



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 08:54 AM UTC

PDB ID : 9M2D / pdb_00009m2d
BMRB ID : 36733
Title : SERF1_HUMAN short isoform of Small EDRK-rich factor 1, serfla at pH 6.8.
Authors : Huang, S.Y.; Shih, O.; Jeng, U.S.; Chang, C.F.; Lin, J.H.; Malliavin, T.E.
Deposited on : 2025-02-27

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

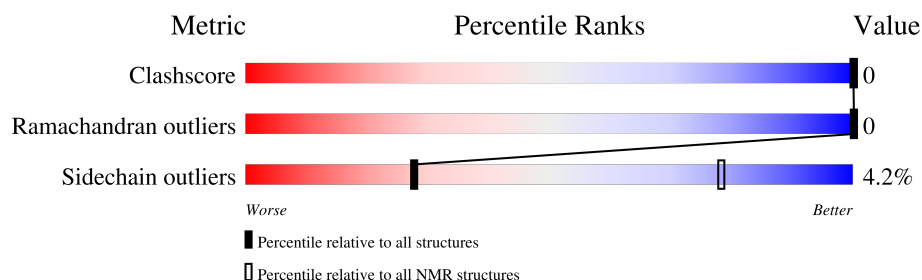
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 56%.

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	64	

2 Ensemble composition and analysis

This entry contains 100 models. Model 51 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:6-A:14 (9)	0.13	61
2	A:34-A:52 (19)	0.20	51

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. No single-model clusters were found.

Cluster number	Models
1	4, 10, 16, 20, 21, 28, 32, 33, 40, 45, 46, 52, 54, 60, 71, 86, 95, 98, 99, 100
2	3, 6, 8, 9, 13, 23, 30, 34, 47, 48, 57, 74, 78, 81, 90, 94, 96
3	7, 18, 24, 37, 38, 50, 67, 68, 77, 79, 80, 85, 89, 91
4	2, 5, 12, 17, 22, 29, 31, 36, 51, 56, 59, 66, 82, 87
5	1, 15, 35, 42, 58, 61, 63, 69, 72, 93
6	14, 26, 41, 43, 44, 55, 64, 88
7	11, 25, 62, 73, 76, 84, 97
8	19, 27, 53, 65, 83, 92
9	39, 49, 70, 75

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1044 atoms, of which 536 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Isoform Short of Small EDRK-rich factor 1.

Mol	Chain	Residues	Atoms						Trace
1	A	62	Total	C	H	N	O	S	0
			1044	299	536	106	99	4	

There are 2 discrepancies between the modelled and reference sequences:

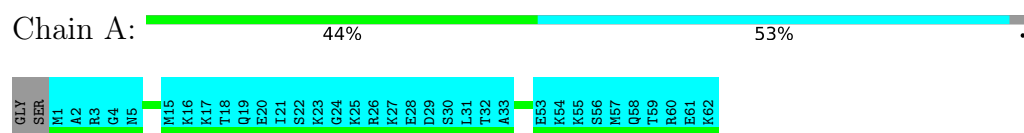
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP O75920
A	0	SER	-	expression tag	UNP O75920

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: Isoform Short of Small EDRK-rich factor 1

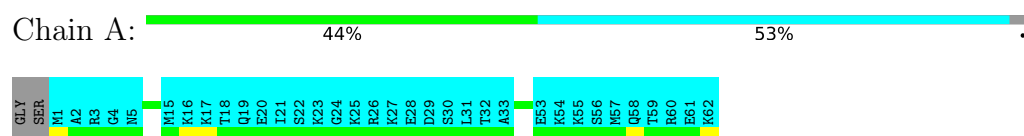


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

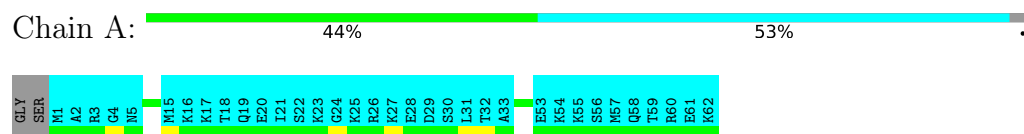
4.2.1 Score per residue for model 1

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



4.2.2 Score per residue for model 2

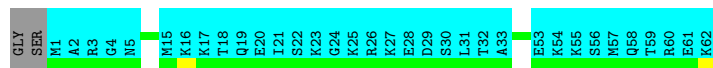
- Molecule 1: Isoform Short of Small EDRK-rich factor 1



4.2.3 Score per residue for model 3

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

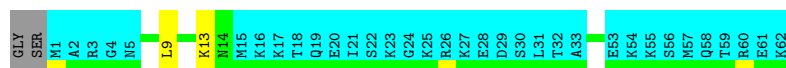
Chain A:  44% 53%



4.2.4 Score per residue for model 4

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  41% 53%



4.2.5 Score per residue for model 5

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  42% 53%



4.2.6 Score per residue for model 6

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

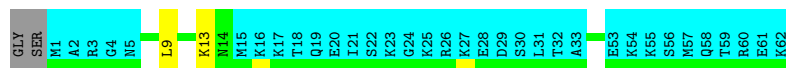
Chain A:  41% 53%



4.2.7 Score per residue for model 7

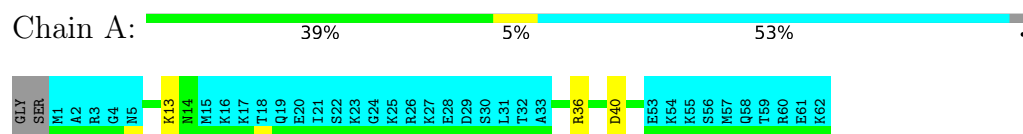
- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  41% 53%



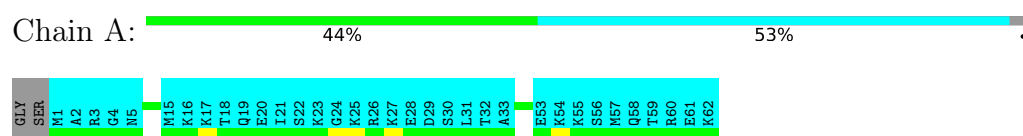
4.2.8 Score per residue for model 8

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



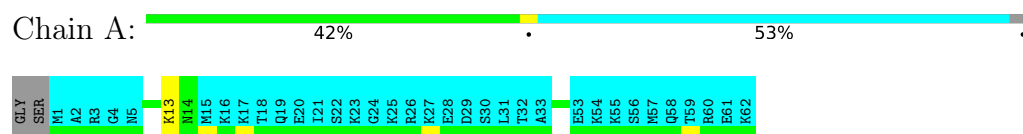
4.2.9 Score per residue for model 9

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



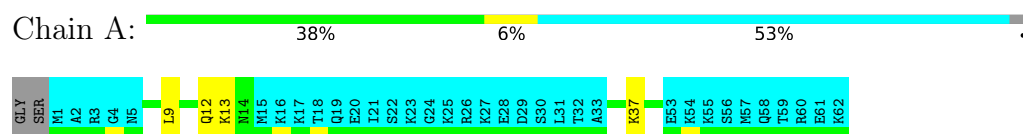
4.2.10 Score per residue for model 10

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



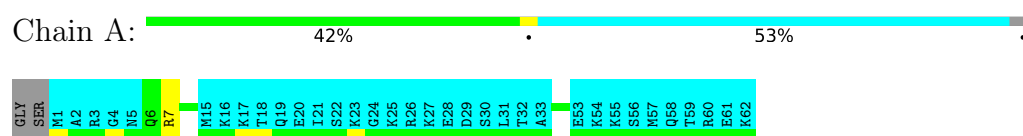
4.2.11 Score per residue for model 11

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



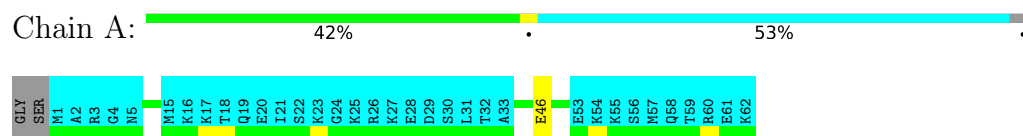
4.2.12 Score per residue for model 12

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



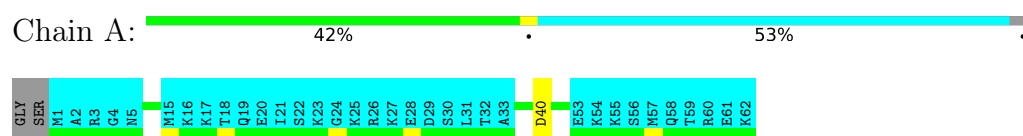
4.2.13 Score per residue for model 13

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



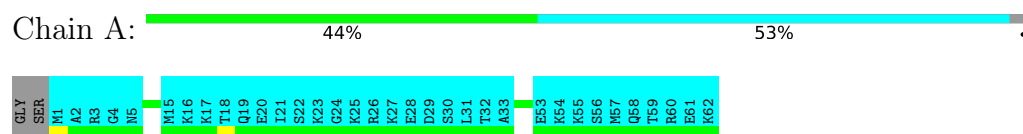
4.2.14 Score per residue for model 14

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



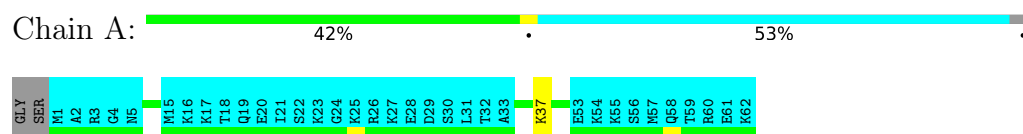
4.2.15 Score per residue for model 15

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



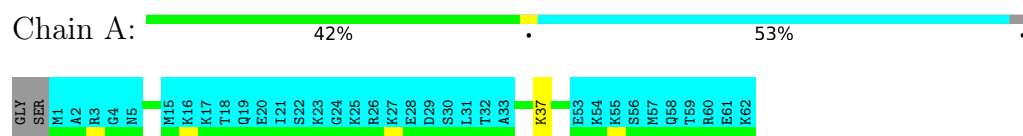
4.2.16 Score per residue for model 16

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



4.2.17 Score per residue for model 17

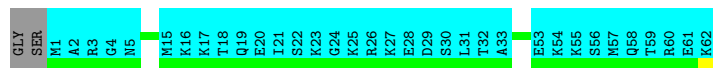
- Molecule 1: Isoform Short of Small EDRK-rich factor 1



4.2.18 Score per residue for model 18

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

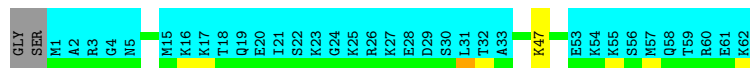
Chain A:  44% 53%



4.2.19 Score per residue for model 19

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  42% 53%



4.2.20 Score per residue for model 20

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  42% 53%



4.2.21 Score per residue for model 21

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  42% 53%



4.2.22 Score per residue for model 22

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

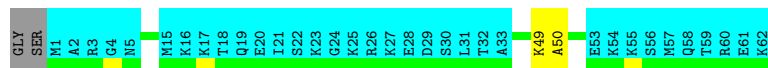
Chain A:  41% 53%



4.2.23 Score per residue for model 23

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  41% 53%



4.2.24 Score per residue for model 24

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

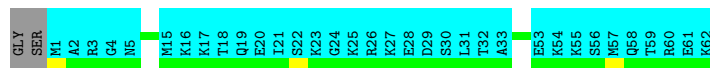
Chain A:  44% 53%



4.2.25 Score per residue for model 25

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  44% 53%



4.2.26 Score per residue for model 26

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  42% 53%



4.2.27 Score per residue for model 27

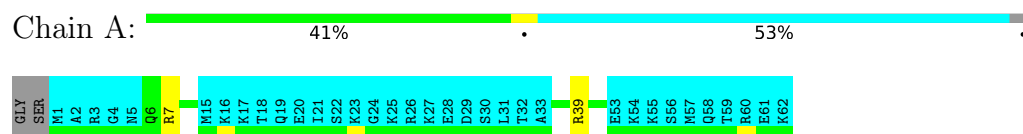
- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  42% 53%



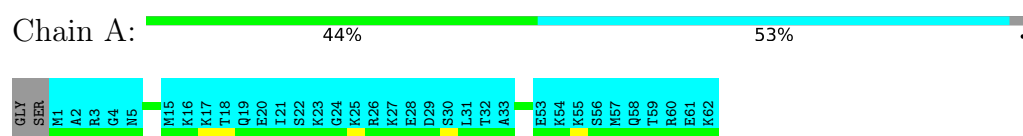
4.2.28 Score per residue for model 28

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



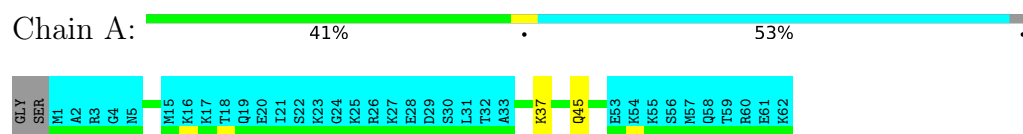
4.2.29 Score per residue for model 29

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



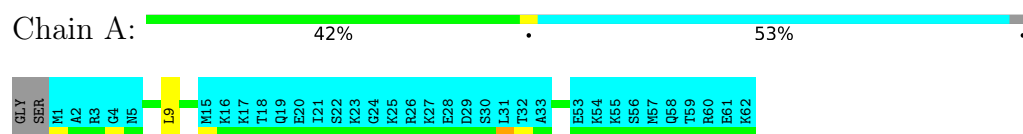
4.2.30 Score per residue for model 30

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



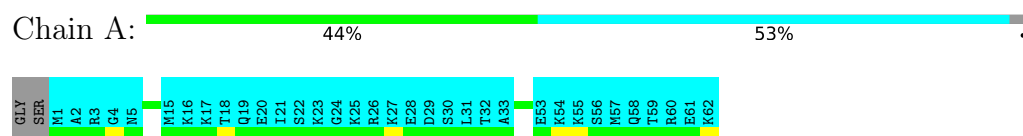
4.2.31 Score per residue for model 31

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



4.2.32 Score per residue for model 32

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



4.2.33 Score per residue for model 33

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

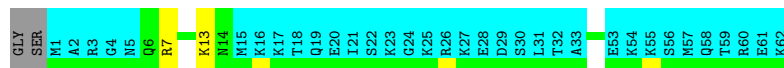
Chain A:  42% 53%



4.2.34 Score per residue for model 34

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  41% 53%



4.2.35 Score per residue for model 35

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  44% 53%



4.2.36 Score per residue for model 36

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  44% 53%



4.2.37 Score per residue for model 37

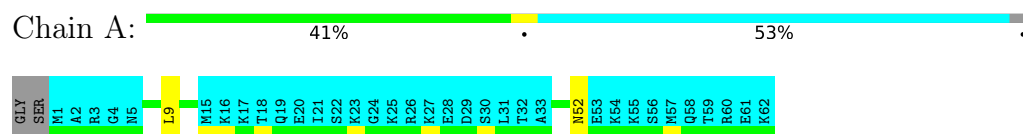
- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  42% 53%



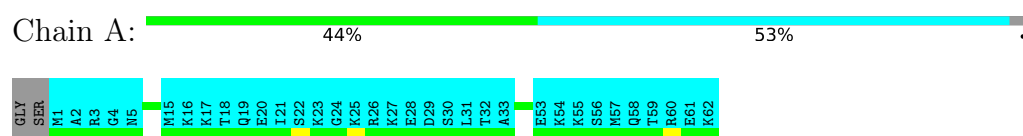
4.2.38 Score per residue for model 38

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



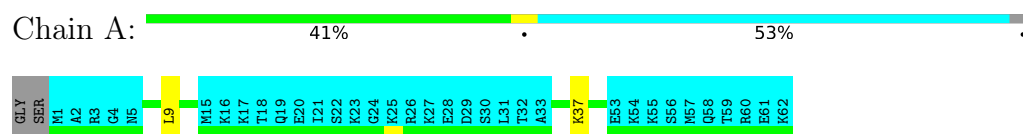
4.2.39 Score per residue for model 39

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



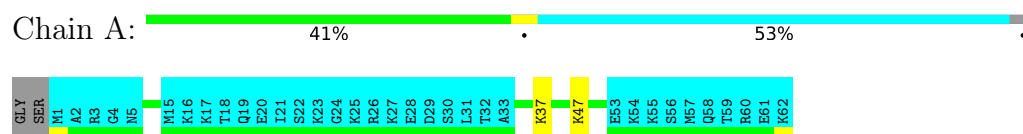
4.2.40 Score per residue for model 40

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



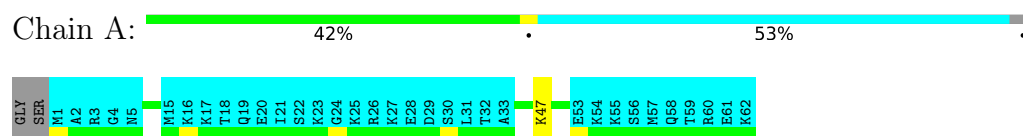
4.2.41 Score per residue for model 41

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



4.2.42 Score per residue for model 42

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



4.2.43 Score per residue for model 43

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

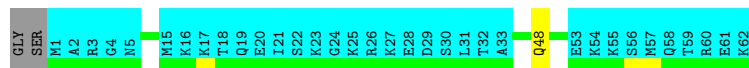
Chain A:  44% 53%



4.2.44 Score per residue for model 44

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  42% 53%



4.2.45 Score per residue for model 45

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

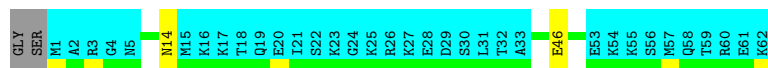
Chain A:  44% 53%



4.2.46 Score per residue for model 46

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  41% 53%



4.2.47 Score per residue for model 47

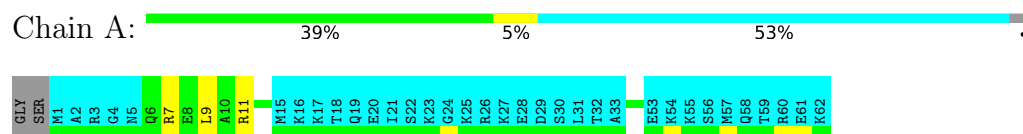
- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  42% 53%



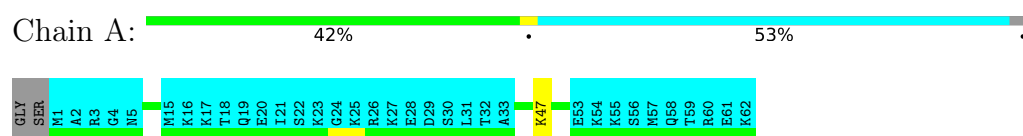
4.2.48 Score per residue for model 48

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



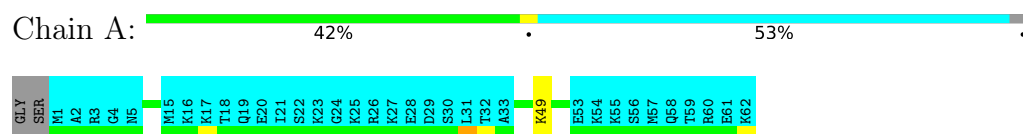
4.2.49 Score per residue for model 49

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



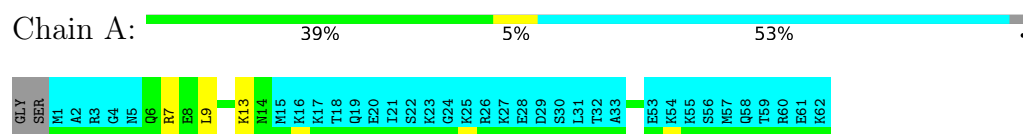
4.2.50 Score per residue for model 50

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



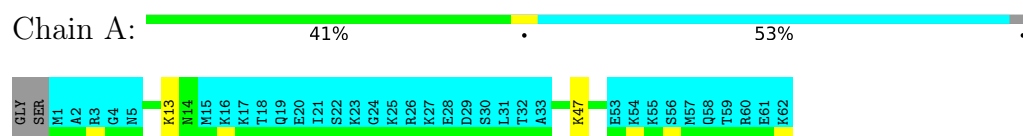
4.2.51 Score per residue for model 51 (medoid)

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



4.2.52 Score per residue for model 52

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



4.2.53 Score per residue for model 53

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  44% 53%



4.2.54 Score per residue for model 54

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  42% 53%



4.2.55 Score per residue for model 55

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

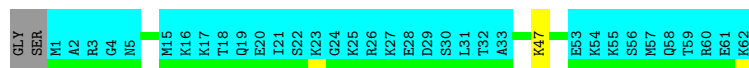
Chain A:  39% 5% 53%



4.2.56 Score per residue for model 56

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

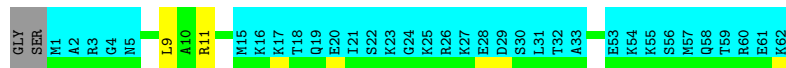
Chain A:  42% 53%



4.2.57 Score per residue for model 57

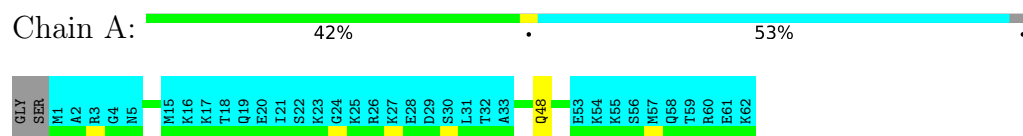
- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  41% 53%



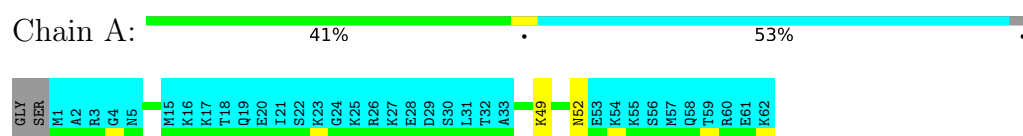
4.2.58 Score per residue for model 58

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



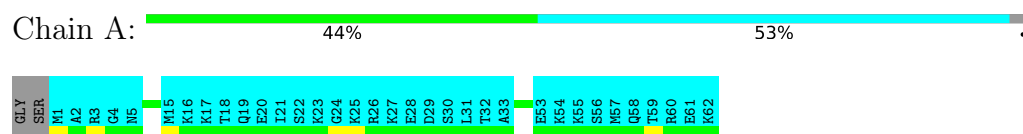
4.2.59 Score per residue for model 59

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



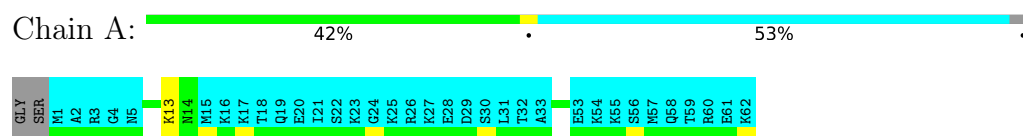
4.2.60 Score per residue for model 60

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



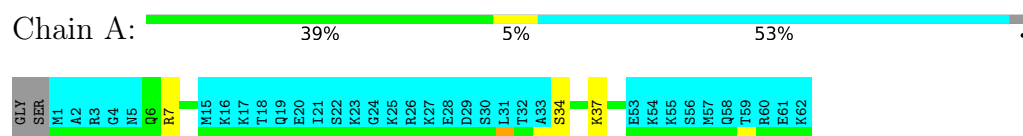
4.2.61 Score per residue for model 61

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



4.2.62 Score per residue for model 62

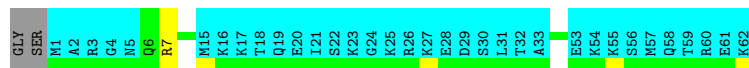
- Molecule 1: Isoform Short of Small EDRK-rich factor 1



4.2.63 Score per residue for model 63

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  42% 53%



4.2.64 Score per residue for model 64

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  42% 53%



4.2.65 Score per residue for model 65

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  44% 53%



4.2.66 Score per residue for model 66

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  44% 53%



4.2.67 Score per residue for model 67

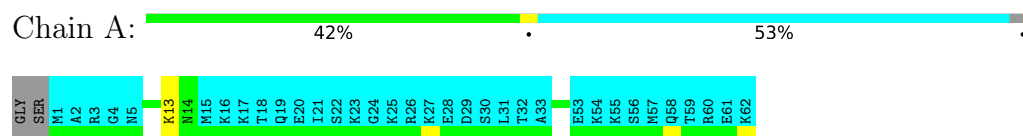
- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  42% 53%



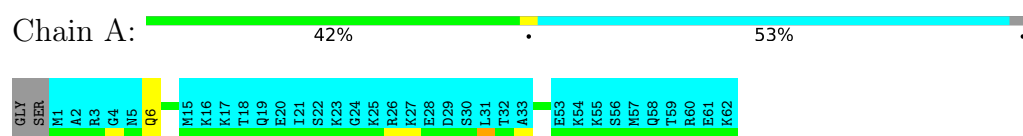
4.2.68 Score per residue for model 68

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



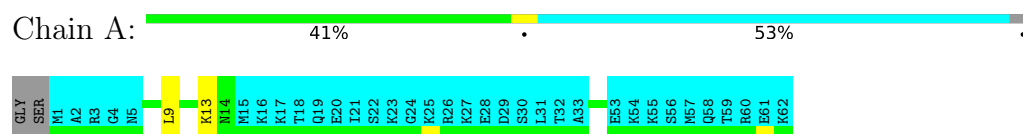
4.2.69 Score per residue for model 69

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



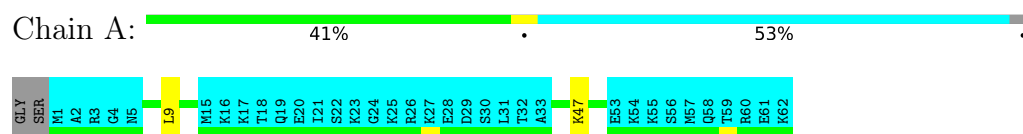
4.2.70 Score per residue for model 70

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



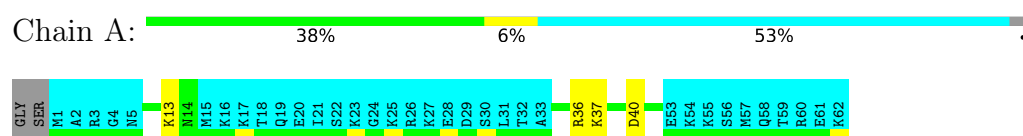
4.2.71 Score per residue for model 71

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



4.2.72 Score per residue for model 72

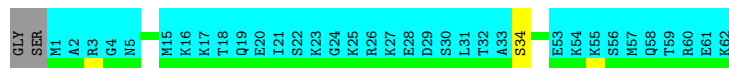
- Molecule 1: Isoform Short of Small EDRK-rich factor 1



4.2.73 Score per residue for model 73

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

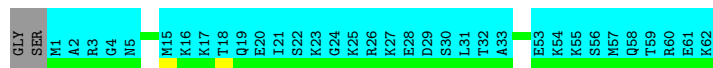
Chain A:  42% 53%



4.2.74 Score per residue for model 74

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  44% 53%



4.2.75 Score per residue for model 75

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  41% 53%



4.2.76 Score per residue for model 76

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  41% 53%



4.2.77 Score per residue for model 77

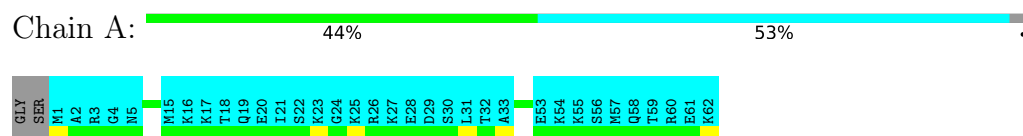
- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  44% 53%



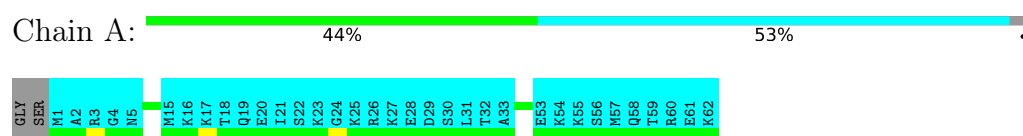
4.2.78 Score per residue for model 78

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



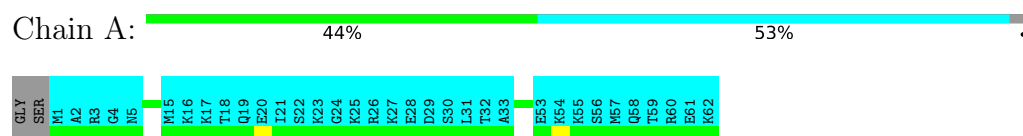
4.2.79 Score per residue for model 79

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



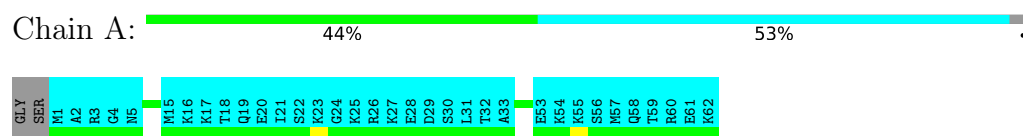
4.2.80 Score per residue for model 80

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



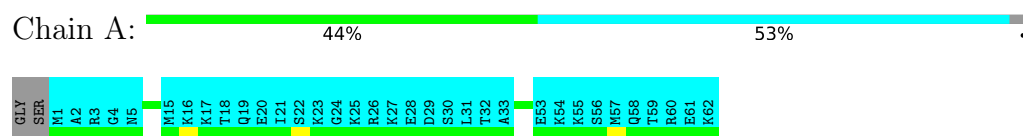
4.2.81 Score per residue for model 81

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



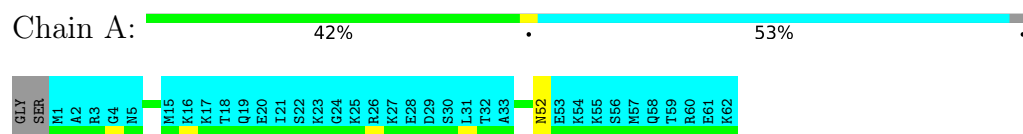
4.2.82 Score per residue for model 82

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



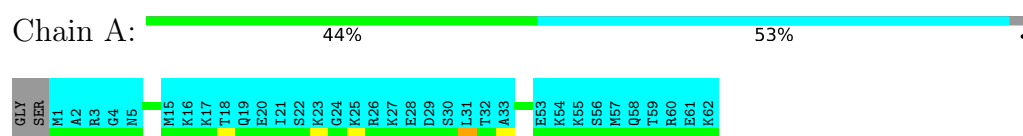
4.2.83 Score per residue for model 83

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



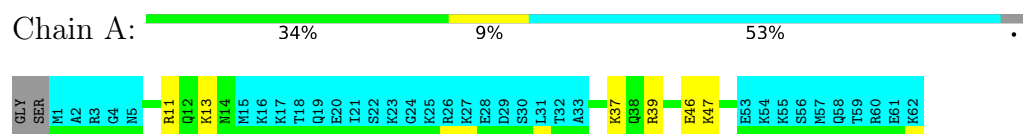
4.2.84 Score per residue for model 84

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



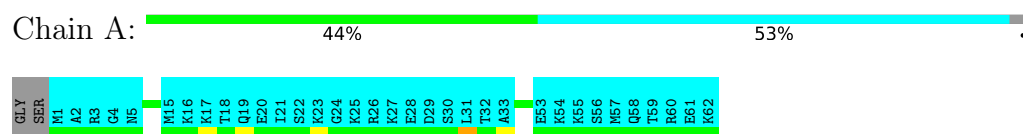
4.2.85 Score per residue for model 85

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



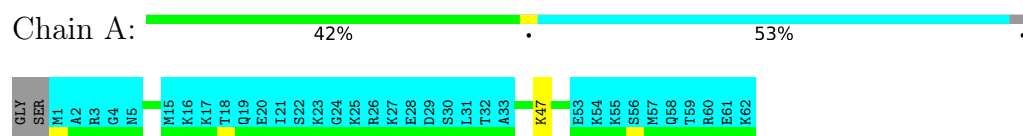
4.2.86 Score per residue for model 86

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



4.2.87 Score per residue for model 87

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



4.2.88 Score per residue for model 88

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

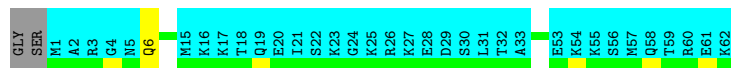
Chain A:  42% 53%



4.2.89 Score per residue for model 89

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

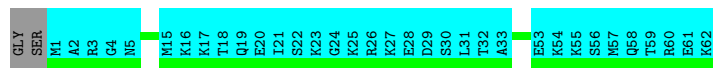
Chain A:  42% 53%



4.2.90 Score per residue for model 90

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

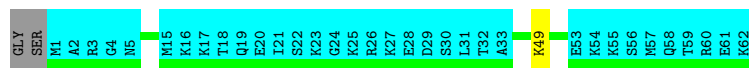
Chain A:  44% 53%



4.2.91 Score per residue for model 91

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  42% 53%



4.2.92 Score per residue for model 92

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

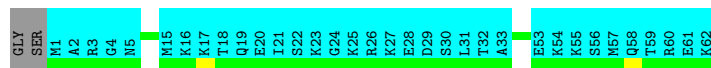
Chain A:  42% 53%



4.2.93 Score per residue for model 93

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

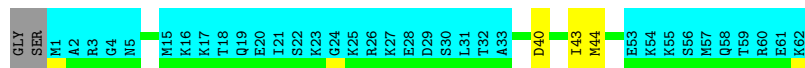
Chain A:  44% 53%



4.2.94 Score per residue for model 94

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  39% 5% 53%



4.2.95 Score per residue for model 95

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  42% 53%



4.2.96 Score per residue for model 96

- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  42% 53%



4.2.97 Score per residue for model 97

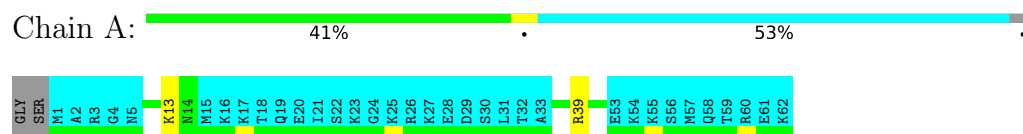
- Molecule 1: Isoform Short of Small EDRK-rich factor 1

Chain A:  44% 53%



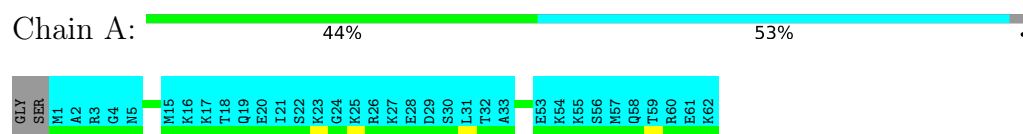
4.2.98 Score per residue for model 98

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



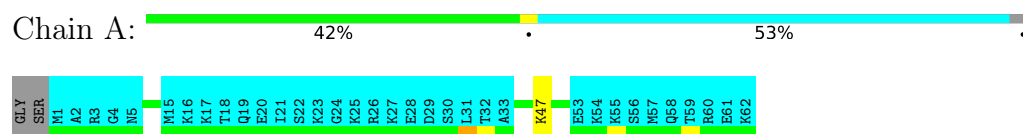
4.2.99 Score per residue for model 99

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



4.2.100 Score per residue for model 100

- Molecule 1: Isoform Short of Small EDRK-rich factor 1



5 Refinement protocol and experimental data overview

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

Of the 2000 calculated structures, 100 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure calculation	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	503
Number of shifts mapped to atoms	503
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	56%

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	236	242	242	0±0
All	All	23600	24200	24200	1

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:ASP:CG	1:A:44:MET:HE2	0.40	2.42	94	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	28/64 (44%)	28±1 (98±2%)	0±1 (2±2%)	0±0 (0±0%)	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2800/6400 (44%)	2757 (98%)	43 (2%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	25/56 (45%)	24±1 (96±4%)	1±1 (4±4%)	28	78
All	All	2500/5600 (45%)	2394 (96%)	106 (4%)	28	78

All 19 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	13	LYS	19
1	A	37	LYS	13
1	A	47	LYS	13
1	A	9	LEU	11
1	A	7	ARG	9
1	A	49	LYS	9
1	A	46	GLU	5
1	A	40	ASP	4
1	A	11	ARG	4
1	A	39	ARG	3
1	A	52	ASN	3
1	A	36	ARG	2
1	A	12	GLN	2
1	A	45	GLN	2
1	A	48	GLN	2
1	A	6	GLN	2
1	A	14	ASN	1
1	A	34	SER	1
1	A	35	GLN	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 56% for the well-defined parts and 56% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

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	503
Number of shifts mapped to atoms	503
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
$^{13}\text{C}_\alpha$	57	-0.07 ± 0.19	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	55	0.18 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}'$	57	-0.39 ± 0.15	None needed (< 0.5 ppm)
^{15}N	54	-1.36 ± 0.17	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 56%, i.e. 234 atoms were assigned a chemical shift out of a possible 417. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	122/140 (87%)	48/56 (86%)	50/56 (89%)	24/28 (86%)
Sidechain	112/277 (40%)	87/172 (51%)	25/81 (31%)	0/24 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Overall	234/417 (56%)	135/228 (59%)	75/137 (55%)	24/52 (46%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 56%, i.e. 503 atoms were assigned a chemical shift out of a possible 897. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	275/312 (88%)	107/126 (85%)	114/124 (92%)	54/62 (87%)
Sidechain	228/585 (39%)	173/366 (47%)	55/175 (31%)	0/44 (0%)
Overall	503/897 (56%)	280/492 (57%)	169/299 (57%)	54/106 (51%)

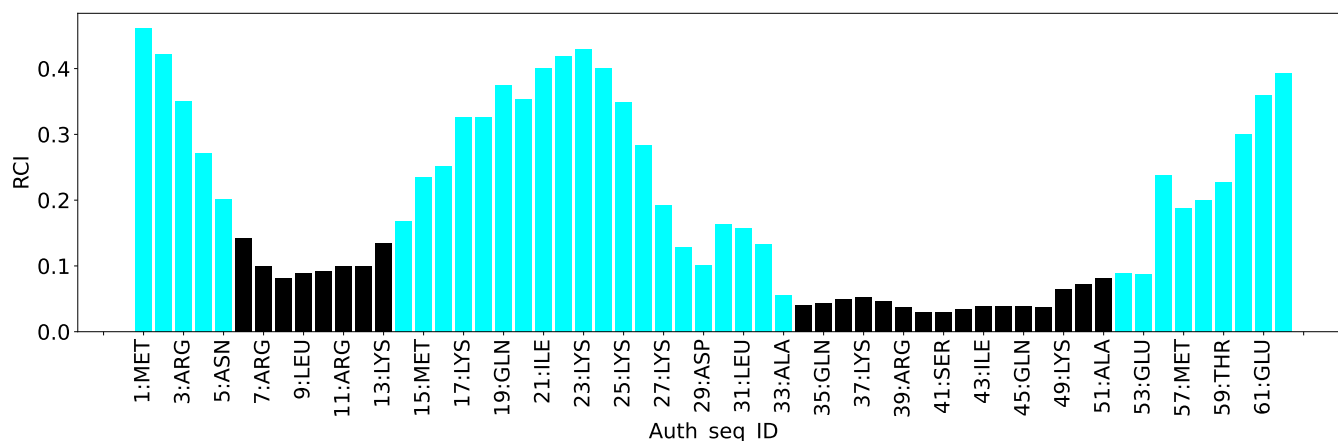
7.1.4 Statistically unusual chemical shifts [i](#)

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	114
Intra-residue ($ i-j =0$)	48
Sequential ($ i-j =1$)	16
Medium range ($ i-j >1$ and $ i-j <5$)	0
Long range ($ i-j \geq 5$)	0
Inter-chain	0
Hydrogen bond restraints	50
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	1.8
Number of long range restraints per residue ¹	0.0

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

8.2 Residual restraint violations [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. There are no distance violations

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 ⓘ

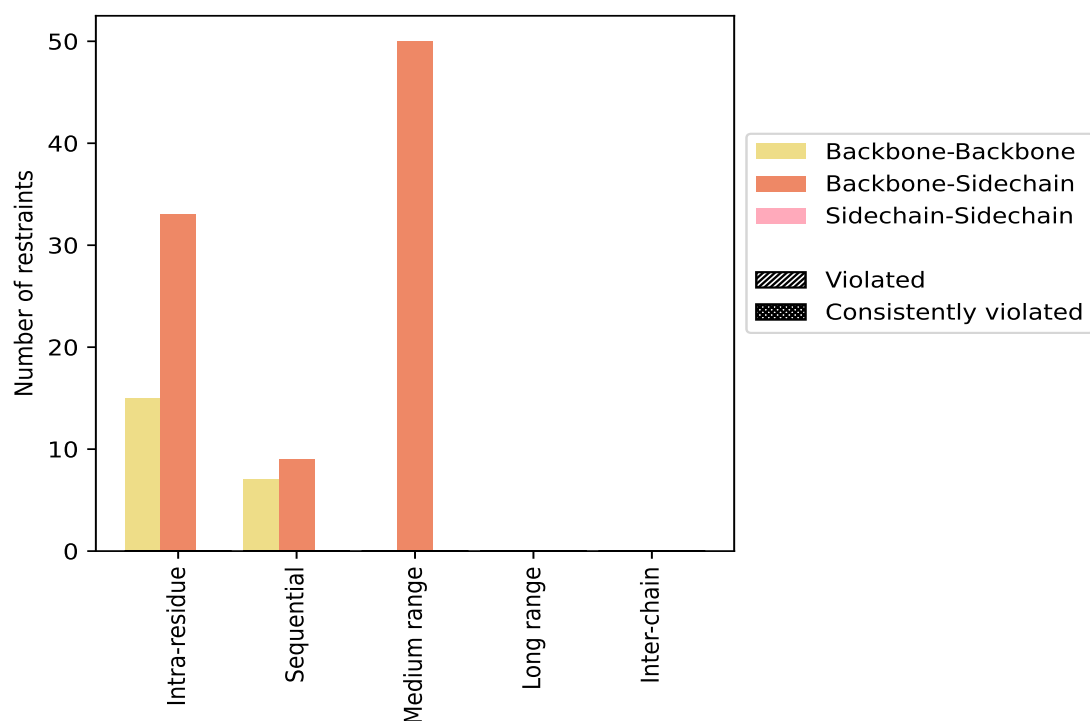
9.1 Summary of distance violations ⓘ

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)	48	42.1	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	15	13.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	33	28.9	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)	16	14.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	7	6.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	9	7.9	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
Medium range (i-j >1 & i-j <5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range (i-j ≥5)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	50	43.9	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	114	100.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	22	19.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	92	80.7	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

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](#)

No violations found

9.3 Distance violation statistics for the ensemble [i](#)

No violations found

9.4 Most violated distance restraints in the ensemble [i](#)

No violations found

9.5 All violated distance restraints [i](#)

No violations found

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found