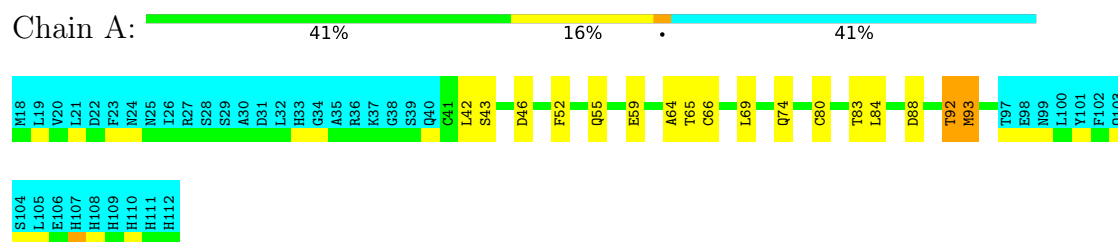
4.2.50 Score per residue for model 50

- Molecule 1: Dickkopf-related protein 4



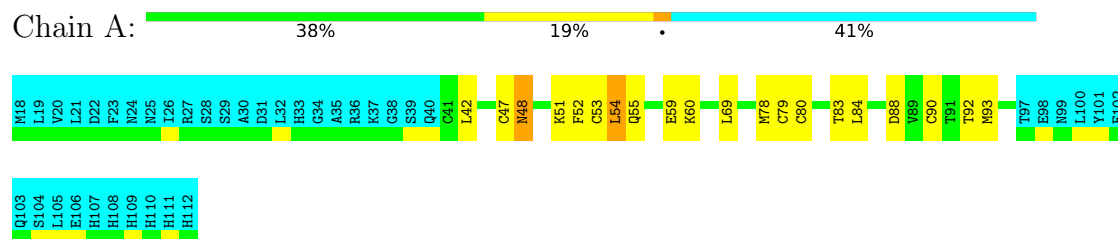
4.2.51 Score per residue for model 51

- Molecule 1: Dickkopf-related protein 4



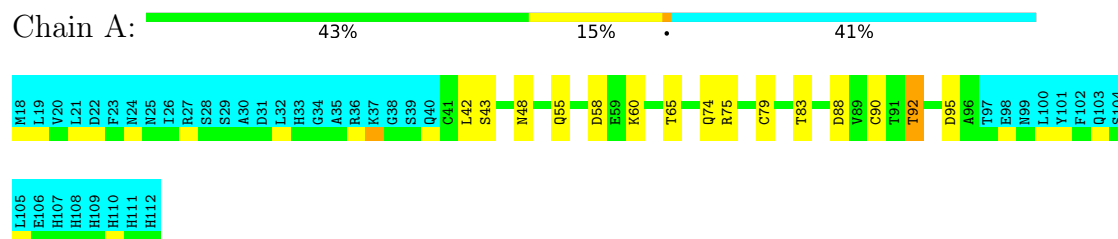
4.2.52 Score per residue for model 52

- Molecule 1: Dickkopf-related protein 4



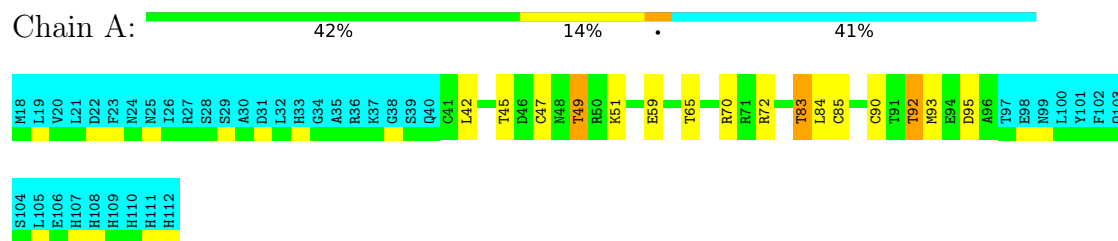
4.2.53 Score per residue for model 53

- Molecule 1: Dickkopf-related protein 4



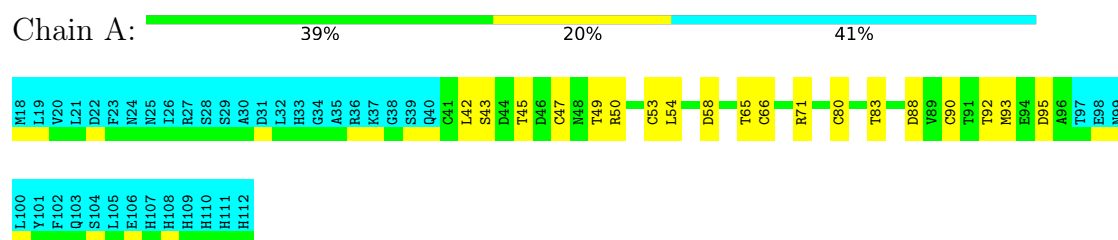
4.2.54 Score per residue for model 54

- Molecule 1: Dickkopf-related protein 4



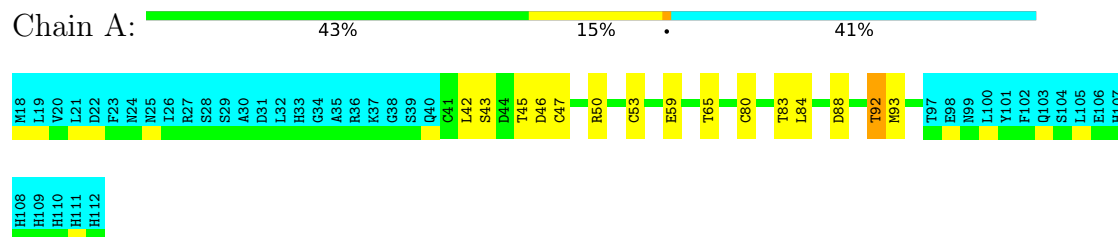
4.2.55 Score per residue for model 55

- Molecule 1: Dickkopf-related protein 4



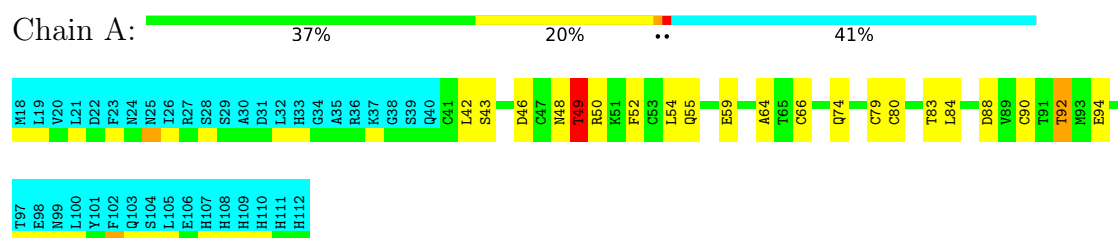
4.2.56 Score per residue for model 56

- Molecule 1: Dickkopf-related protein 4



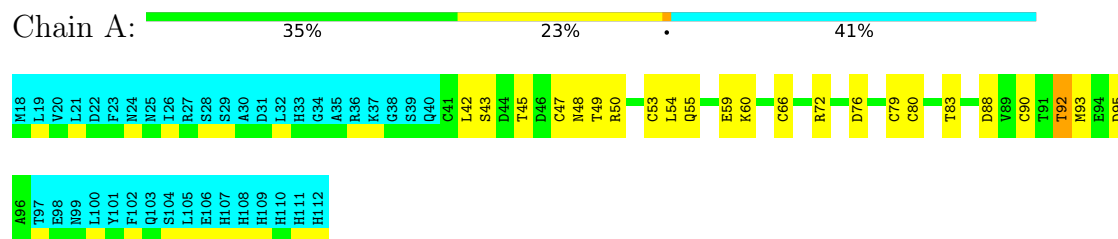
4.2.57 Score per residue for model 57

- Molecule 1: Dickkopf-related protein 4



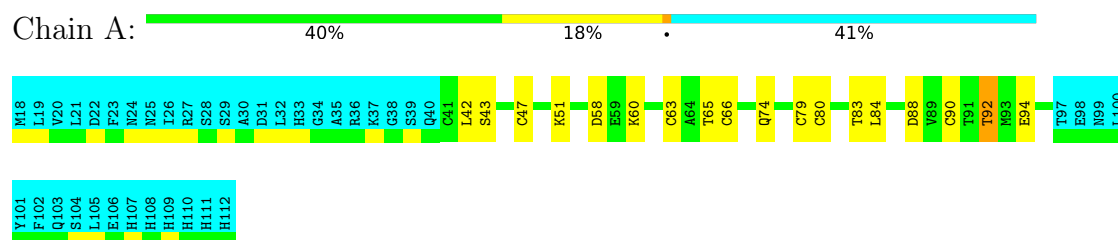
4.2.58 Score per residue for model 58

- Molecule 1: Dickkopf-related protein 4



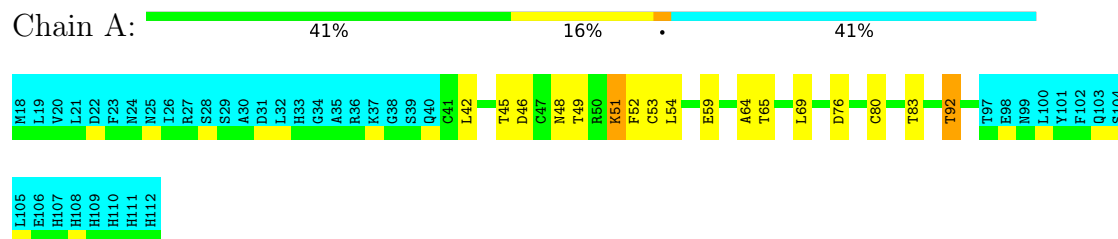
4.2.59 Score per residue for model 59

- Molecule 1: Dickkopf-related protein 4



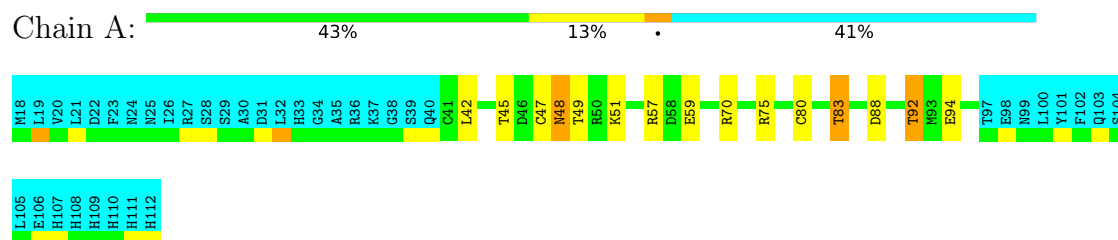
4.2.60 Score per residue for model 60

- Molecule 1: Dickkopf-related protein 4



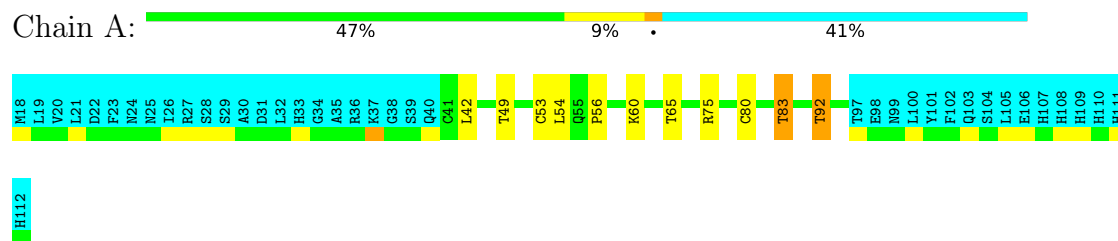
4.2.61 Score per residue for model 61

- Molecule 1: Dickkopf-related protein 4



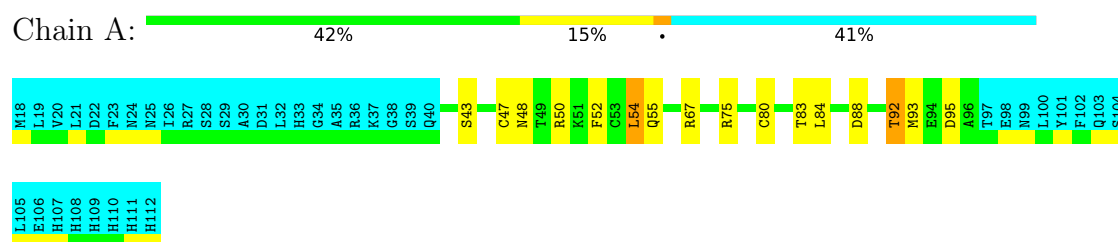
4.2.62 Score per residue for model 62

- Molecule 1: Dickkopf-related protein 4



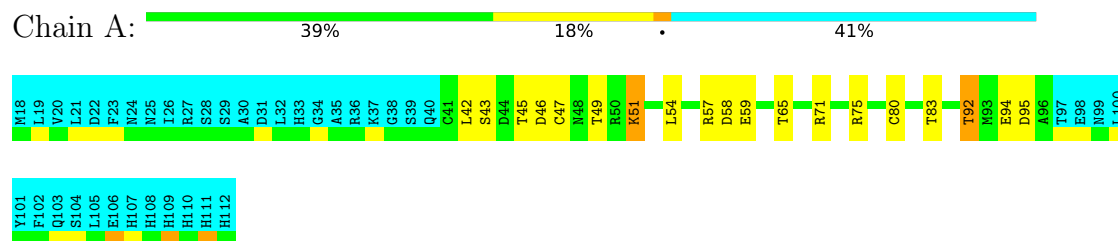
4.2.63 Score per residue for model 63

- Molecule 1: Dickkopf-related protein 4



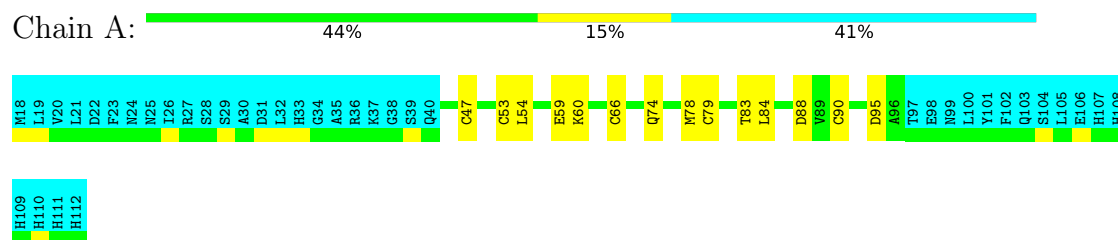
4.2.64 Score per residue for model 64

- Molecule 1: Dickkopf-related protein 4



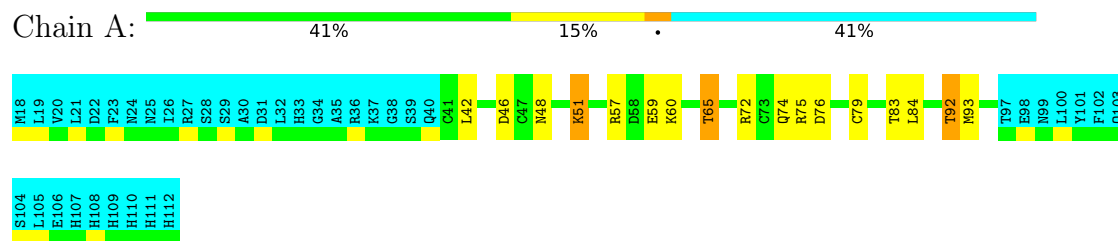
4.2.65 Score per residue for model 65

- Molecule 1: Dickkopf-related protein 4



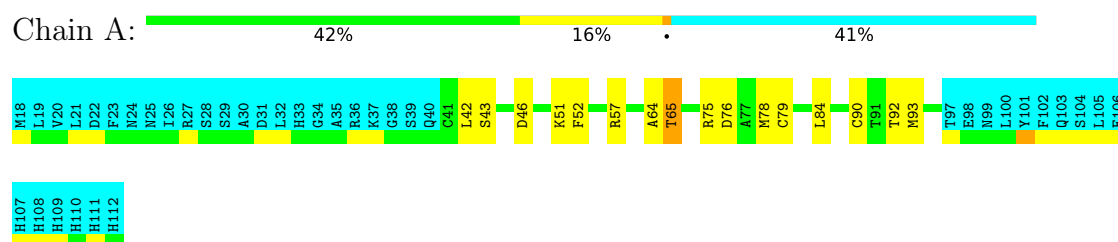
4.2.66 Score per residue for model 66

- Molecule 1: Dickkopf-related protein 4



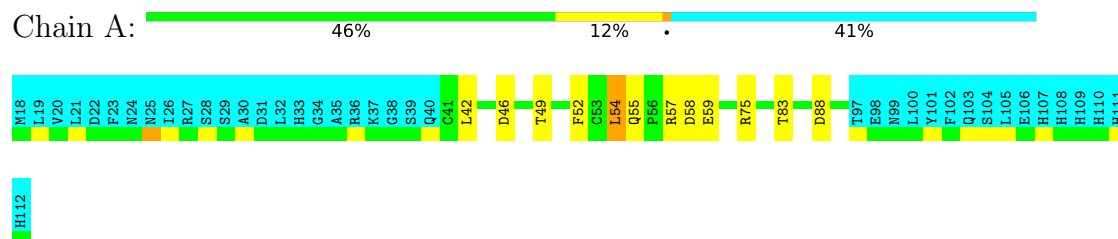
4.2.67 Score per residue for model 67

- Molecule 1: Dickkopf-related protein 4



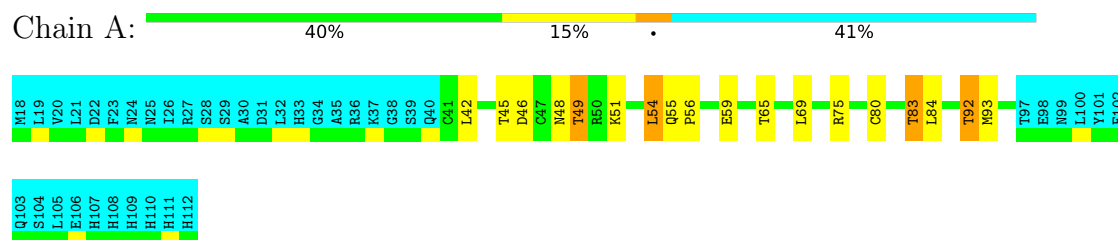
4.2.68 Score per residue for model 68

- Molecule 1: Dickkopf-related protein 4



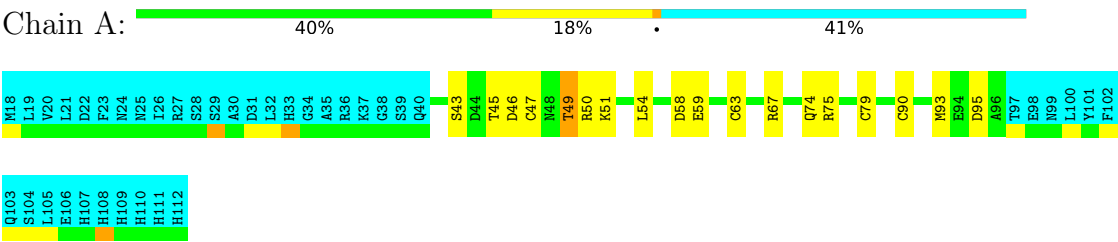
4.2.69 Score per residue for model 69

- Molecule 1: Dickkopf-related protein 4



4.2.70 Score per residue for model 70

● Molecule 1: Dickkopf-related protein 4



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 70 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
CYANA	structure calculation	2.1
CYANA	refinement	2.1

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	912
Number of shifts mapped to atoms	912
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	85%

6 Model quality

6.1 Standard geometry

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

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	431	416	408	2±1
All	All	30170	29120	28560	110

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:PHE:CE1	1:A:64:ALA:HB3	0.66	2.26	51	3
1:A:83:THR:HG22	1:A:92:THR:HG23	0.65	1.67	13	5
1:A:52:PHE:CE1	1:A:54:LEU:HD23	0.63	2.28	63	2
1:A:83:THR:HG22	1:A:92:THR:HA	0.60	1.73	57	37
1:A:83:THR:O	1:A:84:LEU:HD22	0.60	1.94	48	2
1:A:51:LYS:HE3	1:A:65:THR:HG23	0.56	1.77	67	1
1:A:83:THR:C	1:A:84:LEU:HD22	0.55	2.27	51	2
1:A:52:PHE:CE2	1:A:54:LEU:HD23	0.54	2.38	52	6
1:A:51:LYS:HE2	1:A:65:THR:HG23	0.53	1.80	15	4
1:A:51:LYS:HE2	1:A:65:THR:HG22	0.53	1.81	29	3
1:A:69:LEU:CD2	1:A:83:THR:HG21	0.52	2.35	18	3
1:A:51:LYS:CE	1:A:65:THR:HG23	0.51	2.36	60	2
1:A:52:PHE:CE2	1:A:64:ALA:HB3	0.51	2.40	57	5
1:A:54:LEU:HD23	1:A:56:PRO:HD3	0.51	1.83	62	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:LYS:CE	1:A:65:THR:HG22	0.50	2.37	66	1
1:A:69:LEU:HD21	1:A:92:THR:HG23	0.47	1.85	27	3
1:A:54:LEU:CD1	1:A:78:MET:HE3	0.47	2.38	47	1
1:A:84:LEU:HD23	1:A:85:CYS:N	0.47	2.24	54	1
1:A:69:LEU:HD21	1:A:83:THR:HG21	0.47	1.87	69	4
1:A:76:ASP:OD1	1:A:84:LEU:HD12	0.46	2.11	27	2
1:A:84:LEU:HD23	1:A:93:MET:CG	0.45	2.42	38	1
1:A:52:PHE:CZ	1:A:54:LEU:HD12	0.44	2.48	26	3
1:A:70:ARG:O	1:A:89:VAL:HG13	0.44	2.13	31	1
1:A:84:LEU:HD23	1:A:93:MET:HG2	0.44	1.90	51	1
1:A:84:LEU:HD23	1:A:93:MET:HG3	0.43	1.90	33	1
1:A:52:PHE:CD2	1:A:64:ALA:HB3	0.42	2.49	60	1
1:A:54:LEU:HD23	1:A:62:PHE:CE1	0.42	2.49	11	1
1:A:69:LEU:HD13	1:A:92:THR:OG1	0.42	2.15	51	1
1:A:83:THR:HG22	1:A:92:THR:CG2	0.41	2.44	13	2
1:A:48:ASN:O	1:A:49:THR:HG23	0.41	2.15	44	2
1:A:54:LEU:HD23	1:A:62:PHE:CZ	0.41	2.51	5	1
1:A:52:PHE:CE2	1:A:54:LEU:HD12	0.41	2.51	28	1
1:A:54:LEU:HD23	1:A:62:PHE:CE2	0.40	2.51	7	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	56/95 (59%)	52±2 (93±3%)	4±2 (6±3%)	0±1 (1±1%)	18	68
All	All	3920/6650 (59%)	3642 (93%)	247 (6%)	31 (1%)	18	68

All 4 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	49	THR	17
1	A	48	ASN	10
1	A	96	ALA	3

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Mol	Chain	Res	Type	Models (Total)
1	A	47	CYS	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	51/86 (59%)	36±3 (70±6%)	15±3 (30±6%)	1	16
All	All	3570/6020 (59%)	2494 (70%)	1076 (30%)	1	16

All 39 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	42	LEU	56
1	A	92	THR	55
1	A	59	GLU	48
1	A	93	MET	47
1	A	54	LEU	42
1	A	43	SER	39
1	A	47	CYS	37
1	A	65	THR	37
1	A	84	LEU	36
1	A	90	CYS	36
1	A	46	ASP	35
1	A	79	CYS	35
1	A	80	CYS	34
1	A	45	THR	34
1	A	60	LYS	33
1	A	49	THR	33
1	A	88	ASP	32
1	A	58	ASP	31
1	A	83	THR	30
1	A	53	CYS	28
1	A	74	GLN	27
1	A	55	GLN	26
1	A	95	ASP	26
1	A	66	CYS	26

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Mol	Chain	Res	Type	Models (Total)
1	A	75	ARG	25
1	A	63	CYS	24
1	A	57	ARG	23
1	A	51	LYS	22
1	A	48	ASN	21
1	A	50	ARG	19
1	A	76	ASP	13
1	A	67	ARG	12
1	A	72	ARG	12
1	A	78	MET	11
1	A	71	ARG	10
1	A	94	GLU	9
1	A	70	ARG	6
1	A	87	ASN	5
1	A	44	ASP	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 85% for the well-defined parts and 72% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *Dkk4n_BMRB2.txt*

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	912
Number of shifts mapped to atoms	912
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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	79	0.50 ± 0.27	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	74	-0.18 ± 0.29	None needed (< 0.5 ppm)
$^{13}\text{C}'$	74	0.56 ± 0.10	Should be applied
^{15}N	76	1.12 ± 0.38	Should be applied

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 85%, i.e. 615 atoms were assigned a chemical shift out of a possible 726. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	269/276 (97%)	110/111 (99%)	107/112 (96%)	52/53 (98%)
Sidechain	337/430 (78%)	229/274 (84%)	108/129 (84%)	0/27 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	9/20 (45%)	9/10 (90%)	0/10 (0%)	0/0 (—%)
Overall	615/726 (85%)	348/395 (88%)	215/251 (86%)	52/80 (65%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 72%, i.e. 912 atoms were assigned a chemical shift out of a possible 1274. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	392/473 (83%)	163/191 (85%)	153/190 (81%)	76/92 (83%)
Sidechain	497/696 (71%)	342/446 (77%)	155/211 (73%)	0/39 (0%)
Aromatic	23/105 (22%)	23/52 (44%)	0/39 (0%)	0/14 (0%)
Overall	912/1274 (72%)	528/689 (77%)	308/440 (70%)	76/145 (52%)

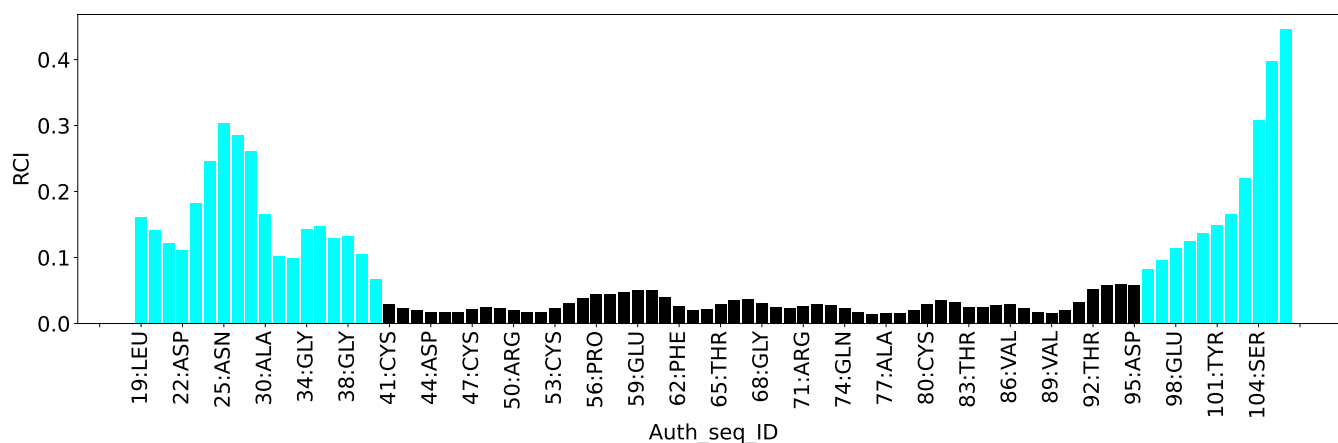
7.1.4 Statistically unusual chemical shifts [i](#)

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

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$)	172
Sequential ($ i-j =1$)	141
Medium range ($ i-j >1$ and $ i-j <5$)	62
Long range ($ i-j \geq 5$)	132
Inter-chain	0
Hydrogen bond restraints	6
Disulfide bond restraints	5
Total dihedral-angle restraints	90
Number of unmapped restraints	0
Number of restraints per residue	6.4
Number of long range restraints per residue ¹	1.5

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)	0.2	0.16
0.2-0.5 (Medium)	0.0	0.29
>0.5 (Large)	None	None

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	1.0	2.47
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

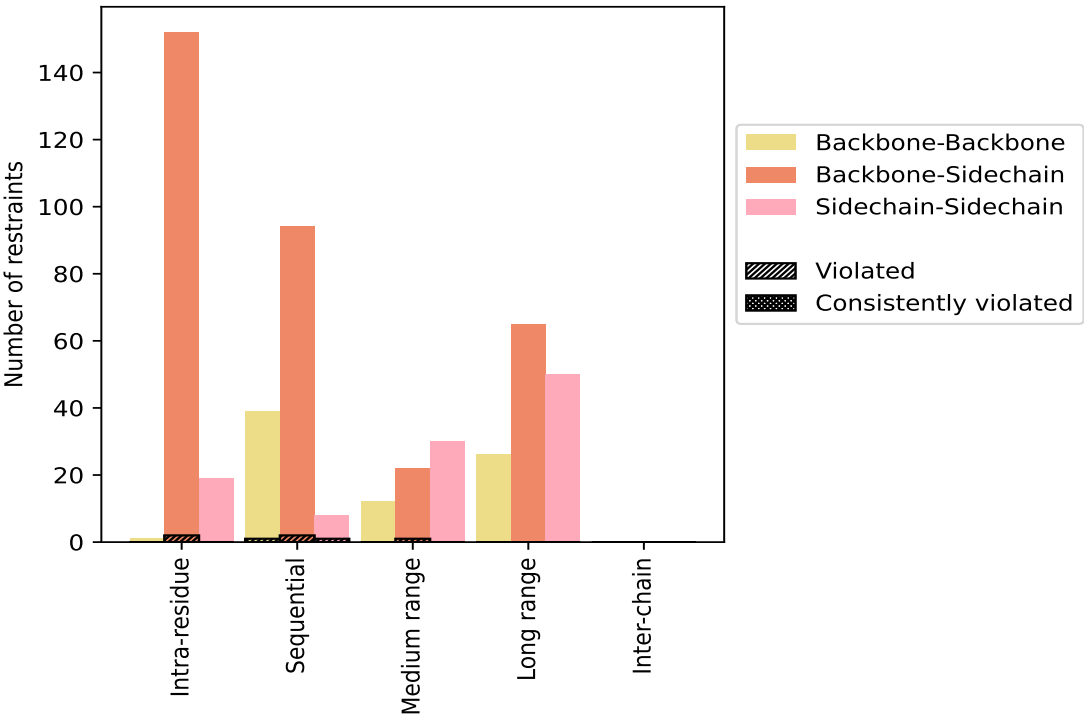
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	172	33.2	2	1.2	0.4	0	0.0	0.0
Backbone-Backbone	1	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	152	29.3	2	1.3	0.4	0	0.0	0.0
Sidechain-Sidechain	19	3.7	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	141	27.2	4	2.8	0.8	0	0.0	0.0
Backbone-Backbone	39	7.5	1	2.6	0.2	0	0.0	0.0
Backbone-Sidechain	94	18.1	2	2.1	0.4	0	0.0	0.0
Sidechain-Sidechain	8	1.5	1	12.5	0.2	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	62	12.0	1	1.6	0.2	0	0.0	0.0
Backbone-Backbone	12	2.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	20	3.9	1	5.0	0.2	0	0.0	0.0
Sidechain-Sidechain	30	5.8	0	0.0	0.0	0	0.0	0.0
Long range ($i-j \geq 5$)	132	25.5	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	26	5.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	61	11.8	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	45	8.7	0	0.0	0.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	6	1.2	0	0.0	0.0	0	0.0	0.0
Disulfide bond	5	1.0	0	0.0	0.0	0	0.0	0.0
Total	518	100.0	7	1.4	1.4	0	0.0	0.0
Backbone-Backbone	78	15.1	1	1.3	0.2	0	0.0	0.0
Backbone-Sidechain	333	64.3	5	1.5	1.0	0	0.0	0.0
Sidechain-Sidechain	107	20.7	1	0.9	0.2	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	0	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0	0	0	0.0	0.0	0.0	0.0
6	0	0	0	0	0	0	0.0	0.0	0.0	0.0
7	0	0	0	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	0	0	0	0.0	0.0	0.0	0.0
10	0	0	0	0	0	0	0.0	0.0	0.0	0.0

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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	0	0	0	0	0.0	0.0	0.0	0.0
12	0	0	0	0	0	0	0.0	0.0	0.0	0.0
13	0	0	0	0	0	0	0.0	0.0	0.0	0.0
14	0	0	0	0	0	0	0.0	0.0	0.0	0.0
15	0	0	0	0	0	0	0.0	0.0	0.0	0.0
16	0	0	0	0	0	0	0.0	0.0	0.0	0.0
17	0	0	0	0	0	0	0.0	0.0	0.0	0.0
18	0	0	0	0	0	0	0.0	0.0	0.0	0.0
19	0	0	0	0	0	0	0.0	0.0	0.0	0.0
20	0	0	0	0	0	0	0.0	0.0	0.0	0.0
21	0	0	0	0	0	0	0.0	0.0	0.0	0.0
22	0	0	0	0	0	0	0.0	0.0	0.0	0.0
23	0	0	0	0	0	0	0.0	0.0	0.0	0.0
24	0	0	0	0	0	0	0.0	0.0	0.0	0.0
25	0	0	0	0	0	0	0.0	0.0	0.0	0.0
26	1	0	0	0	0	1	0.11	0.11	0.0	0.11
27	0	0	0	0	0	0	0.0	0.0	0.0	0.0
28	0	0	0	0	0	0	0.0	0.0	0.0	0.0
29	0	0	0	0	0	0	0.0	0.0	0.0	0.0
30	0	0	0	0	0	0	0.0	0.0	0.0	0.0
31	0	0	0	0	0	0	0.0	0.0	0.0	0.0
32	0	0	0	0	0	0	0.0	0.0	0.0	0.0
33	1	0	0	0	0	1	0.14	0.14	0.0	0.14
34	1	0	0	0	0	1	0.14	0.14	0.0	0.14
35	0	0	0	0	0	0	0.0	0.0	0.0	0.0
36	1	0	0	0	0	1	0.14	0.14	0.0	0.14
37	0	0	0	0	0	0	0.0	0.0	0.0	0.0
38	0	0	0	0	0	0	0.0	0.0	0.0	0.0
39	0	0	0	0	0	0	0.0	0.0	0.0	0.0
40	1	0	0	0	0	1	0.14	0.14	0.0	0.14
41	0	0	0	0	0	0	0.0	0.0	0.0	0.0
42	1	0	0	0	0	1	0.14	0.14	0.0	0.14
43	1	0	0	0	0	1	0.16	0.16	0.0	0.16
44	0	0	0	0	0	0	0.0	0.0	0.0	0.0
45	0	0	0	0	0	0	0.0	0.0	0.0	0.0
46	0	0	0	0	0	0	0.0	0.0	0.0	0.0
47	0	0	0	0	0	0	0.0	0.0	0.0	0.0
48	0	0	0	0	0	0	0.0	0.0	0.0	0.0
49	0	0	0	0	0	0	0.0	0.0	0.0	0.0
50	0	0	0	0	0	0	0.0	0.0	0.0	0.0
51	0	1	0	0	0	1	0.16	0.16	0.0	0.16

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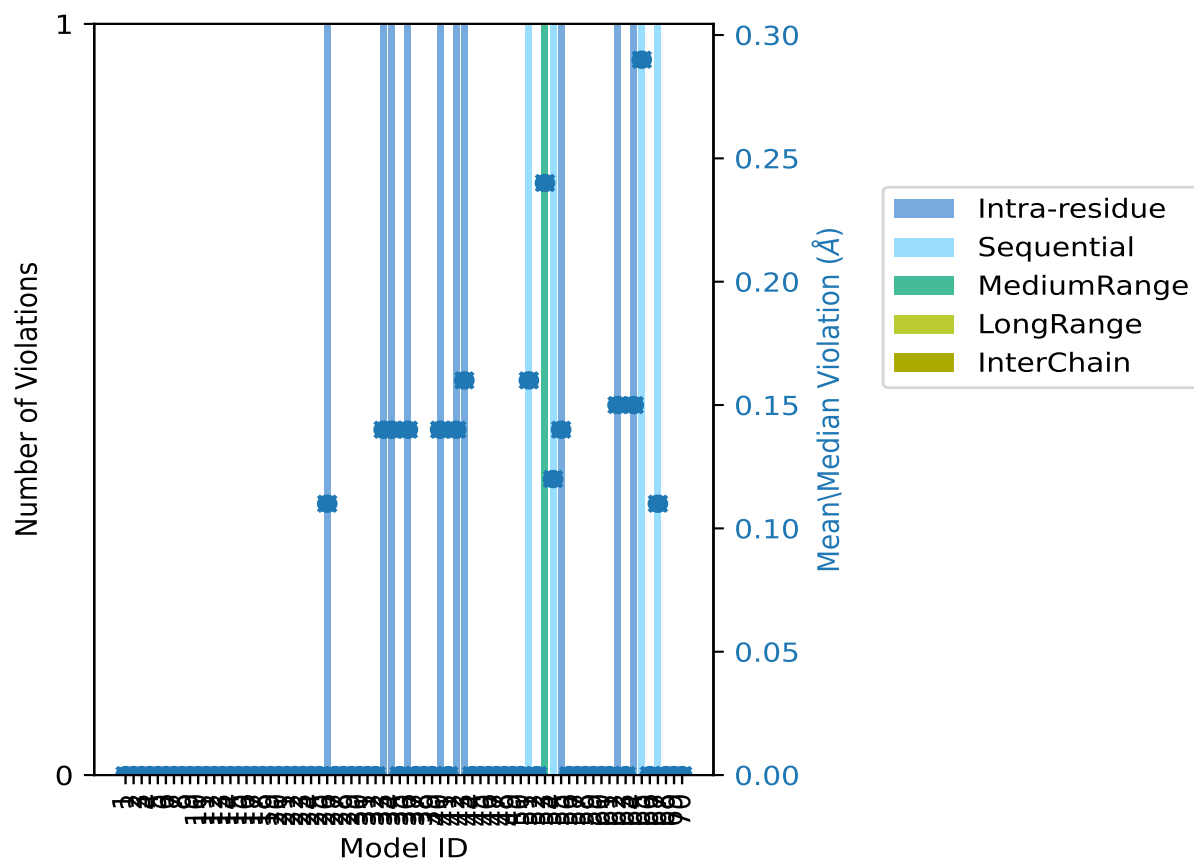
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
52	0	0	0	0	0	0	0.0	0.0	0.0	0.0
53	0	0	1	0	0	1	0.24	0.24	0.0	0.24
54	0	1	0	0	0	1	0.12	0.12	0.0	0.12
55	1	0	0	0	0	1	0.14	0.14	0.0	0.14
56	0	0	0	0	0	0	0.0	0.0	0.0	0.0
57	0	0	0	0	0	0	0.0	0.0	0.0	0.0
58	0	0	0	0	0	0	0.0	0.0	0.0	0.0
59	0	0	0	0	0	0	0.0	0.0	0.0	0.0
60	0	0	0	0	0	0	0.0	0.0	0.0	0.0
61	0	0	0	0	0	0	0.0	0.0	0.0	0.0
62	1	0	0	0	0	1	0.15	0.15	0.0	0.15
63	0	0	0	0	0	0	0.0	0.0	0.0	0.0
64	1	0	0	0	0	1	0.15	0.15	0.0	0.15
65	0	1	0	0	0	1	0.29	0.29	0.0	0.29
66	0	0	0	0	0	0	0.0	0.0	0.0	0.0
67	0	1	0	0	0	1	0.11	0.11	0.0	0.11
68	0	0	0	0	0	0	0.0	0.0	0.0	0.0
69	0	0	0	0	0	0	0.0	0.0	0.0	0.0
70	0	0	0	0	0	0	0.0	0.0	0.0	0.0

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, 500(IR:170, SQ:137, MR:61, LR:132, 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	%
1	4	1	0	0	6	1	1.4
0	0	0	0	0	0	2	2.9
0	0	0	0	0	0	3	4.3
0	0	0	0	0	0	4	5.7
0	0	0	0	0	0	5	7.1
0	0	0	0	0	0	6	8.6

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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	0	0	0	0	7	10.0
0	0	0	0	0	0	8	11.4
1	0	0	0	0	1	9	12.9
0	0	0	0	0	0	10	14.3
0	0	0	0	0	0	11	15.7
0	0	0	0	0	0	12	17.1
0	0	0	0	0	0	13	18.6
0	0	0	0	0	0	14	20.0
0	0	0	0	0	0	15	21.4
0	0	0	0	0	0	16	22.9
0	0	0	0	0	0	17	24.3
0	0	0	0	0	0	18	25.7
0	0	0	0	0	0	19	27.1
0	0	0	0	0	0	20	28.6
0	0	0	0	0	0	21	30.0
0	0	0	0	0	0	22	31.4
0	0	0	0	0	0	23	32.9
0	0	0	0	0	0	24	34.3
0	0	0	0	0	0	25	35.7
0	0	0	0	0	0	26	37.1
0	0	0	0	0	0	27	38.6
0	0	0	0	0	0	28	40.0
0	0	0	0	0	0	29	41.4
0	0	0	0	0	0	30	42.9
0	0	0	0	0	0	31	44.3
0	0	0	0	0	0	32	45.7
0	0	0	0	0	0	33	47.1
0	0	0	0	0	0	34	48.6
0	0	0	0	0	0	35	50.0
0	0	0	0	0	0	36	51.4
0	0	0	0	0	0	37	52.9
0	0	0	0	0	0	38	54.3
0	0	0	0	0	0	39	55.7
0	0	0	0	0	0	40	57.1
0	0	0	0	0	0	41	58.6
0	0	0	0	0	0	42	60.0
0	0	0	0	0	0	43	61.4
0	0	0	0	0	0	44	62.9
0	0	0	0	0	0	45	64.3
0	0	0	0	0	0	46	65.7
0	0	0	0	0	0	47	67.1

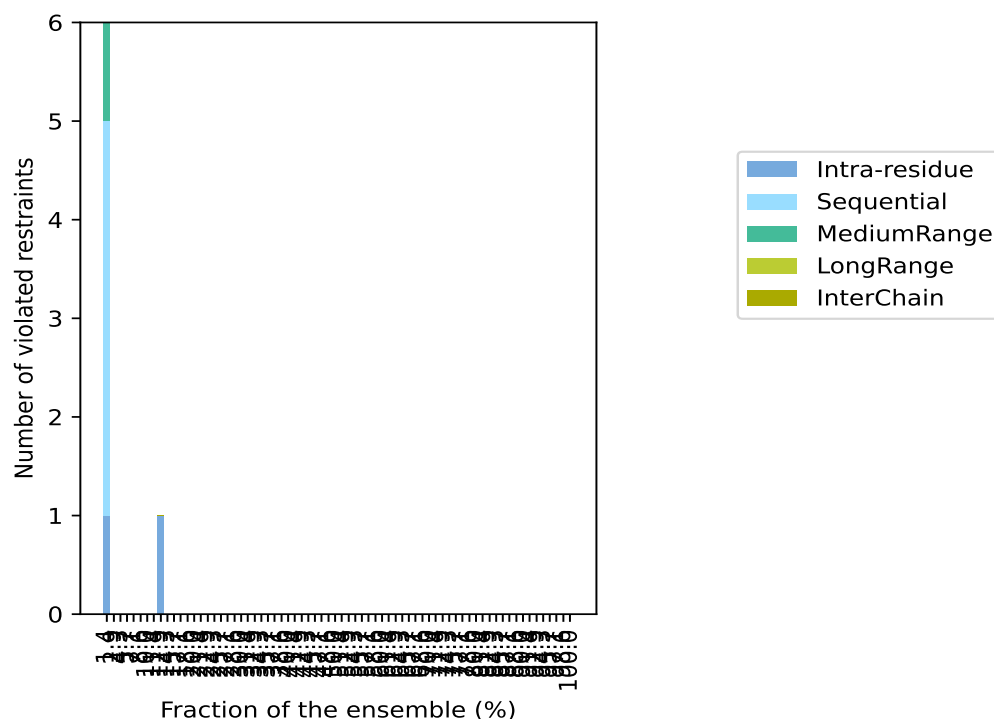
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	48	68.6
0	0	0	0	0	0	49	70.0
0	0	0	0	0	0	50	71.4
0	0	0	0	0	0	51	72.9
0	0	0	0	0	0	52	74.3
0	0	0	0	0	0	53	75.7
0	0	0	0	0	0	54	77.1
0	0	0	0	0	0	55	78.6
0	0	0	0	0	0	56	80.0
0	0	0	0	0	0	57	81.4
0	0	0	0	0	0	58	82.9
0	0	0	0	0	0	59	84.3
0	0	0	0	0	0	60	85.7
0	0	0	0	0	0	61	87.1
0	0	0	0	0	0	62	88.6
0	0	0	0	0	0	63	90.0
0	0	0	0	0	0	64	91.4
0	0	0	0	0	0	65	92.9
0	0	0	0	0	0	66	94.3
0	0	0	0	0	0	67	95.7
0	0	0	0	0	0	68	97.1
0	0	0	0	0	0	69	98.6
0	0	0	0	0	0	70	100.0

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

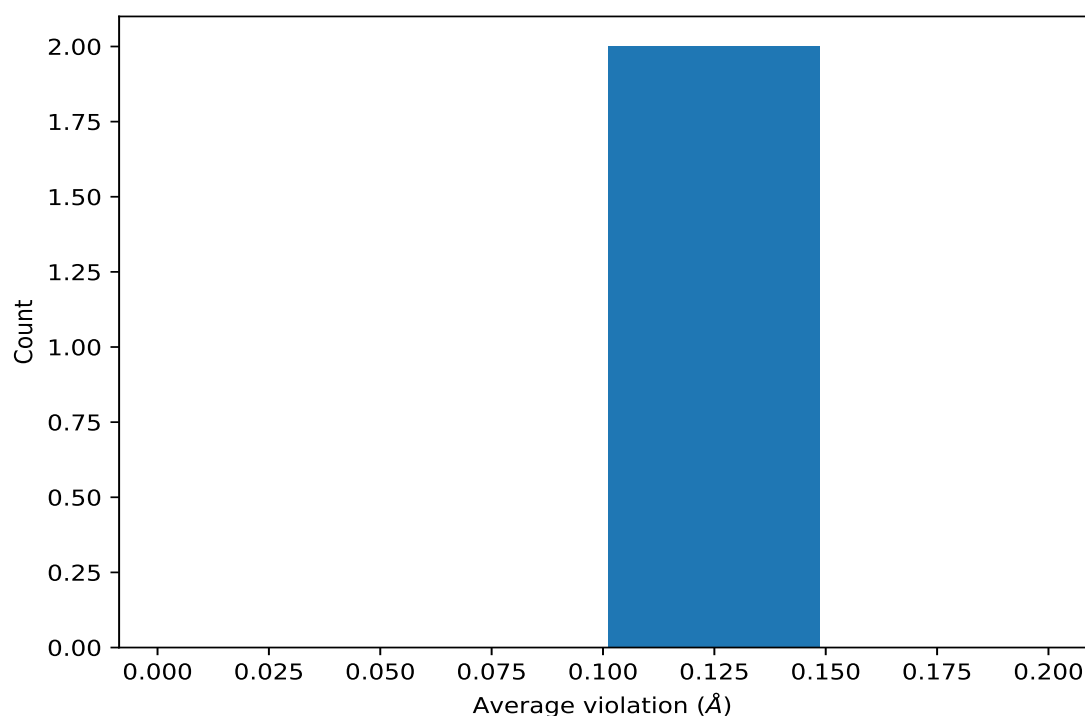
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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.

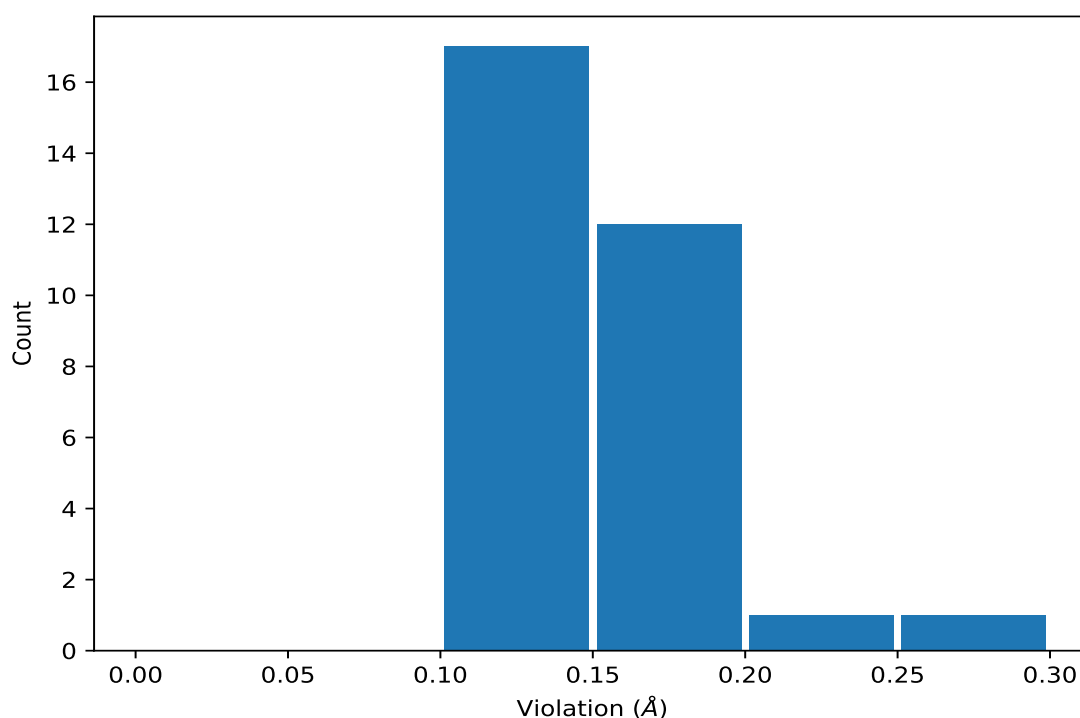
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,364)	1:55:A:GLN:H	1:55:A:GLN:HG2	9	0.14	0.01	0.14
(3,364)	1:55:A:GLN:H	1:55:A:GLN:HG3	9	0.14	0.01	0.14

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)
(3,25)	1:97:A:THR:H	1:98:A:GLU:H	65	0.29
(3,172)	1:92:A:THR:HB	1:94:A:GLU:H	53	0.24
(3,448)	1:76:A:ASP:HB2	1:77:A:ALA:HB1	51	0.16
(3,448)	1:76:A:ASP:HB2	1:77:A:ALA:HB2	51	0.16
(3,448)	1:76:A:ASP:HB2	1:77:A:ALA:HB3	51	0.16
(3,448)	1:76:A:ASP:HB3	1:77:A:ALA:HB1	51	0.16
(3,448)	1:76:A:ASP:HB3	1:77:A:ALA:HB2	51	0.16
(3,448)	1:76:A:ASP:HB3	1:77:A:ALA:HB3	51	0.16
(3,364)	1:55:A:GLN:H	1:55:A:GLN:HG2	43	0.16
(3,364)	1:55:A:GLN:H	1:55:A:GLN:HG3	43	0.16
(3,364)	1:55:A:GLN:H	1:55:A:GLN:HG2	62	0.15
(3,364)	1:55:A:GLN:H	1:55:A:GLN:HG3	62	0.15
(3,364)	1:55:A:GLN:H	1:55:A:GLN:HG2	64	0.15
(3,364)	1:55:A:GLN:H	1:55:A:GLN:HG3	64	0.15
(3,364)	1:55:A:GLN:H	1:55:A:GLN:HG2	33	0.14
(3,364)	1:55:A:GLN:H	1:55:A:GLN:HG3	33	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,364)	1:55:A:GLN:H	1:55:A:GLN:HG2	34	0.14
(3,364)	1:55:A:GLN:H	1:55:A:GLN:HG3	34	0.14
(3,364)	1:55:A:GLN:H	1:55:A:GLN:HG2	36	0.14
(3,364)	1:55:A:GLN:H	1:55:A:GLN:HG3	36	0.14
(3,364)	1:55:A:GLN:H	1:55:A:GLN:HG2	40	0.14
(3,364)	1:55:A:GLN:H	1:55:A:GLN:HG3	40	0.14
(3,364)	1:55:A:GLN:H	1:55:A:GLN:HG2	42	0.14
(3,364)	1:55:A:GLN:H	1:55:A:GLN:HG3	42	0.14
(3,364)	1:55:A:GLN:H	1:55:A:GLN:HG2	55	0.14
(3,364)	1:55:A:GLN:H	1:55:A:GLN:HG3	55	0.14
(3,306)	1:52:A:PHE:HD1	1:53:A:CYS:HA	54	0.12
(3,306)	1:52:A:PHE:HD2	1:53:A:CYS:HA	54	0.12
(3,499)	1:100:A:LEU:H	1:100:A:LEU:HB2	26	0.11
(3,499)	1:100:A:LEU:H	1:100:A:LEU:HB3	26	0.11
(3,7)	1:49:A:THR:HB	1:50:A:ARG:H	67	0.11

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

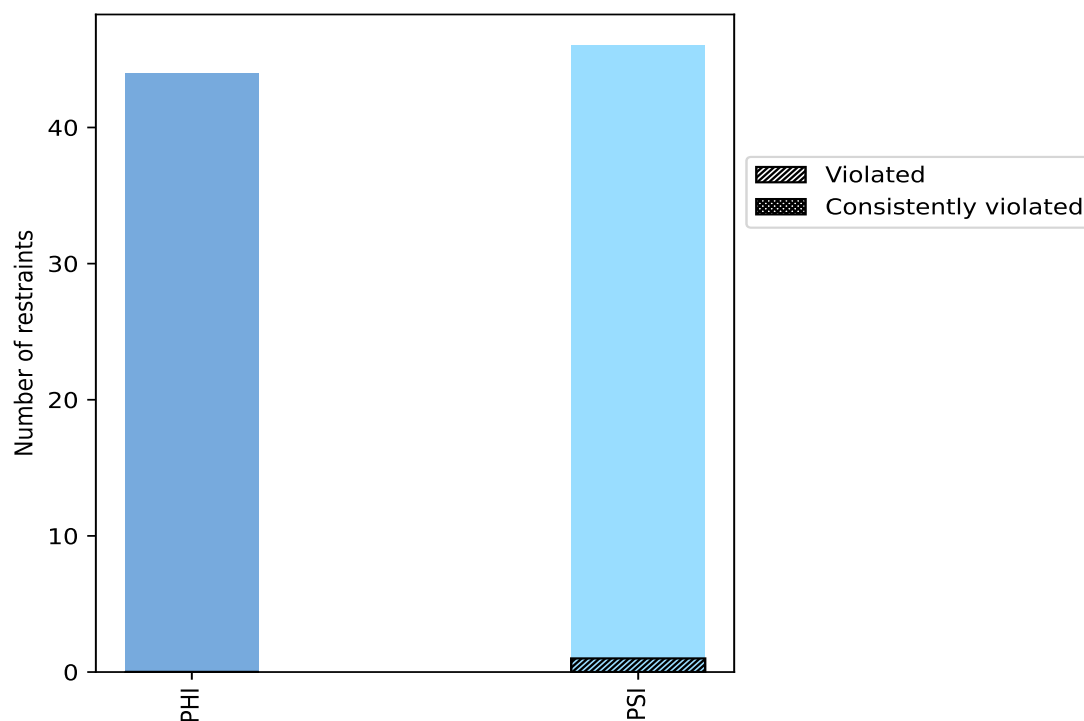
10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	44	48.9	0	0.0	0.0	0	0.0	0.0
PSI	46	51.1	1	2.2	1.1	0	0.0	0.0
Total	90	100.0	1	1.1	1.1	0	0.0	0.0

¹ percentage calculated with respect to total number of dihedral-angle restraints, ² percentage calculated with respect to number of restraints in a particular dihedral-angle type, ³ violated in at least one model, ⁴ violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



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

10.2 Dihedral-angle violation statistics for each model [i](#)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

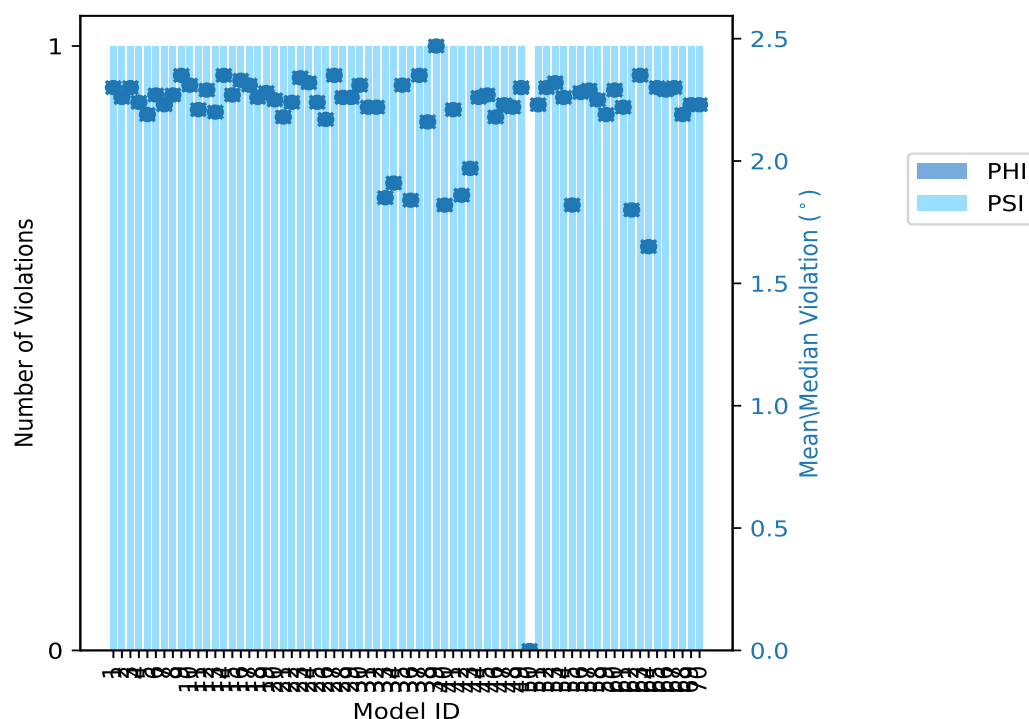
Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	0	1	1	2.3	2.3	0.0	2.3
2	0	1	1	2.26	2.26	0.0	2.26
3	0	1	1	2.3	2.3	0.0	2.3
4	0	1	1	2.24	2.24	0.0	2.24
5	0	1	1	2.19	2.19	0.0	2.19
6	0	1	1	2.27	2.27	0.0	2.27
7	0	1	1	2.23	2.23	0.0	2.23
8	0	1	1	2.27	2.27	0.0	2.27
9	0	1	1	2.35	2.35	0.0	2.35
10	0	1	1	2.31	2.31	0.0	2.31
11	0	1	1	2.21	2.21	0.0	2.21
12	0	1	1	2.29	2.29	0.0	2.29
13	0	1	1	2.2	2.2	0.0	2.2
14	0	1	1	2.35	2.35	0.0	2.35
15	0	1	1	2.27	2.27	0.0	2.27
16	0	1	1	2.33	2.33	0.0	2.33
17	0	1	1	2.31	2.31	0.0	2.31
18	0	1	1	2.26	2.26	0.0	2.26
19	0	1	1	2.28	2.28	0.0	2.28
20	0	1	1	2.25	2.25	0.0	2.25
21	0	1	1	2.18	2.18	0.0	2.18
22	0	1	1	2.24	2.24	0.0	2.24
23	0	1	1	2.34	2.34	0.0	2.34
24	0	1	1	2.32	2.32	0.0	2.32
25	0	1	1	2.24	2.24	0.0	2.24
26	0	1	1	2.17	2.17	0.0	2.17
27	0	1	1	2.35	2.35	0.0	2.35
28	0	1	1	2.26	2.26	0.0	2.26
29	0	1	1	2.26	2.26	0.0	2.26
30	0	1	1	2.31	2.31	0.0	2.31
31	0	1	1	2.22	2.22	0.0	2.22
32	0	1	1	2.22	2.22	0.0	2.22
33	0	1	1	1.85	1.85	0.0	1.85
34	0	1	1	1.91	1.91	0.0	1.91
35	0	1	1	2.31	2.31	0.0	2.31
36	0	1	1	1.84	1.84	0.0	1.84
37	0	1	1	2.35	2.35	0.0	2.35
38	0	1	1	2.16	2.16	0.0	2.16

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Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
39	0	1	1	2.47	2.47	0.0	2.47
40	0	1	1	1.82	1.82	0.0	1.82
41	0	1	1	2.21	2.21	0.0	2.21
42	0	1	1	1.86	1.86	0.0	1.86
43	0	1	1	1.97	1.97	0.0	1.97
44	0	1	1	2.26	2.26	0.0	2.26
45	0	1	1	2.27	2.27	0.0	2.27
46	0	1	1	2.18	2.18	0.0	2.18
47	0	1	1	2.23	2.23	0.0	2.23
48	0	1	1	2.22	2.22	0.0	2.22
49	0	1	1	2.3	2.3	0.0	2.3
50	0	0	0	0.0	0.0	0.0	0.0
51	0	1	1	2.23	2.23	0.0	2.23
52	0	1	1	2.3	2.3	0.0	2.3
53	0	1	1	2.32	2.32	0.0	2.32
54	0	1	1	2.26	2.26	0.0	2.26
55	0	1	1	1.82	1.82	0.0	1.82
56	0	1	1	2.28	2.28	0.0	2.28
57	0	1	1	2.29	2.29	0.0	2.29
58	0	1	1	2.25	2.25	0.0	2.25
59	0	1	1	2.19	2.19	0.0	2.19
60	0	1	1	2.29	2.29	0.0	2.29
61	0	1	1	2.22	2.22	0.0	2.22
62	0	1	1	1.8	1.8	0.0	1.8
63	0	1	1	2.35	2.35	0.0	2.35
64	0	1	1	1.65	1.65	0.0	1.65
65	0	1	1	2.3	2.3	0.0	2.3
66	0	1	1	2.29	2.29	0.0	2.29
67	0	1	1	2.3	2.3	0.0	2.3
68	0	1	1	2.19	2.19	0.0	2.19
69	0	1	1	2.23	2.23	0.0	2.23
70	0	1	1	2.23	2.23	0.0	2.23

10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



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

10.3 Dihedral-angle violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	1	1.4
0	0	0	2	2.9
0	0	0	3	4.3
0	0	0	4	5.7
0	0	0	5	7.1
0	0	0	6	8.6
0	0	0	7	10.0
0	0	0	8	11.4
0	0	0	9	12.9
0	0	0	10	14.3
0	0	0	11	15.7

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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	12	17.1
0	0	0	13	18.6
0	0	0	14	20.0
0	0	0	15	21.4
0	0	0	16	22.9
0	0	0	17	24.3
0	0	0	18	25.7
0	0	0	19	27.1
0	0	0	20	28.6
0	0	0	21	30.0
0	0	0	22	31.4
0	0	0	23	32.9
0	0	0	24	34.3
0	0	0	25	35.7
0	0	0	26	37.1
0	0	0	27	38.6
0	0	0	28	40.0
0	0	0	29	41.4
0	0	0	30	42.9
0	0	0	31	44.3
0	0	0	32	45.7
0	0	0	33	47.1
0	0	0	34	48.6
0	0	0	35	50.0
0	0	0	36	51.4
0	0	0	37	52.9
0	0	0	38	54.3
0	0	0	39	55.7
0	0	0	40	57.1
0	0	0	41	58.6
0	0	0	42	60.0
0	0	0	43	61.4
0	0	0	44	62.9
0	0	0	45	64.3
0	0	0	46	65.7
0	0	0	47	67.1
0	0	0	48	68.6
0	0	0	49	70.0
0	0	0	50	71.4
0	0	0	51	72.9
0	0	0	52	74.3

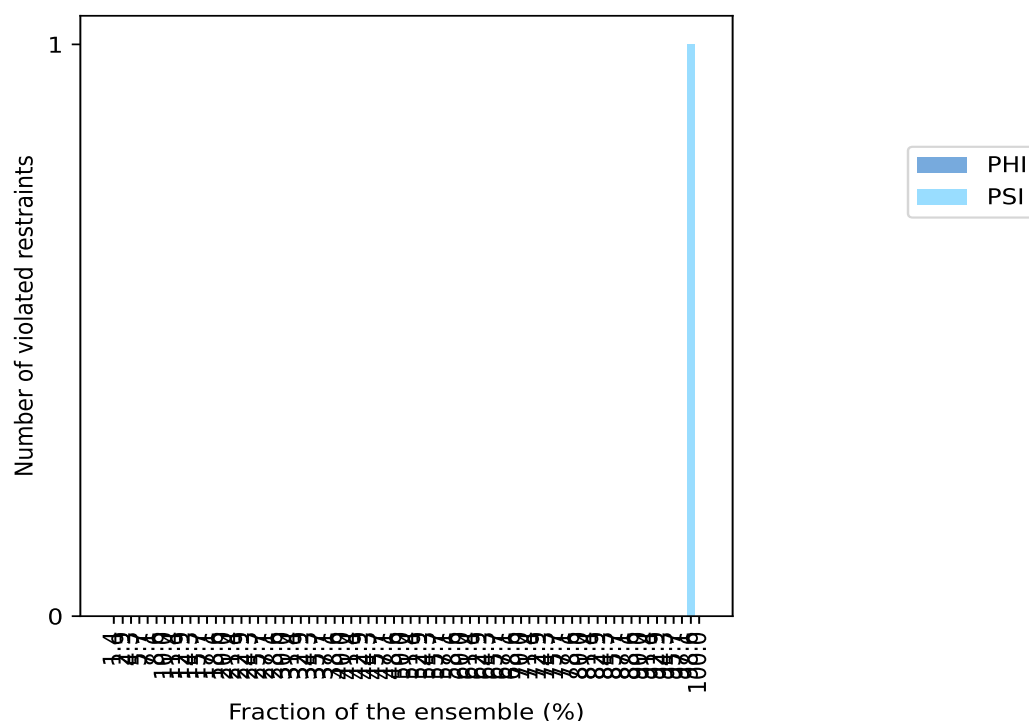
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	53	75.7
0	0	0	54	77.1
0	0	0	55	78.6
0	0	0	56	80.0
0	0	0	57	81.4
0	0	0	58	82.9
0	0	0	59	84.3
0	0	0	60	85.7
0	0	0	61	87.1
0	0	0	62	88.6
0	0	0	63	90.0
0	0	0	64	91.4
0	0	0	65	92.9
0	0	0	66	94.3
0	0	0	67	95.7
0	0	0	68	97.1
0	1	1	69	98.6
0	0	0	70	100.0

¹ Number of models with violations

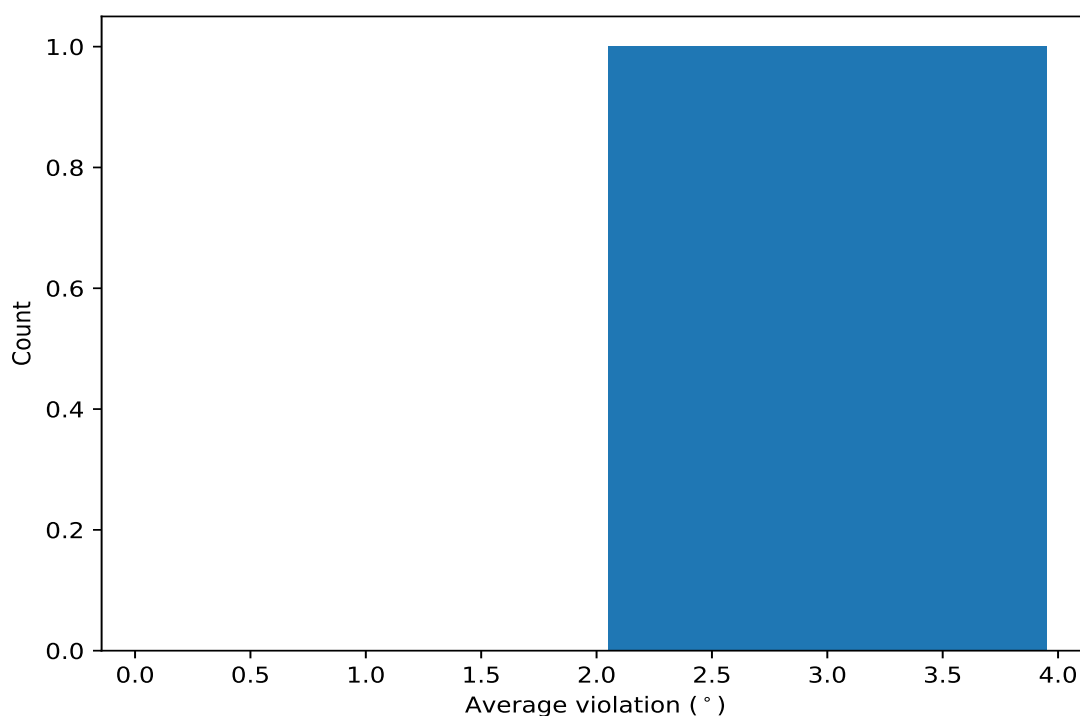
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



10.4.2 Table: Most violated dihedral-angle restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

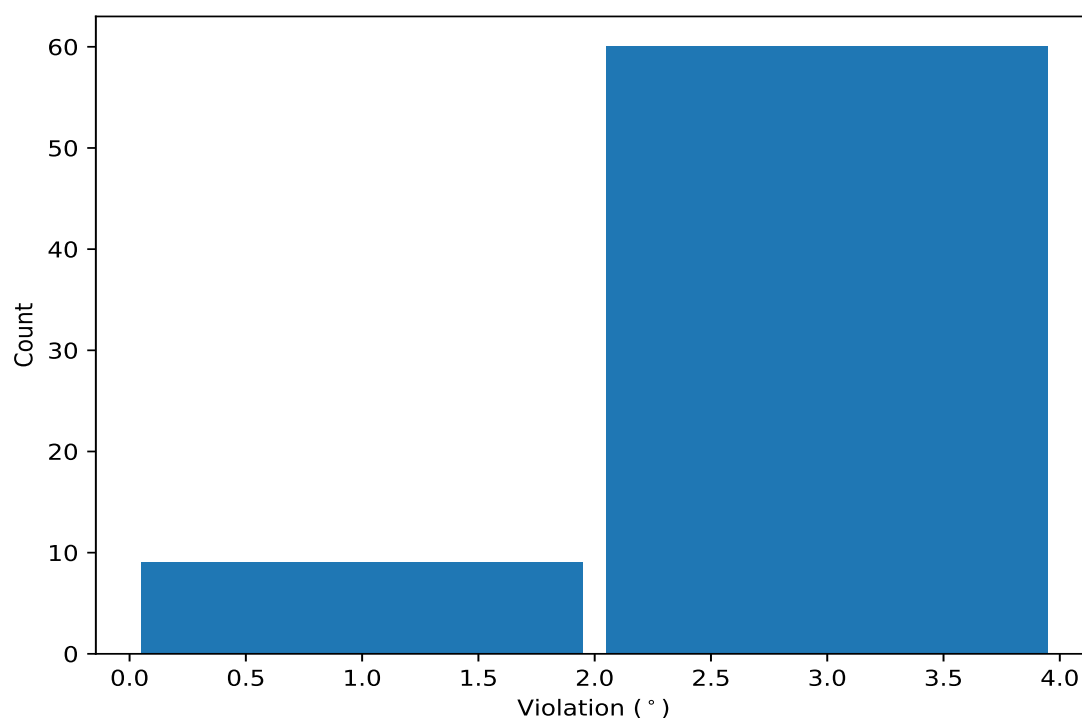
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	69	2.21	0.16	2.26

¹ Number of violated models, ²Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

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



10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	39	2.47
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	9	2.35
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	14	2.35
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	27	2.35
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	37	2.35
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	63	2.35
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	23	2.34
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	16	2.33
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	24	2.32
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	53	2.32
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	10	2.31
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	17	2.31
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	30	2.31
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	35	2.31
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	1	2.3
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	3	2.3
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	49	2.3
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	52	2.3
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	65	2.3
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	67	2.3
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	12	2.29

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	57	2.29
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	60	2.29
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	66	2.29
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	19	2.28
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	56	2.28
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	6	2.27
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	8	2.27
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	15	2.27
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	45	2.27
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	2	2.26
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	18	2.26
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	28	2.26
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	29	2.26
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	44	2.26
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	54	2.26
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	20	2.25
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	58	2.25
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	4	2.24
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	22	2.24
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	25	2.24
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	7	2.23
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	47	2.23
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	51	2.23
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	69	2.23
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	70	2.23
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	31	2.22
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	32	2.22
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	48	2.22
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	61	2.22
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	11	2.21
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	41	2.21
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	13	2.2
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	5	2.19
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	59	2.19
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	68	2.19
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	21	2.18
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	46	2.18
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	26	2.17
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	38	2.16
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	43	1.97
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	34	1.91
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	42	1.86
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	33	1.85
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	36	1.84
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	40	1.82
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	55	1.82
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	62	1.8
(1,22)	1:55:A:GLN:N	1:55:A:GLN:CA	1:55:A:GLN:C	1:56:A:PRO:N	64	1.65