Full wwPDB NMR Structure Validation Report (i)

May 29, 2020 – 01:03 am BST

PDB ID	:	2N8A
Title	:	1H, 13C and 15N chemical shift assignments and solution structure for PARP-1 F1F2 domains in complex with a DNA single-strand break
Authors	:	Neuhaus, D.; Eustermann, S.; Yang, J.; Wu, W.
Deposited on	:	2015-10-08

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

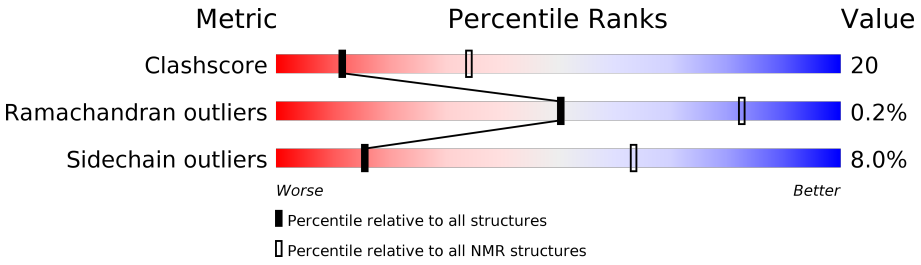
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 29%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	214	63% 21% • 15%
2	B	45	31% 69%

2 Ensemble composition and analysis

This entry contains 78 models. Model 36 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:5-A:91 (87)	0.05	65
2	A:108-A:201 (94)	0.06	36

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 11 clusters and 17 single-model clusters were found.

Cluster number	Models
1	6, 10, 13, 14, 15, 16, 20, 21, 23, 24, 26, 28, 30, 31, 39, 55
2	40, 43, 45, 56, 57, 58, 64, 65, 70
3	4, 11, 18, 44, 47, 50, 53, 66
4	7, 8, 17, 22, 34, 37, 74
5	12, 27, 29, 51, 52
6	1, 32, 42, 54
7	9, 25, 60
8	2, 3, 35
9	48, 61
10	5, 63
11	68, 71
Single-model clusters	19; 33; 36; 38; 41; 46; 49; 59; 62; 67; 69; 72; 73; 75; 76; 77; 78

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4788 atoms, of which 2176 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Poly [ADP-ribose] polymerase 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	214	3356	1055	1670	299	319	13	0

- Molecule 2 is a DNA chain called DNA (45-MER).

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
2	B	45	1430	436	506	170	273	45	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
3	A	2	2	2

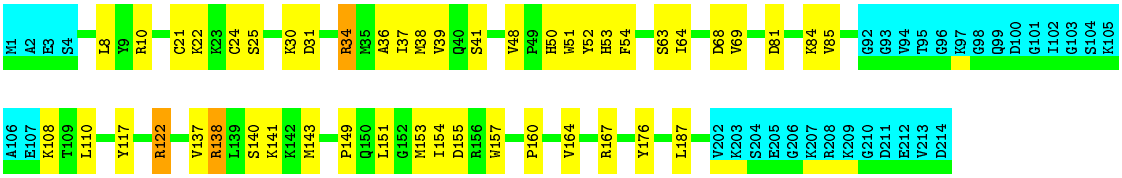
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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.

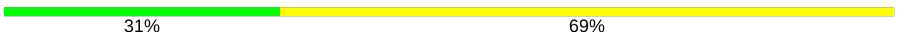
• Molecule 1: Poly [ADP-ribose] polymerase 1

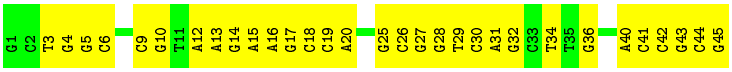
Chain A:



• Molecule 2: DNA (45-MER)

Chain B:





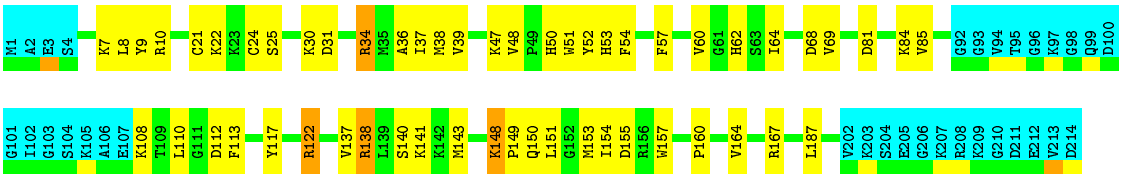
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

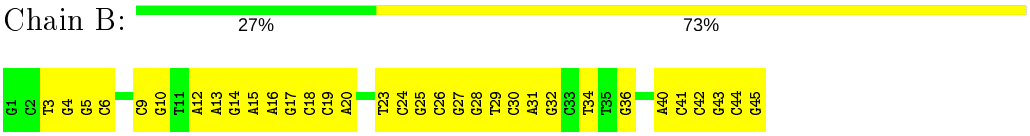
• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

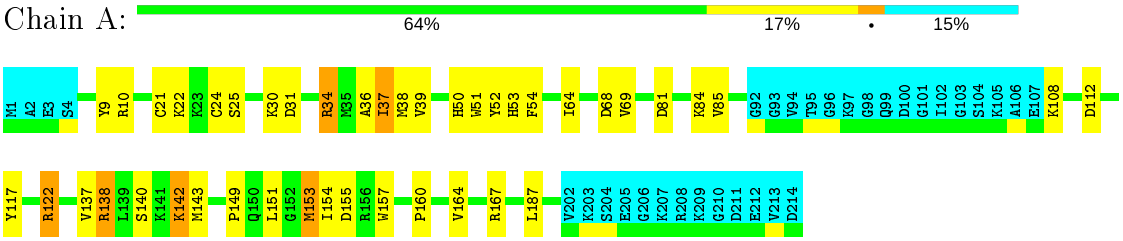
Chain B:



4.2.2 Score per residue for model 2

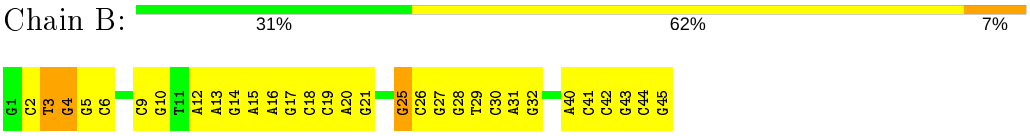
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

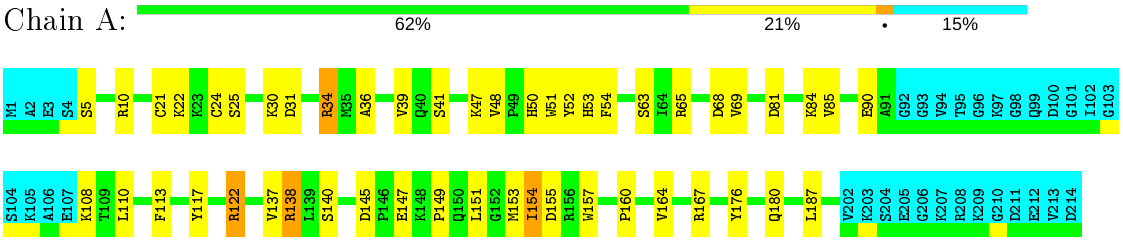
Chain B:



4.2.3 Score per residue for model 3

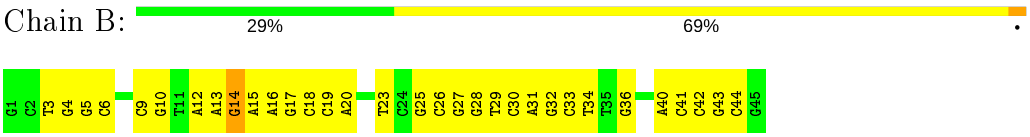
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

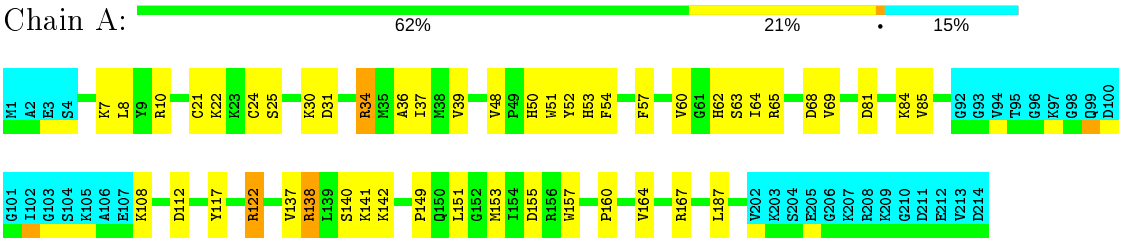
Chain B:



4.2.4 Score per residue for model 4

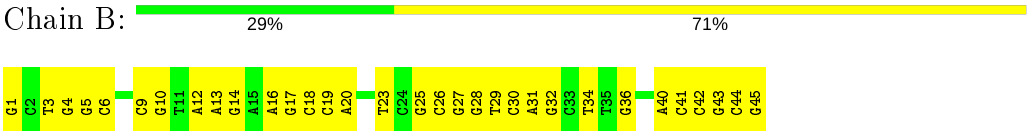
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

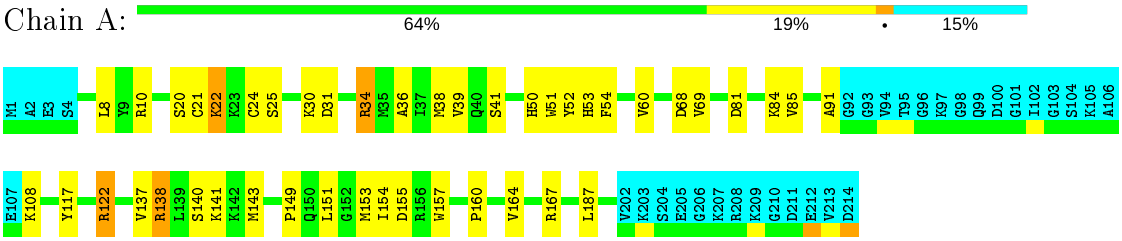
Chain B:



4.2.5 Score per residue for model 5

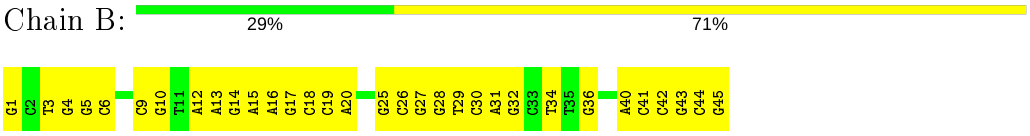
• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

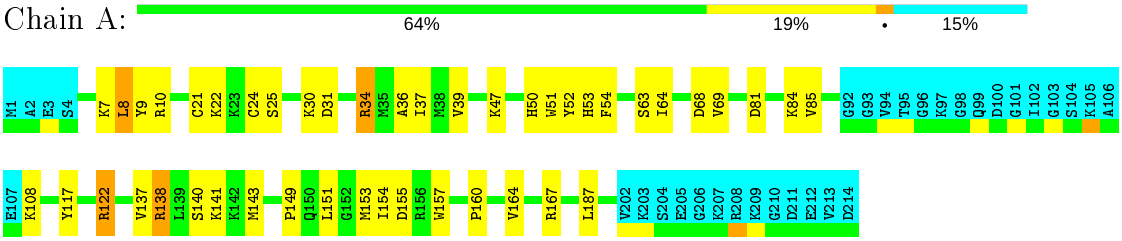
Chain B:



4.2.6 Score per residue for model 6

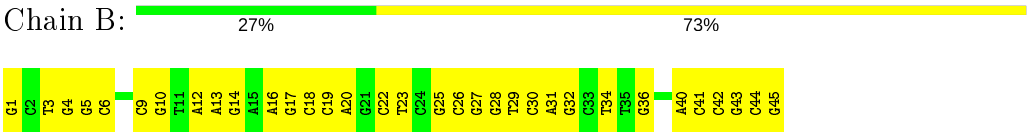
• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

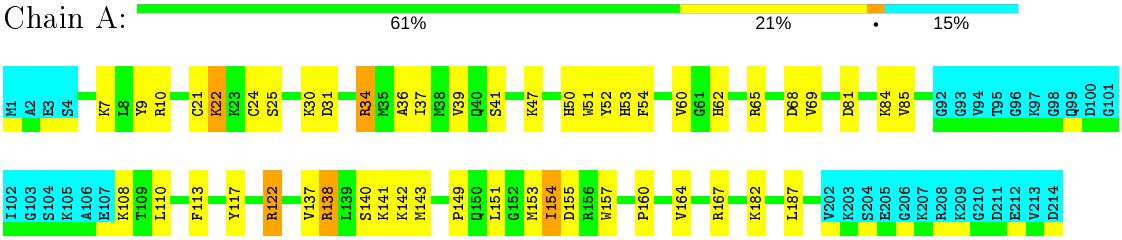
Chain B:



4.2.7 Score per residue for model 7

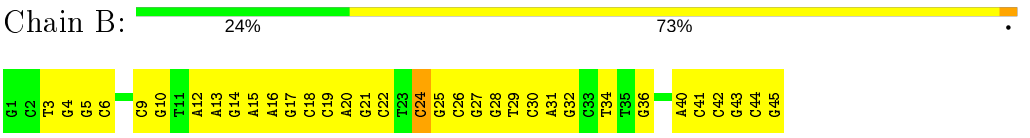
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

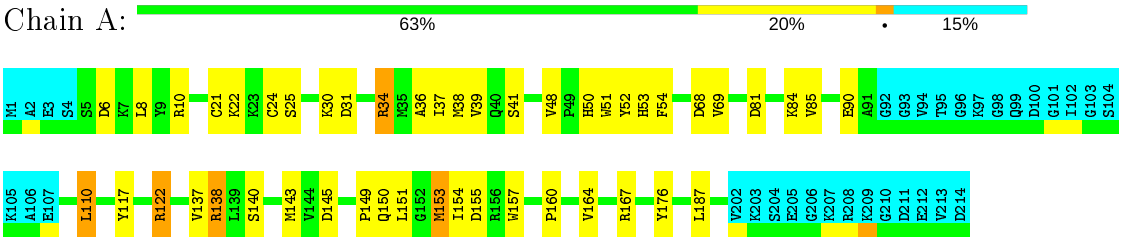
Chain B:



4.2.8 Score per residue for model 8

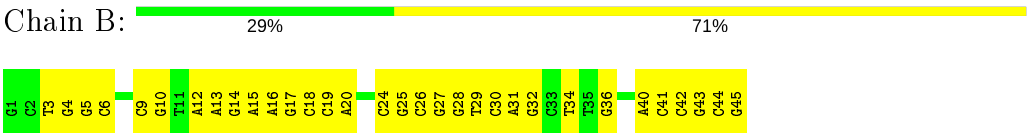
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

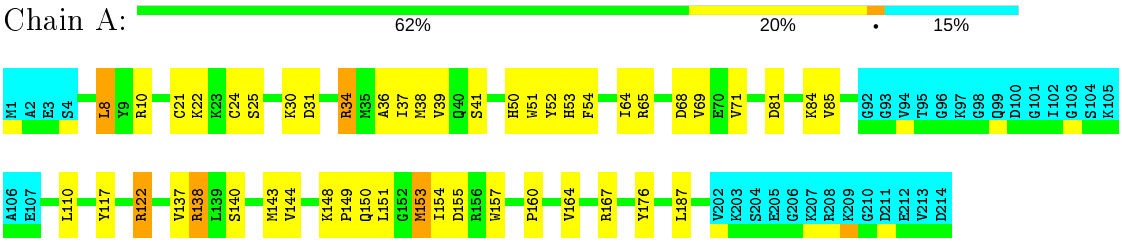
Chain B:



4.2.9 Score per residue for model 9

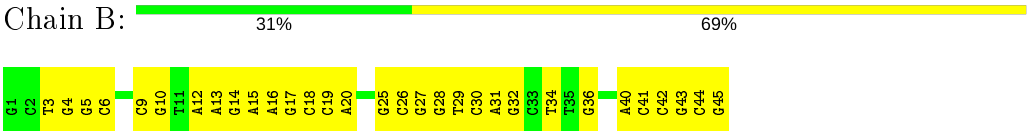
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

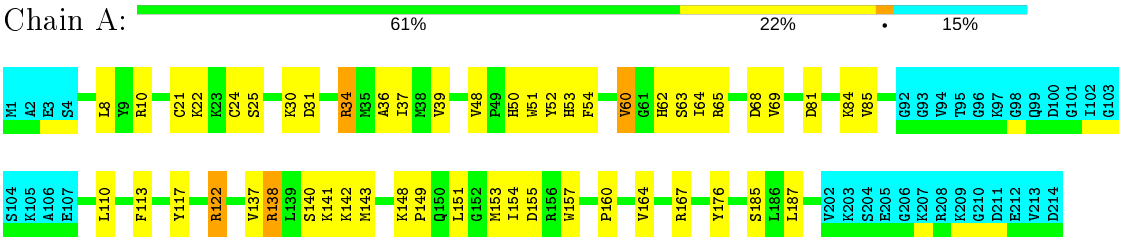
Chain B:



4.2.10 Score per residue for model 10

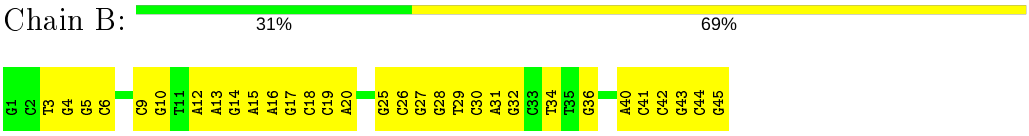
• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

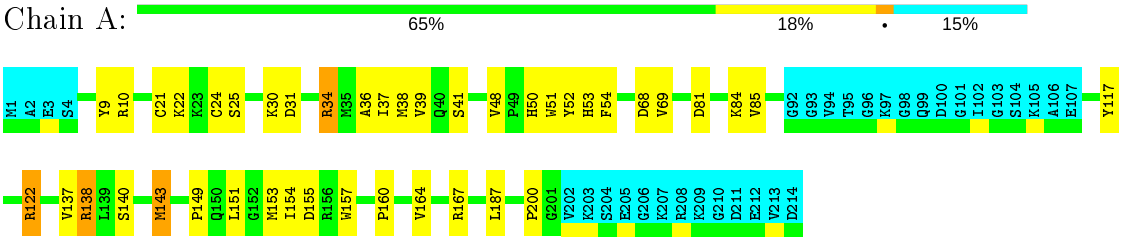
Chain B:



4.2.11 Score per residue for model 11

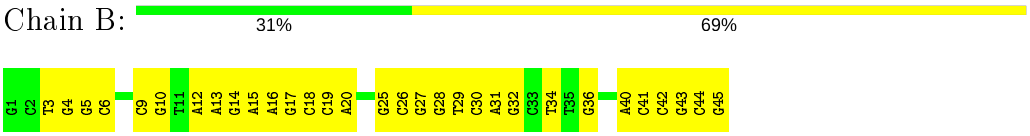
• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

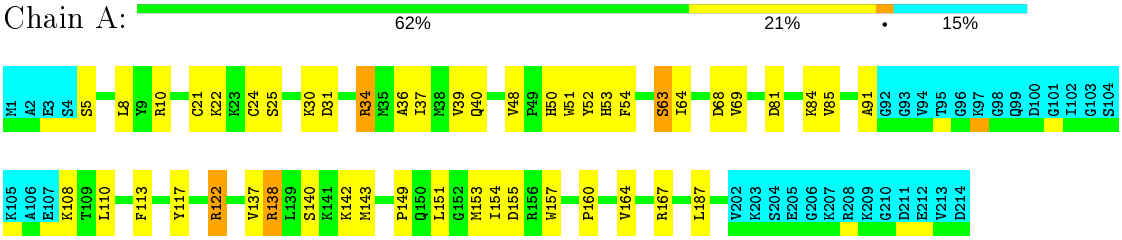
Chain B:



4.2.12 Score per residue for model 12

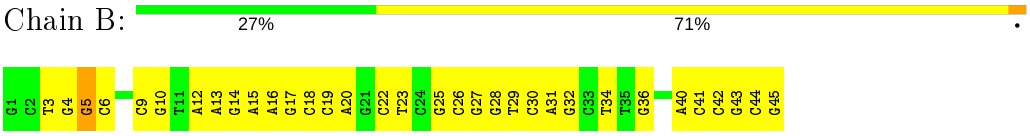
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

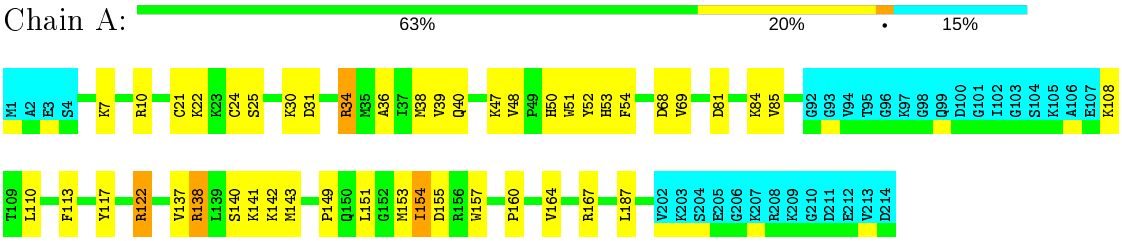
Chain B:



4.2.13 Score per residue for model 13

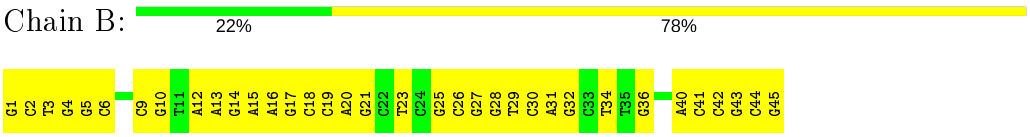
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

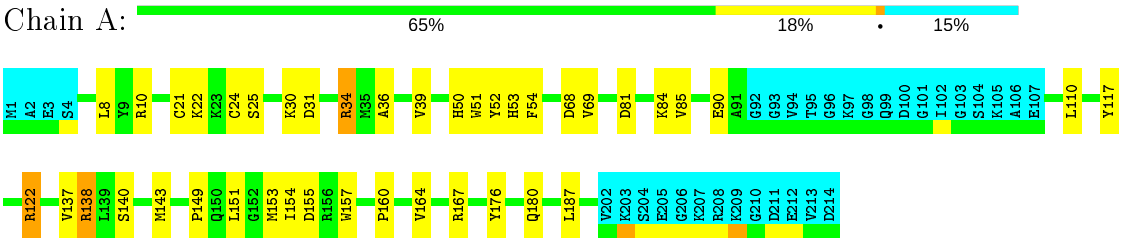
Chain B:



4.2.14 Score per residue for model 14

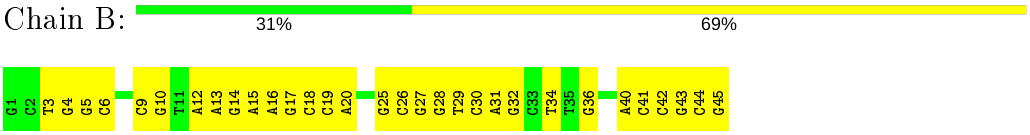
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

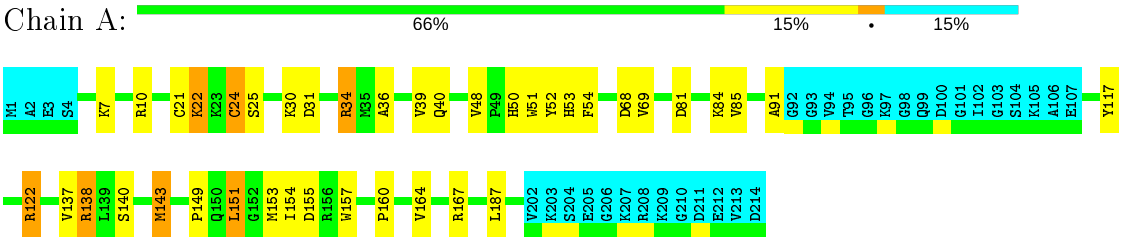
Chain B:



4.2.15 Score per residue for model 15

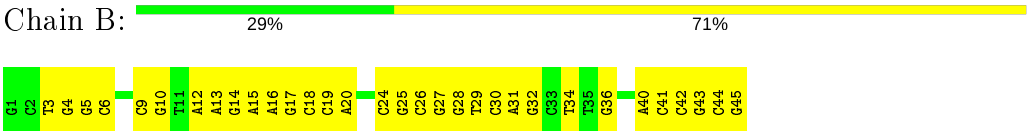
• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

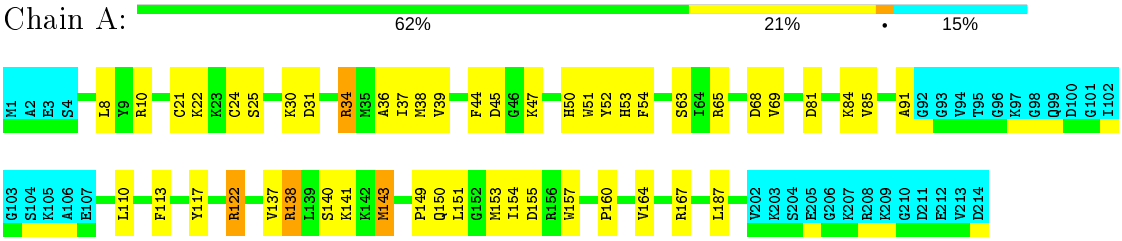
Chain B:



4.2.16 Score per residue for model 16

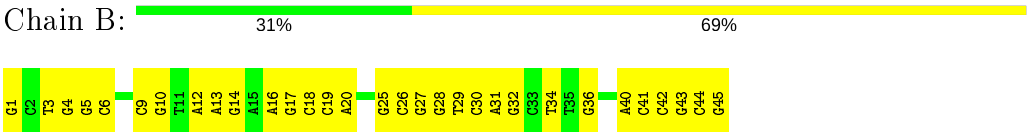
• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

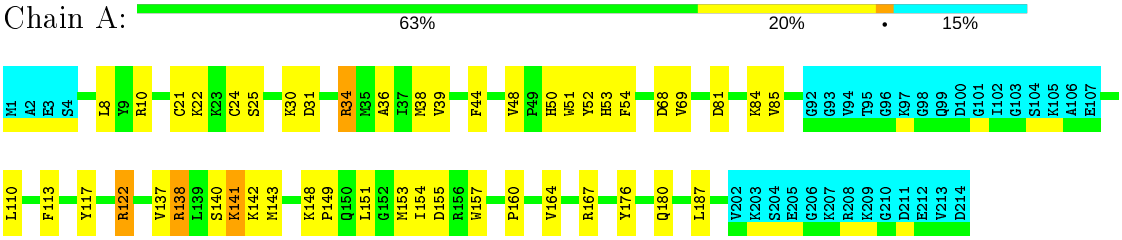
Chain B:



4.2.17 Score per residue for model 17

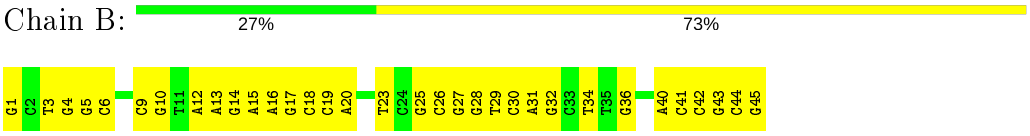
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

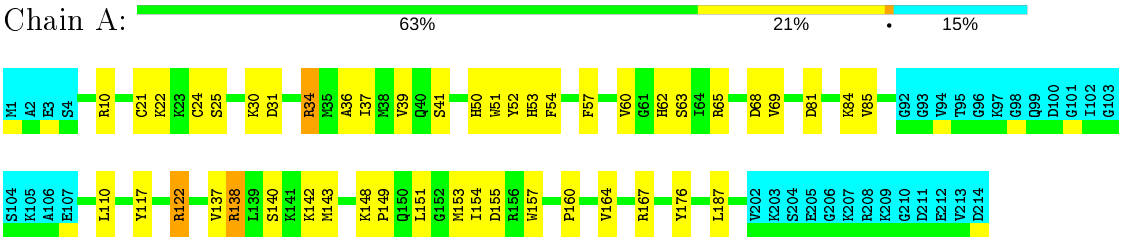
Chain B:



4.2.18 Score per residue for model 18

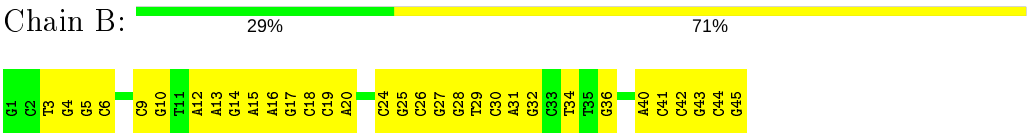
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

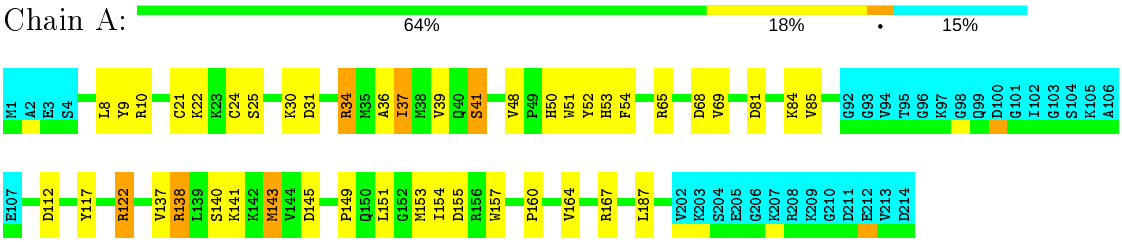
Chain B:



4.2.19 Score per residue for model 19

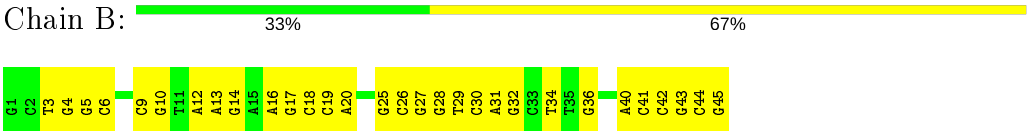
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

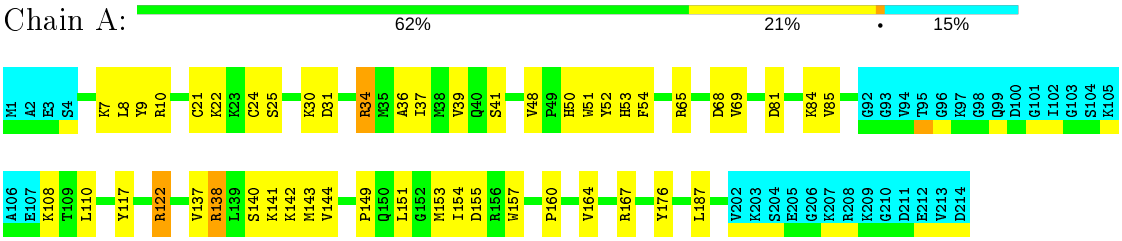
Chain B:



4.2.20 Score per residue for model 20

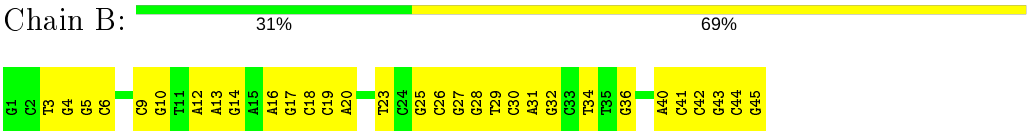
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

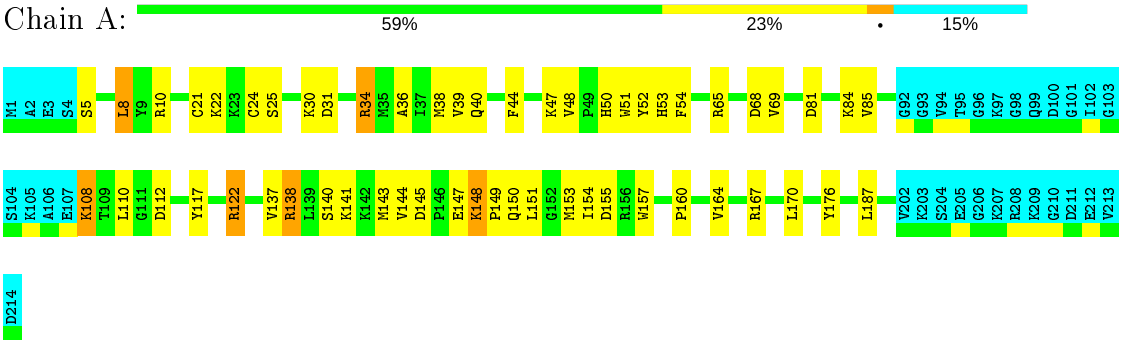
Chain B:



4.2.21 Score per residue for model 21

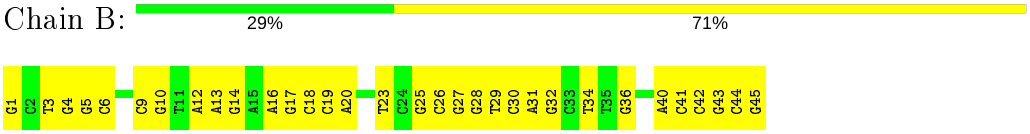
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

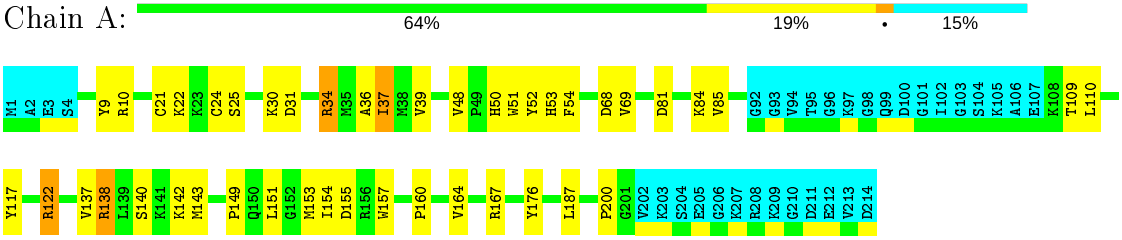
Chain B:



4.2.22 Score per residue for model 22

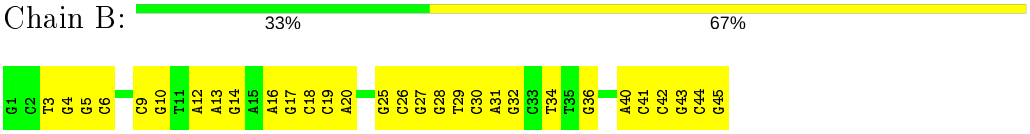
• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

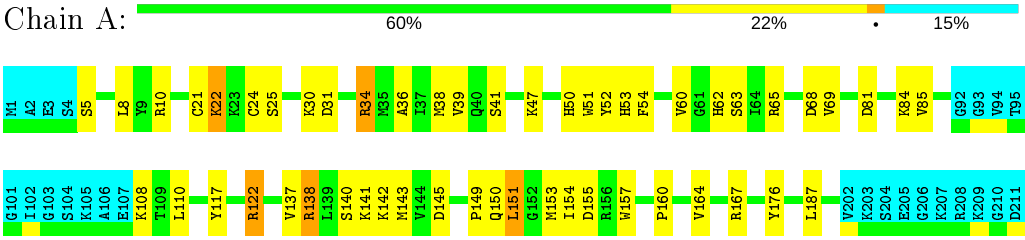
Chain B:



4.2.23 Score per residue for model 23

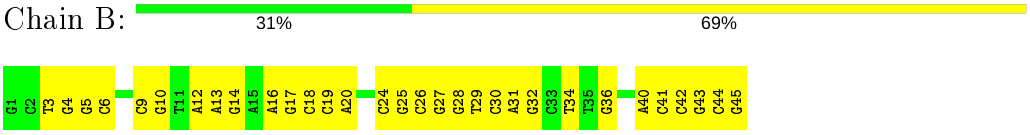
• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

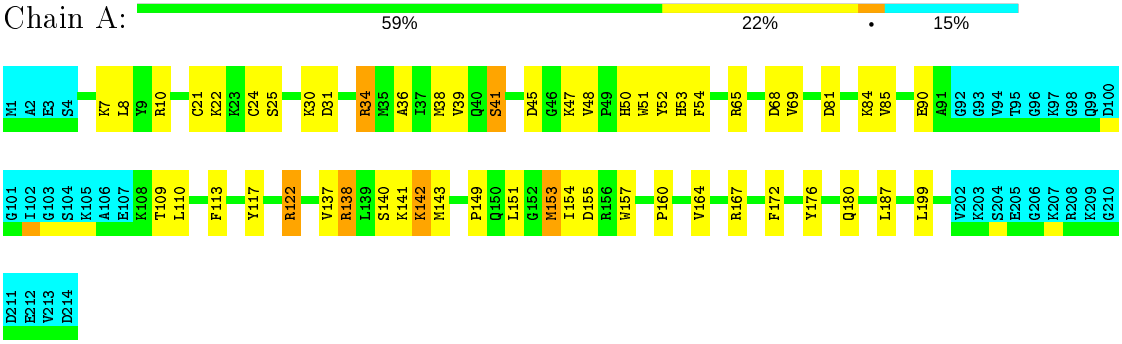
Chain B:



4.2.24 Score per residue for model 24

- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



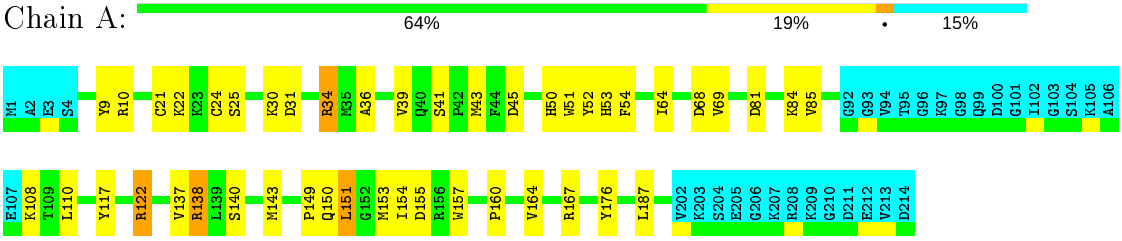
- Molecule 2: DNA (45-MER)

Chain B:

4.2.25 Score per residue for model 25

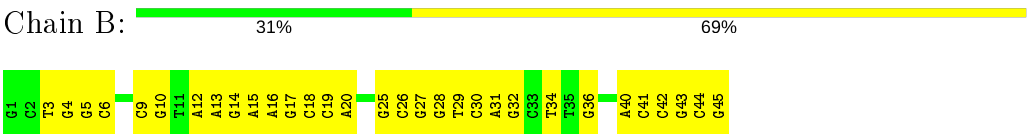
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

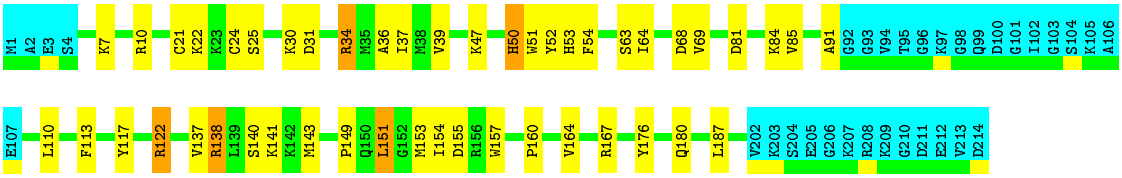
Chain B:



4.2.26 Score per residue for model 26

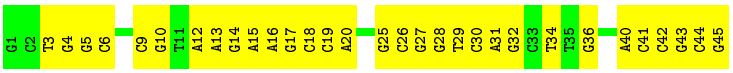
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

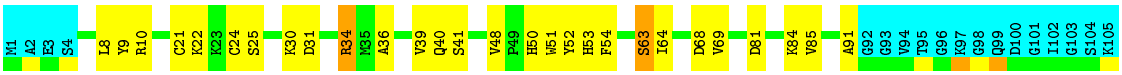
Chain B:

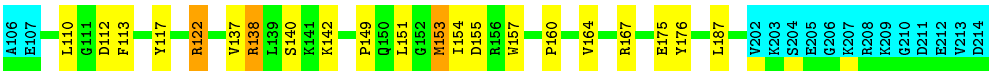


4.2.27 Score per residue for model 27

- Molecule 1: Poly [ADP-ribose] polymerase 1

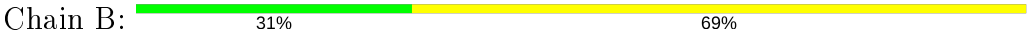
Chain A:

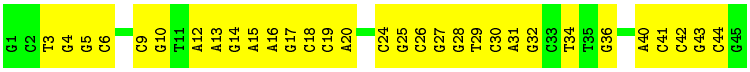




- Molecule 2: DNA (45-MER)

Chain B:

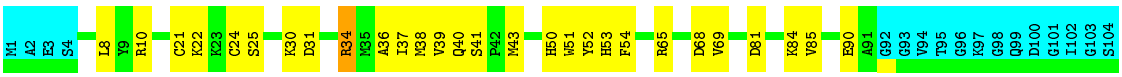


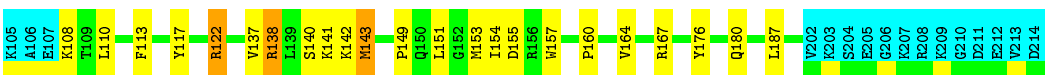


4.2.28 Score per residue for model 28

- Molecule 1: Poly [ADP-ribose] polymerase 1

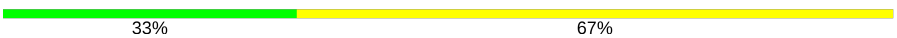
Chain A:

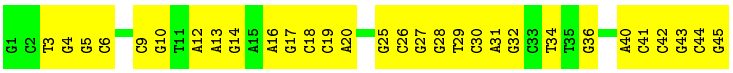




- Molecule 2: DNA (45-MER)

Chain B:

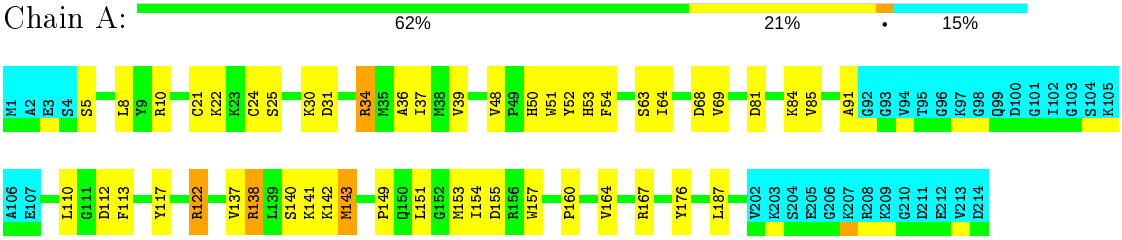




4.2.29 Score per residue for model 29

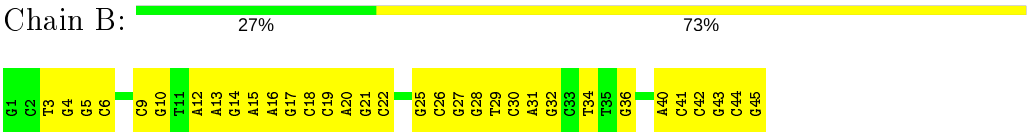
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

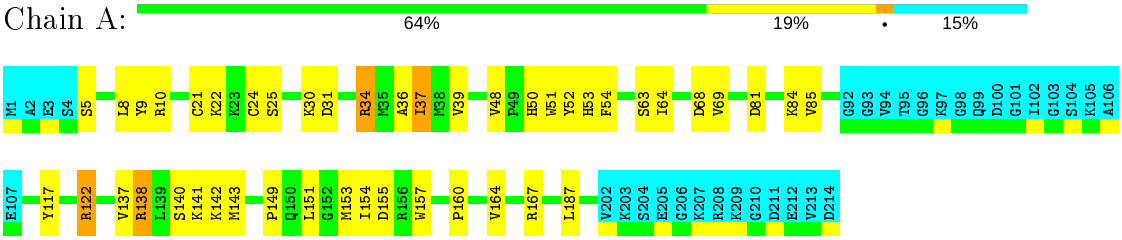
Chain B:



4.2.30 Score per residue for model 30

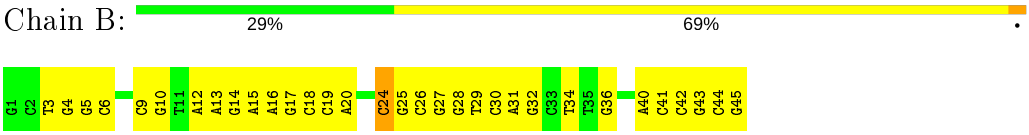
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

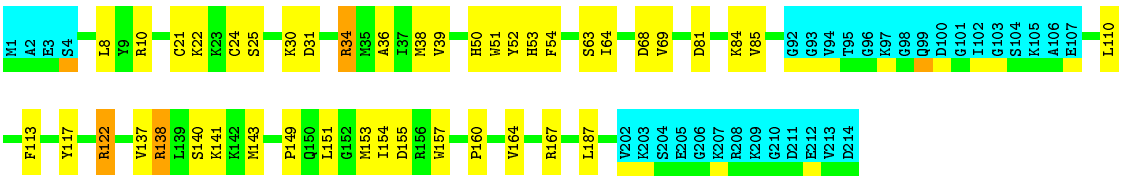
Chain B:



4.2.31 Score per residue for model 31

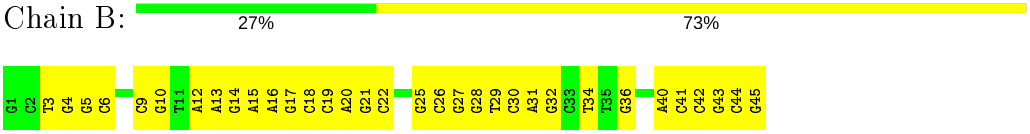
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

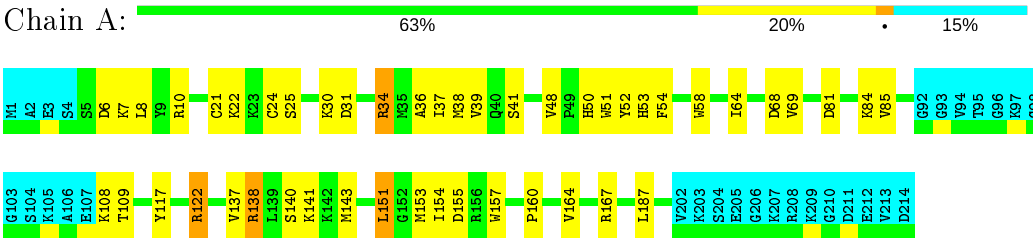
Chain B:



4.2.32 Score per residue for model 32

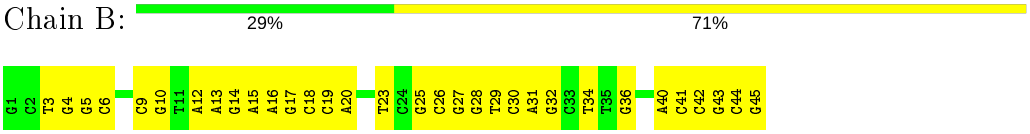
• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

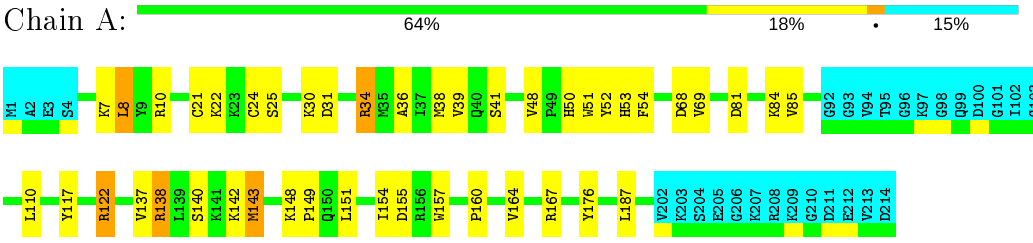
Chain B:



4.2.33 Score per residue for model 33

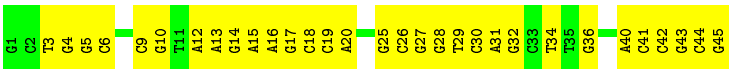
• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

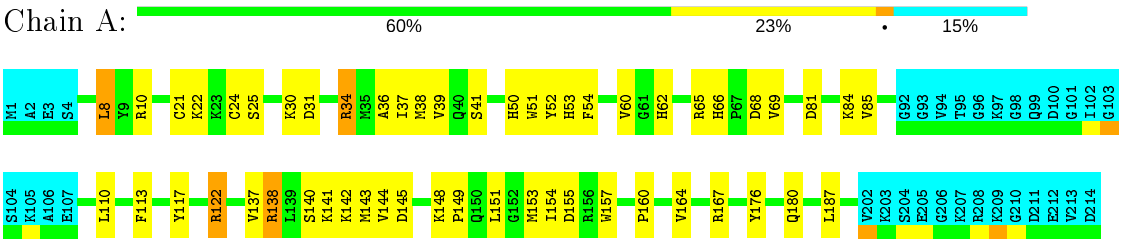
Chain B:



4.2.34 Score per residue for model 34

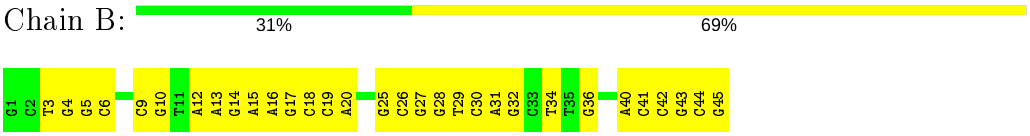
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

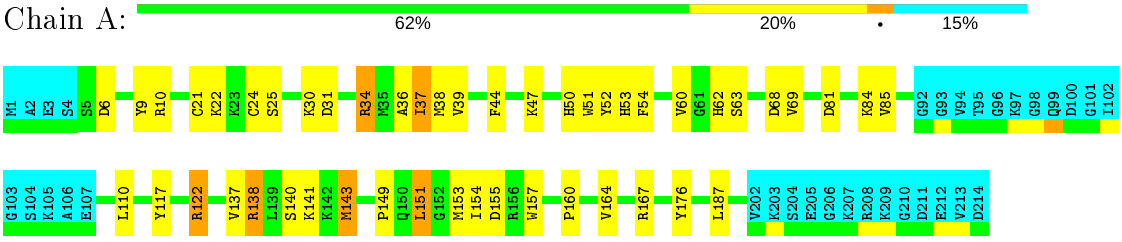
Chain B:



4.2.35 Score per residue for model 35

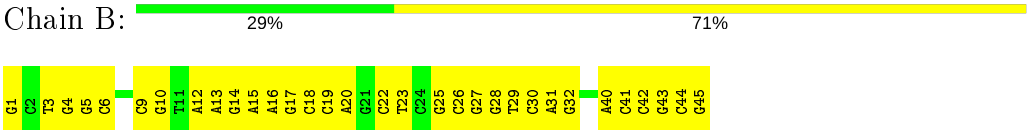
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

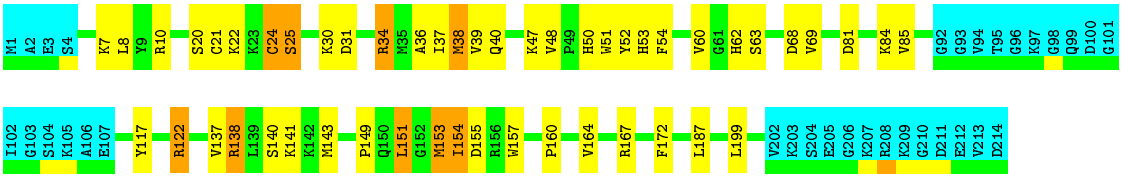
Chain B:



4.2.36 Score per residue for model 36 (medoid)

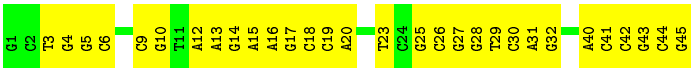
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

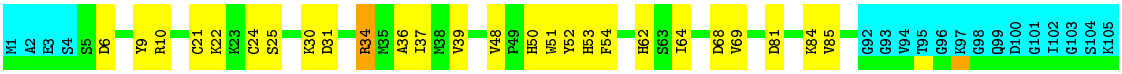
Chain B:



4.2.37 Score per residue for model 37

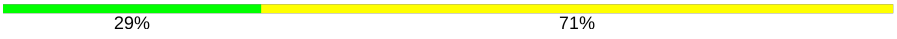
• Molecule 1: Poly [ADP-ribose] polymerase 1

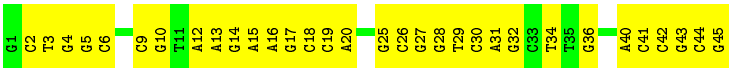
Chain A:



• Molecule 2: DNA (45-MER)

Chain B:

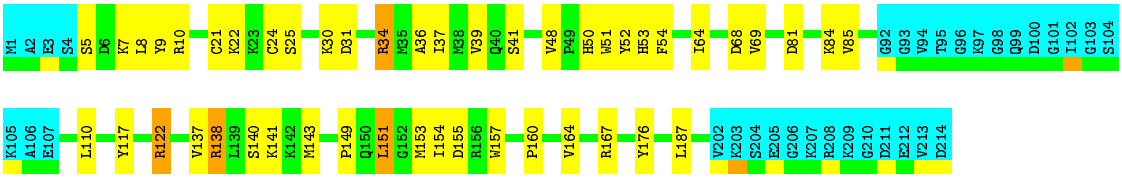




4.2.38 Score per residue for model 38

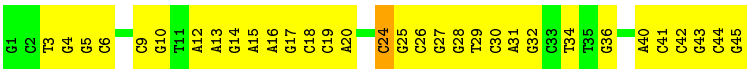
• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

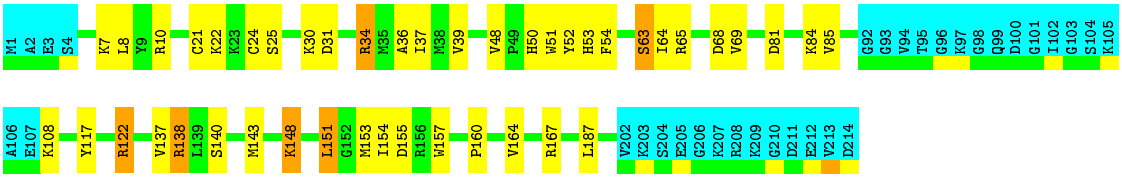
Chain B:



4.2.39 Score per residue for model 39

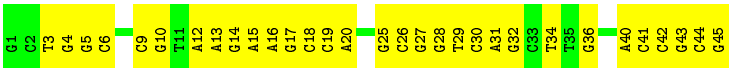
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

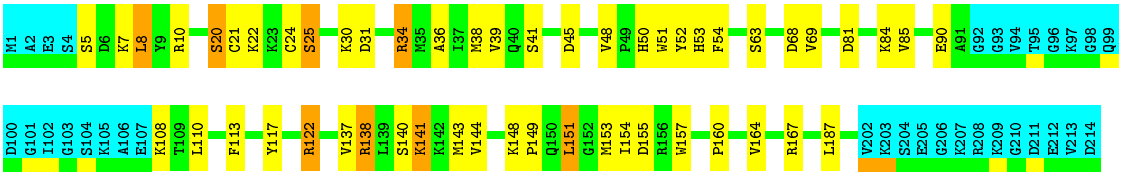
Chain B:



4.2.40 Score per residue for model 40

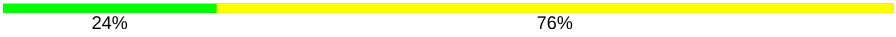
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

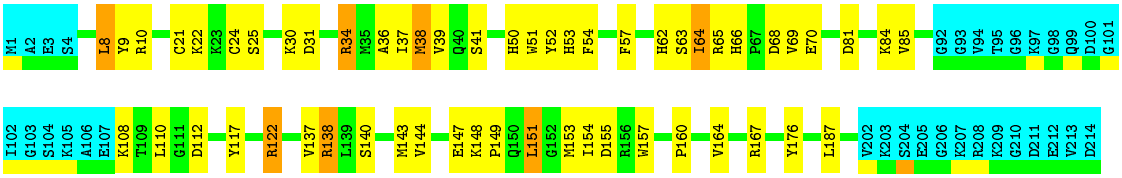
Chain B:



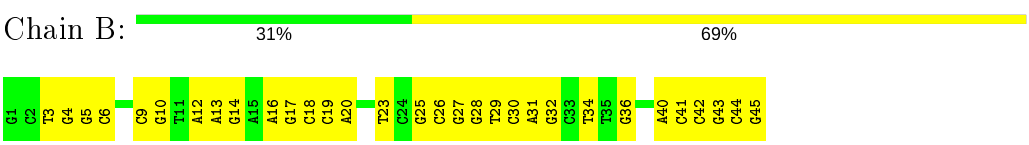
4.2.41 Score per residue for model 41

- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:

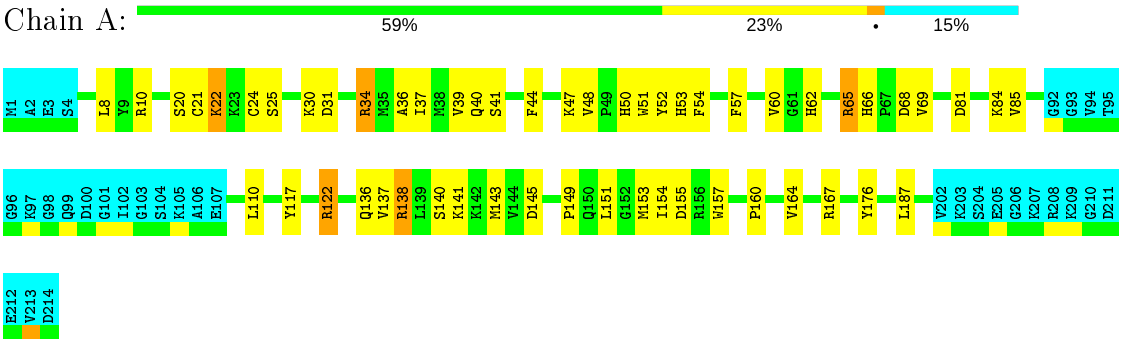


- Molecule 2: DNA (45-MER)

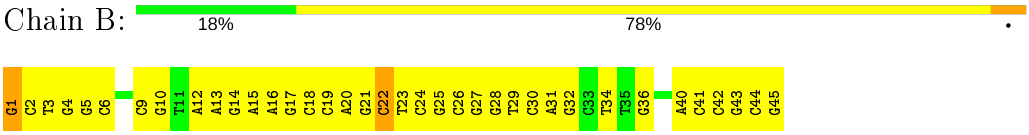


4.2.42 Score per residue for model 42

- Molecule 1: Poly [ADP-ribose] polymerase 1

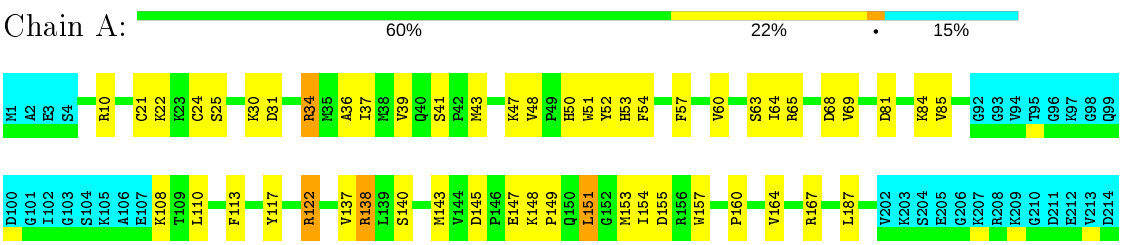


- Molecule 2: DNA (45-MER)



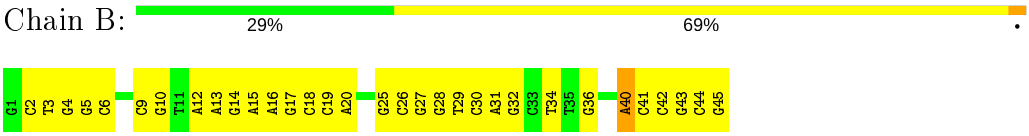
4.2.43 Score per residue for model 43

- Molecule 1: Poly [ADP-ribose] polymerase 1



- Molecule 2: DNA (45-MER)

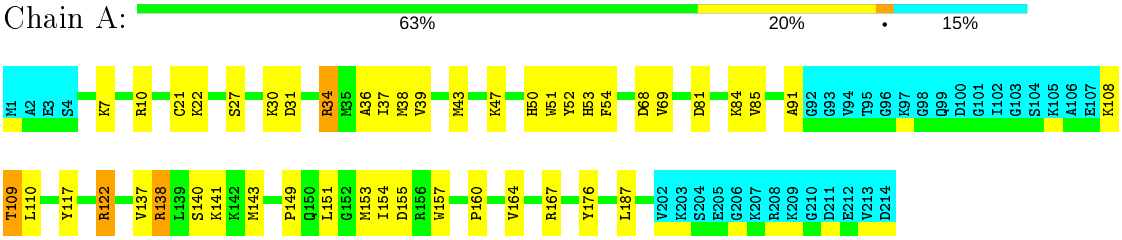
Chain B:



4.2.44 Score per residue for model 44

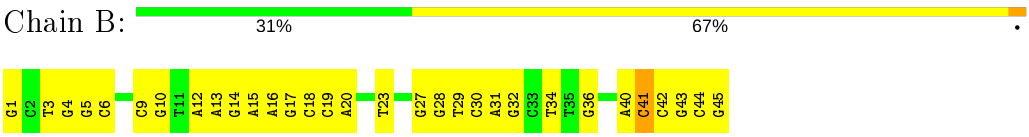
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

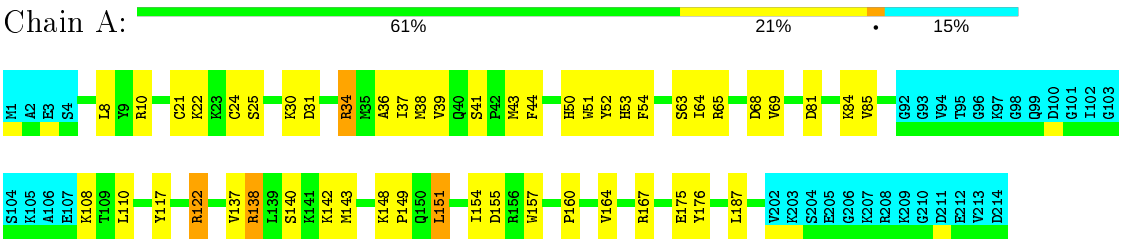
Chain B:



4.2.45 Score per residue for model 45

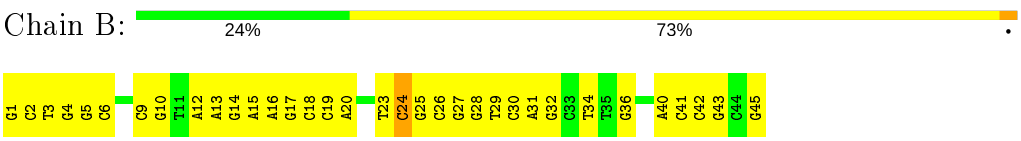
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

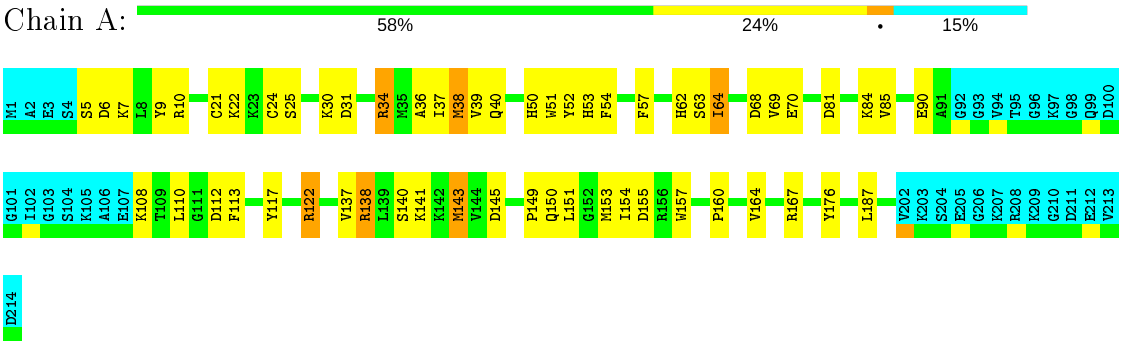
Chain B:



4.2.46 Score per residue for model 46

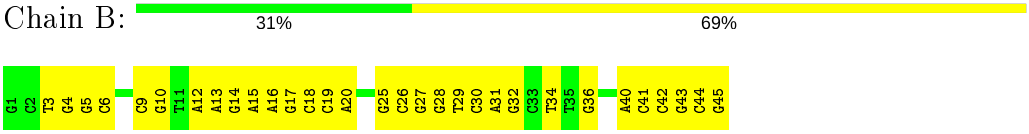
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

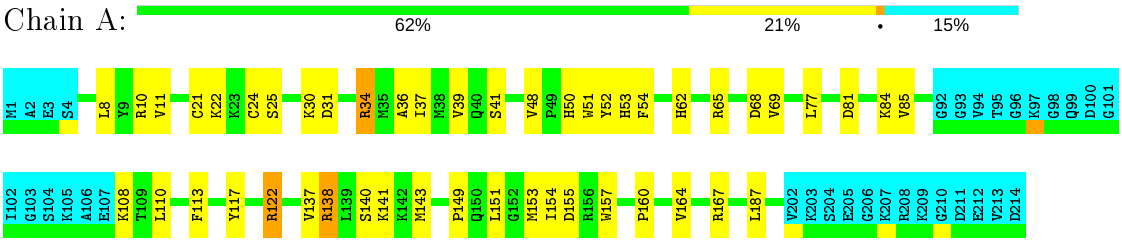
Chain B:



4.2.47 Score per residue for model 47

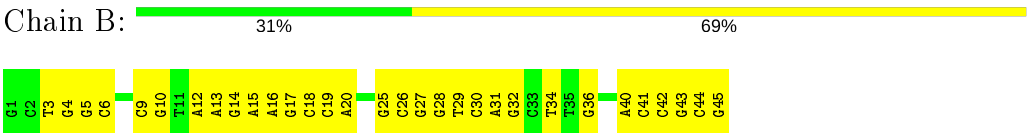
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

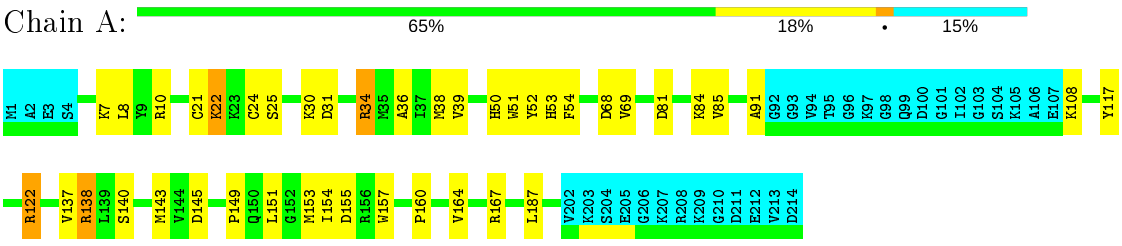
Chain B:



4.2.48 Score per residue for model 48

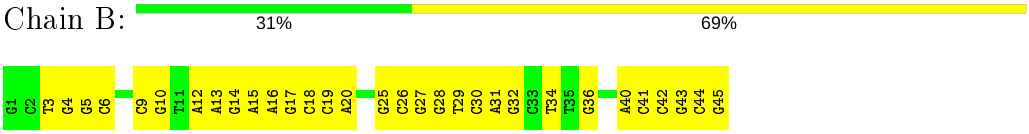
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

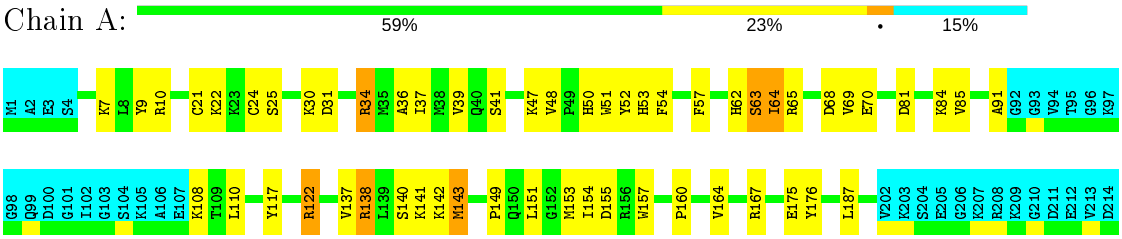
Chain B:



4.2.49 Score per residue for model 49

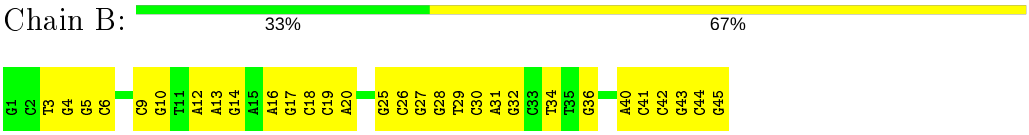
• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

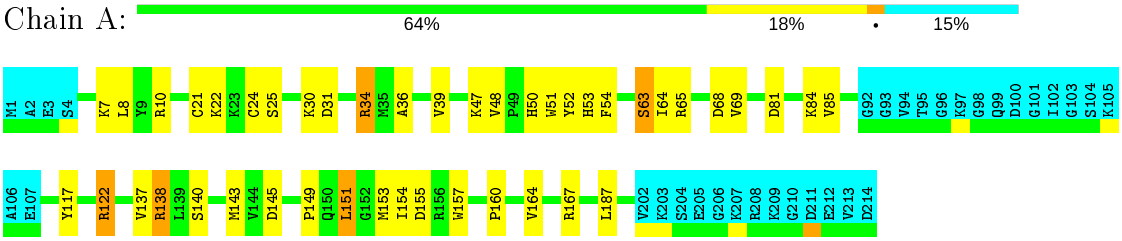
Chain B:



4.2.50 Score per residue for model 50

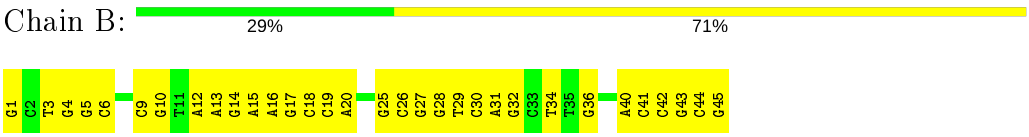
• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

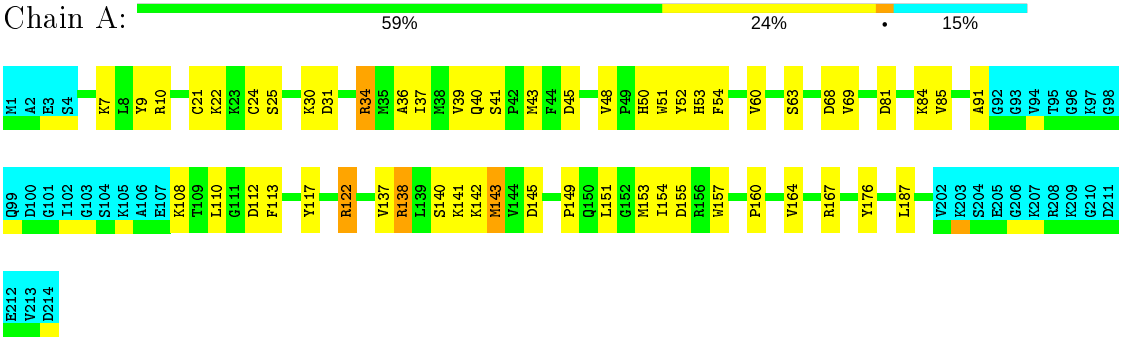
Chain B:



4.2.51 Score per residue for model 51

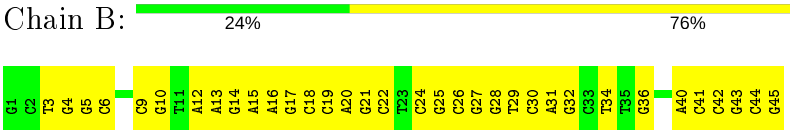
• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

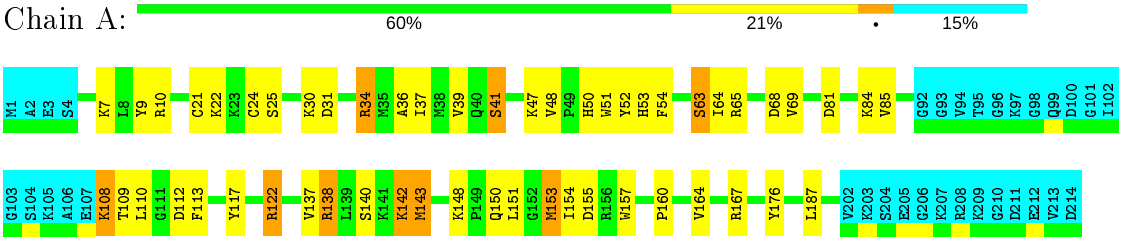
Chain B:



4.2.52 Score per residue for model 52

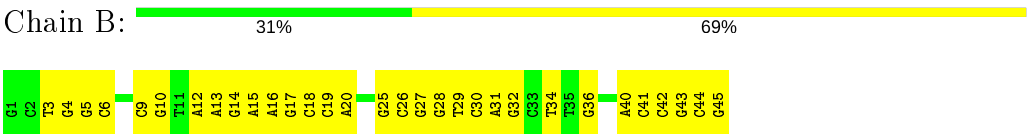
• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

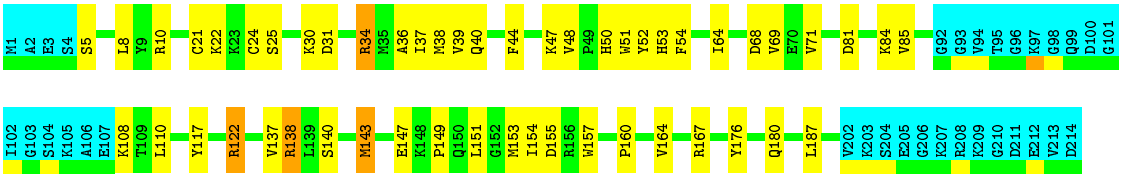
Chain B:



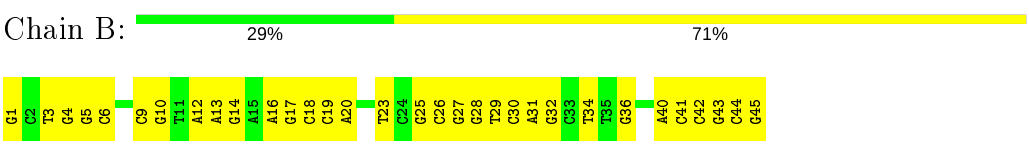
4.2.53 Score per residue for model 53

• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:

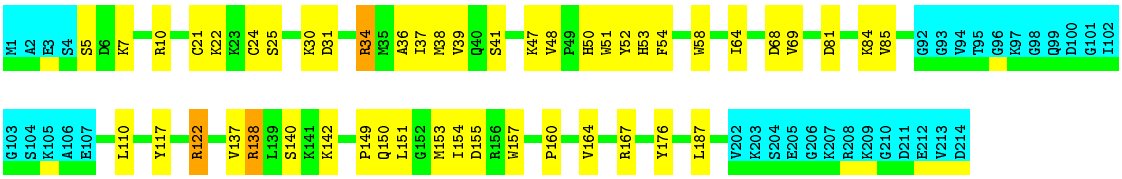


- Molecule 2: DNA (45-MER)

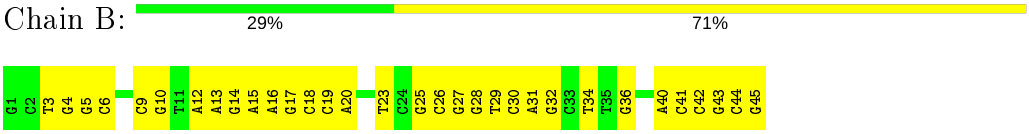


4.2.54 Score per residue for model 54

- Molecule 1: Poly [ADP-ribose] polymerase 1



- Molecule 2: DNA (45-MER)

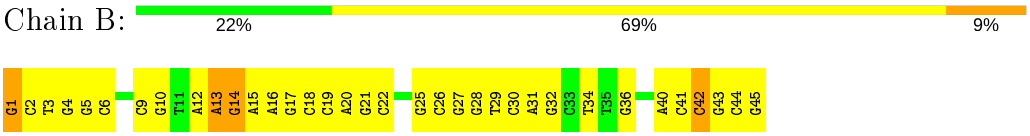


4.2.55 Score per residue for model 55

- Molecule 1: Poly [ADP-ribose] polymerase 1

- Molecule 2: DNA (45-MER)

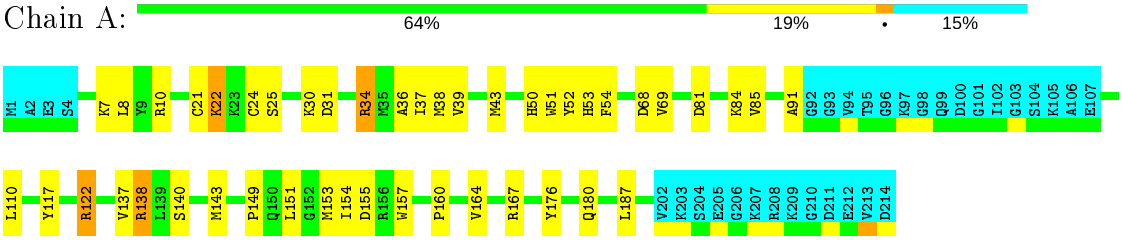
Chain B:



4.2.56 Score per residue for model 56

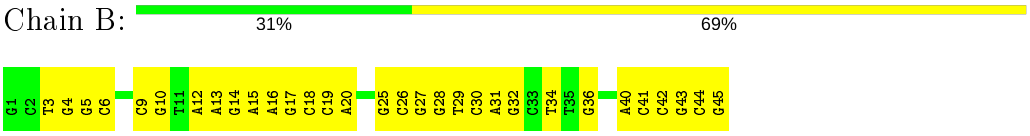
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

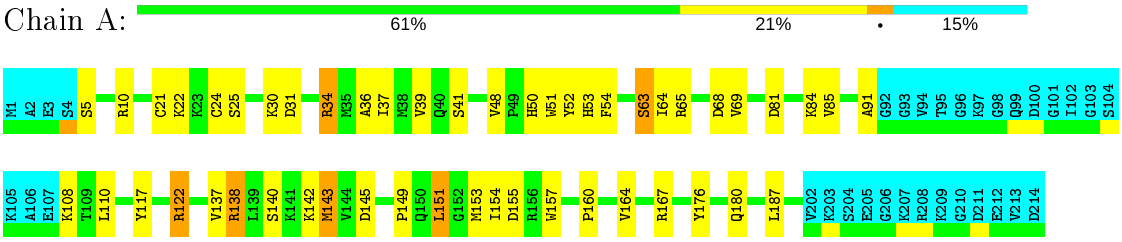
Chain B:



4.2.57 Score per residue for model 57

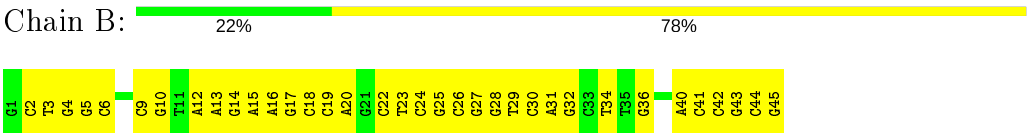
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

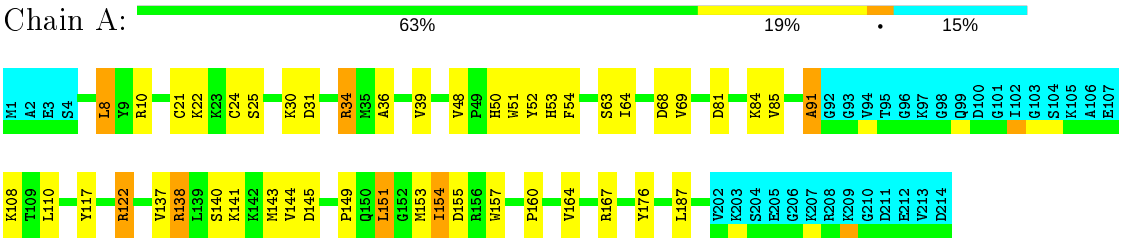
Chain B:



4.2.58 Score per residue for model 58

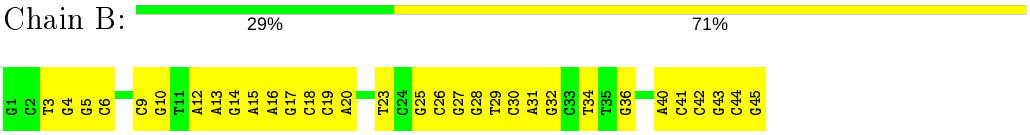
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

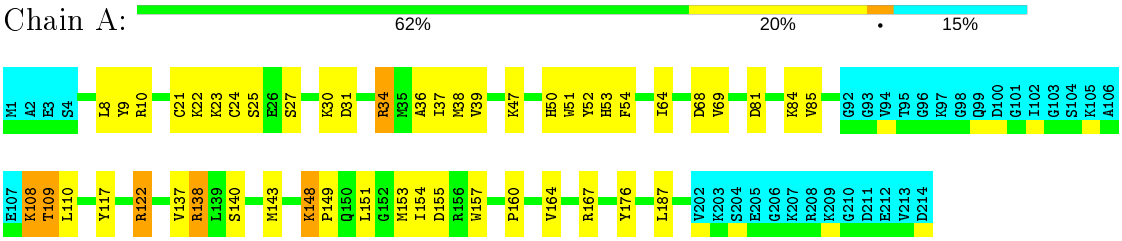
Chain B:



4.2.59 Score per residue for model 59

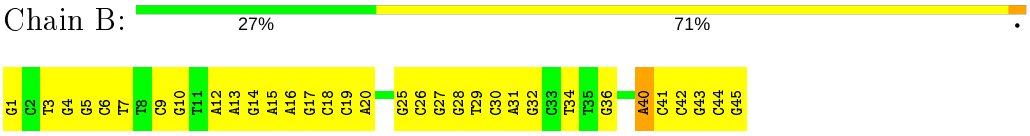
• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

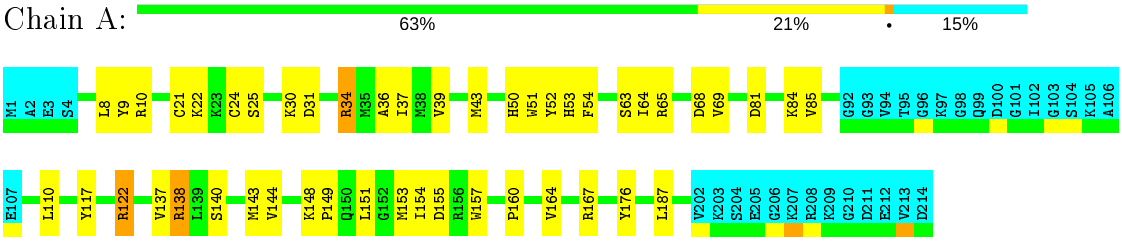
Chain B:



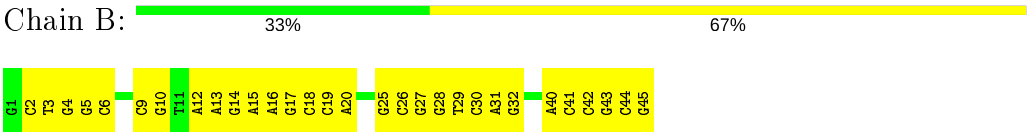
4.2.60 Score per residue for model 60

• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:

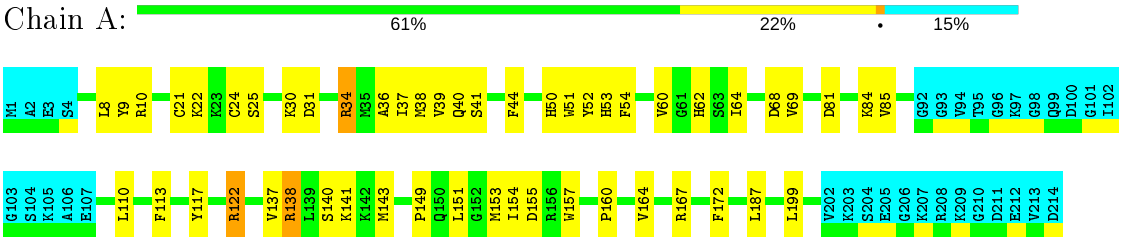


• Molecule 2: DNA (45-MER)

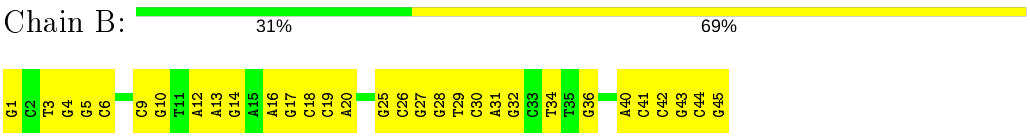


4.2.61 Score per residue for model 61

• Molecule 1: Poly [ADP-ribose] polymerase 1

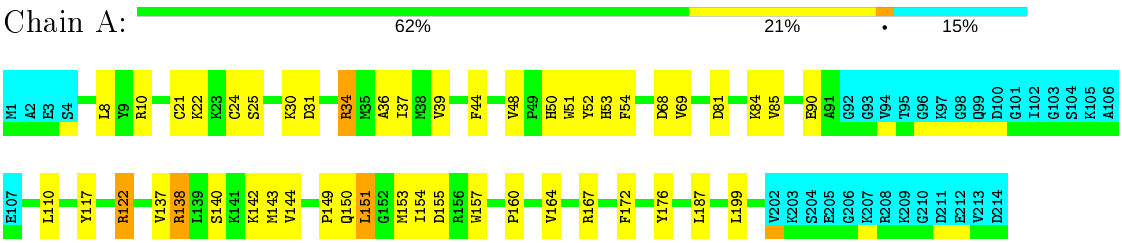


• Molecule 2: DNA (45-MER)

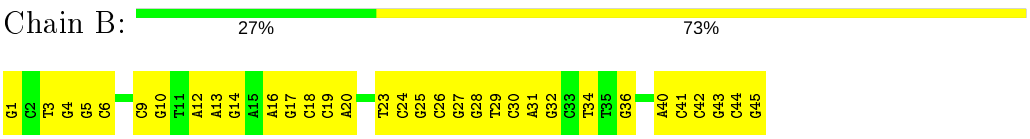


4.2.62 Score per residue for model 62

• Molecule 1: Poly [ADP-ribose] polymerase 1



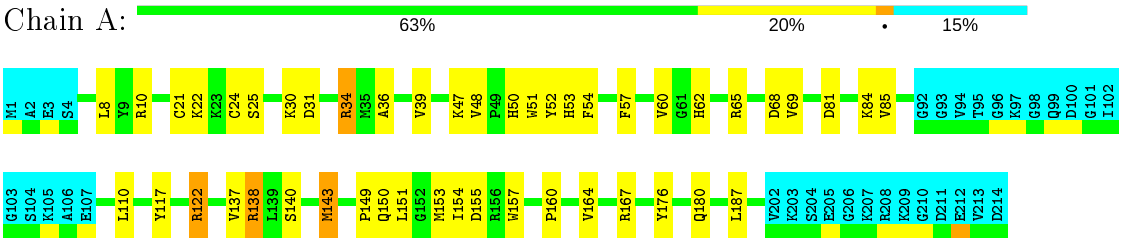
• Molecule 2: DNA (45-MER)



4.2.63 Score per residue for model 63

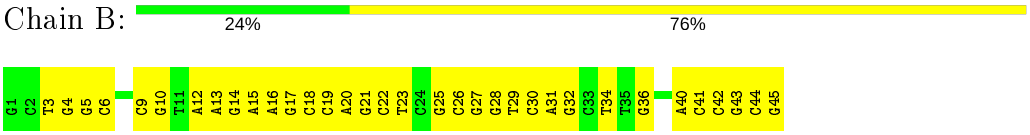
• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

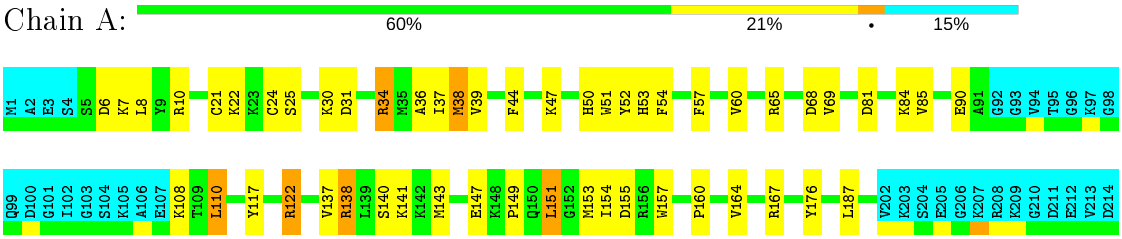
Chain B:



4.2.64 Score per residue for model 64

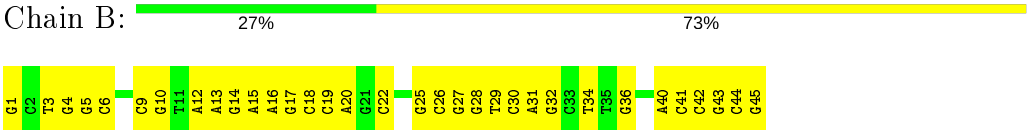
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

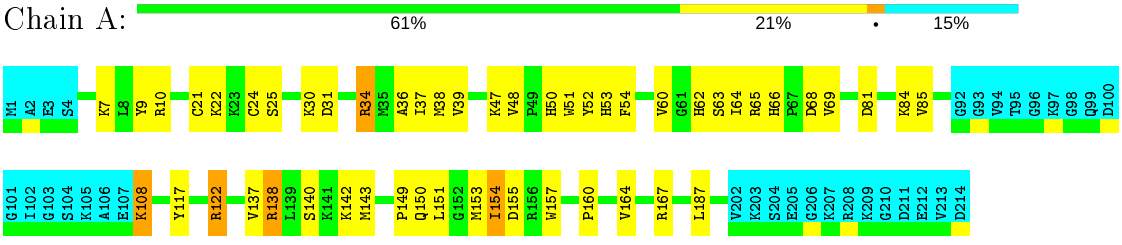
Chain B:



4.2.65 Score per residue for model 65

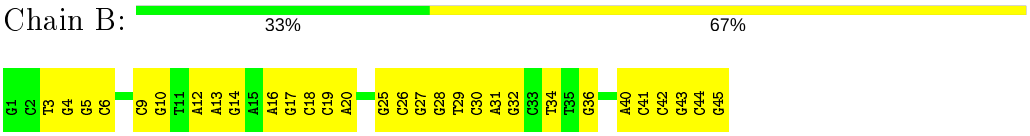
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

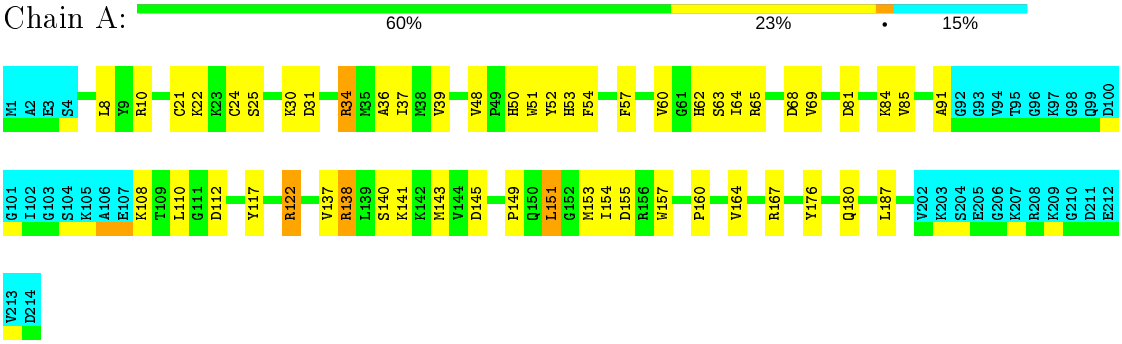
Chain B:



4.2.66 Score per residue for model 66

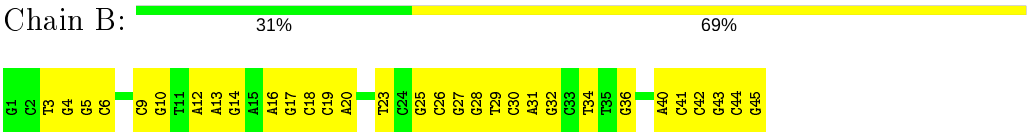
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

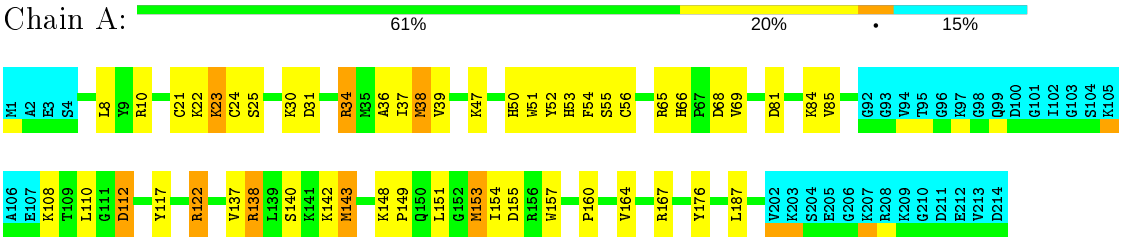
Chain B:



4.2.67 Score per residue for model 67

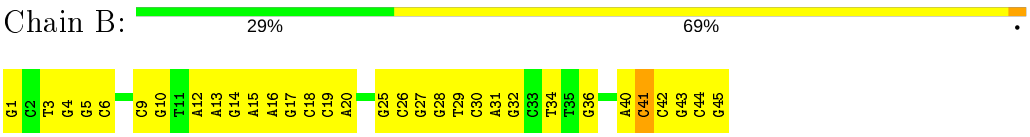
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

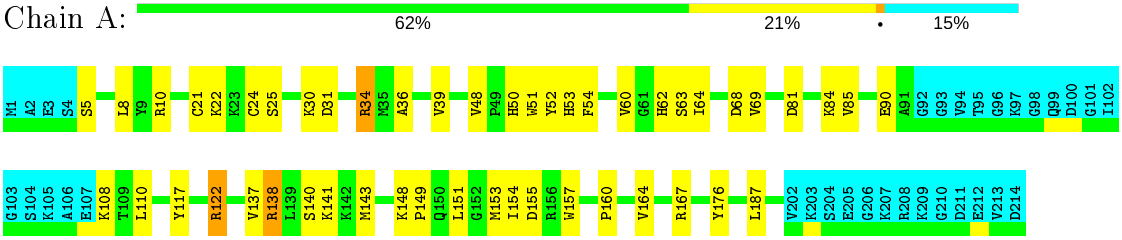
Chain B:



4.2.68 Score per residue for model 68

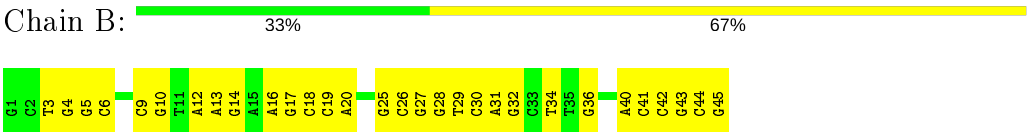
• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

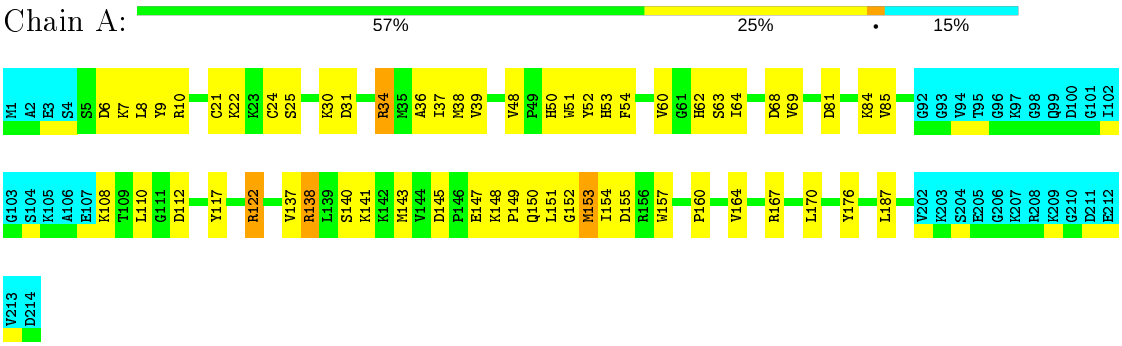
Chain B:



4.2.69 Score per residue for model 69

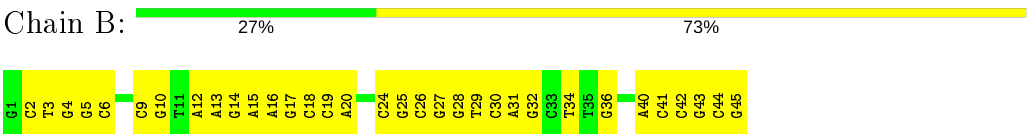
• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

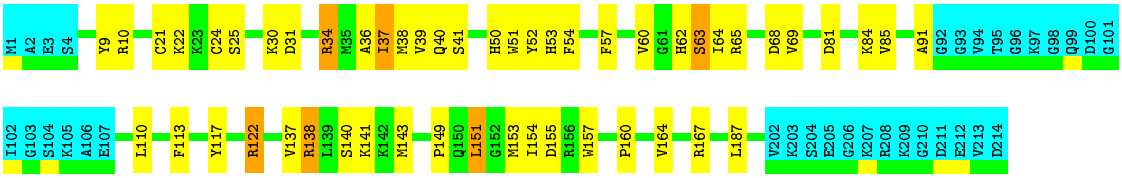
Chain B:



4.2.70 Score per residue for model 70

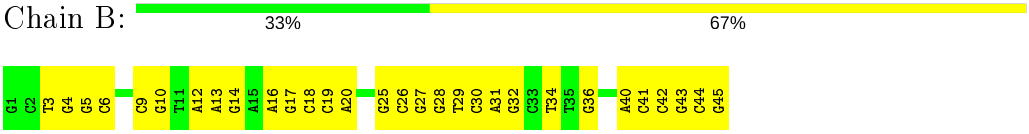
• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

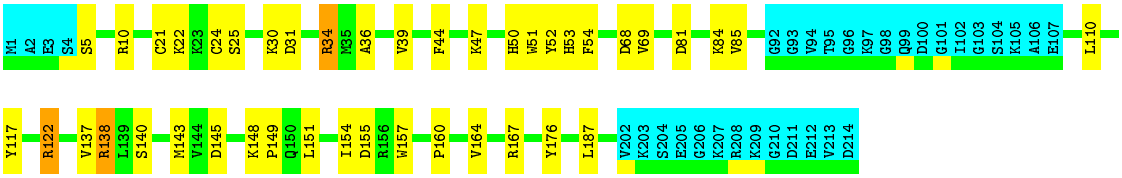
Chain B:



4.2.71 Score per residue for model 71

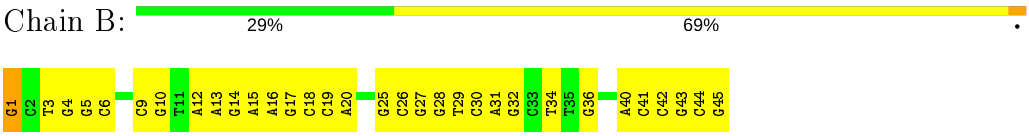
• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

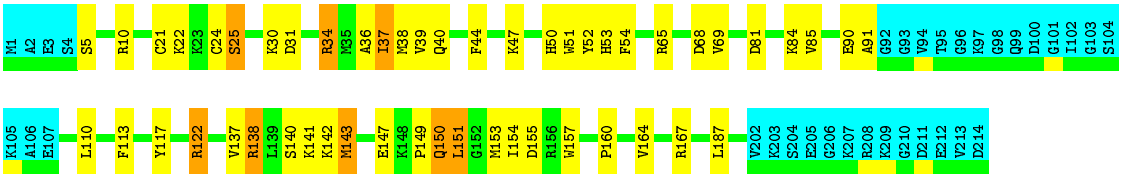
Chain B:



4.2.72 Score per residue for model 72

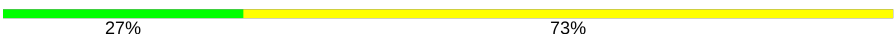
• Molecule 1: Poly [ADP-ribose] polymerase 1

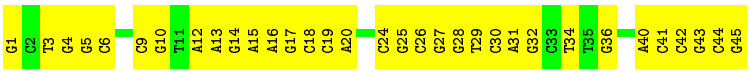
Chain A:



• Molecule 2: DNA (45-MER)

Chain B:

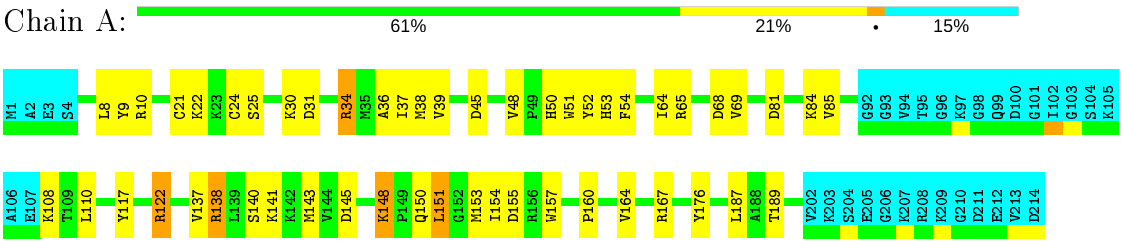




4.2.73 Score per residue for model 73

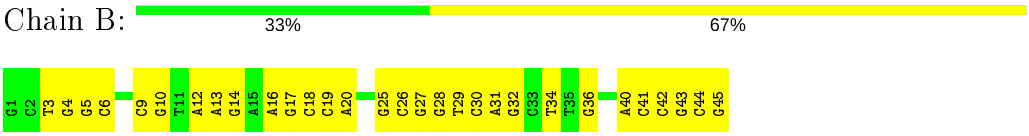
• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

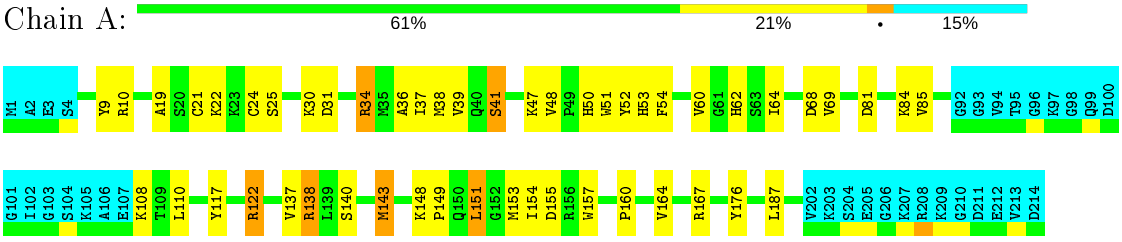
Chain B:



4.2.74 Score per residue for model 74

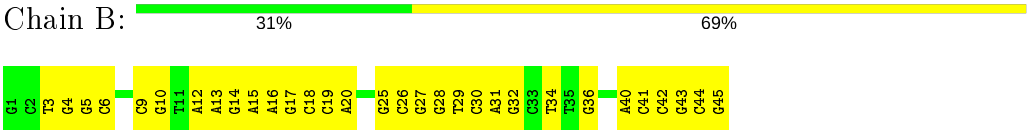
• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

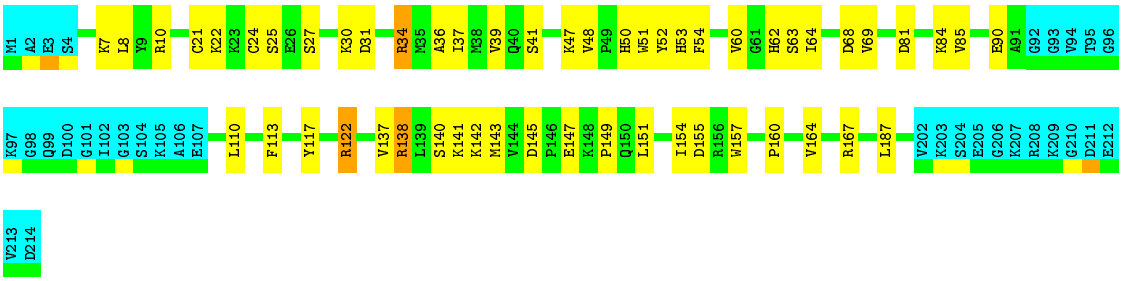
Chain B:



4.2.75 Score per residue for model 75

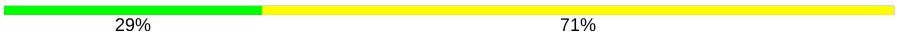
• Molecule 1: Poly [ADP-ribose] polymerase 1

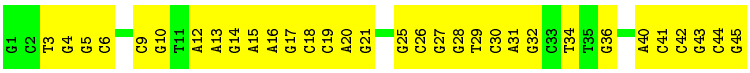
Chain A:



• Molecule 2: DNA (45-MER)

Chain B:

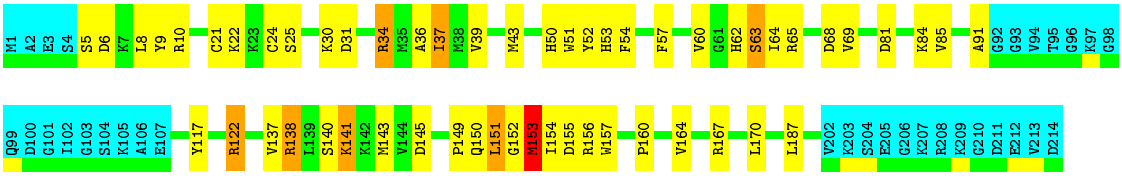




4.2.76 Score per residue for model 76

• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



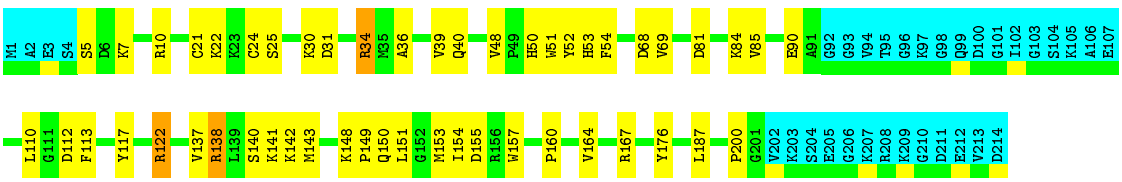
• Molecule 2: DNA (45-MER)

Chain B:

4.2.77 Score per residue for model 77

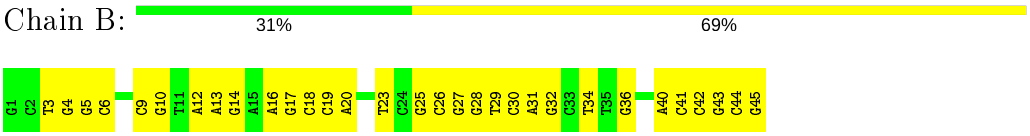
• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



• Molecule 2: DNA (45-MER)

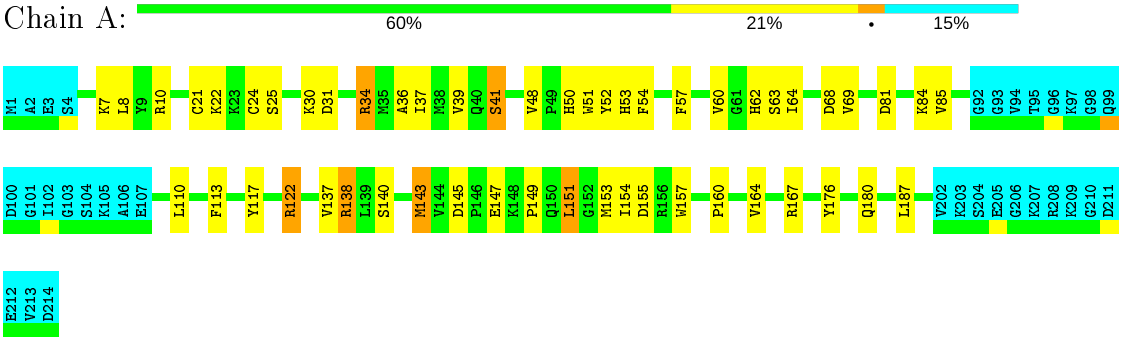
Chain B:



4.2.78 Score per residue for model 78

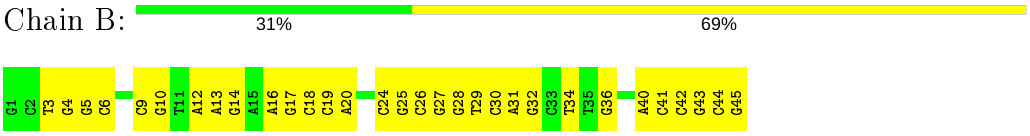
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 2: DNA (45-MER)

Chain B:



5 Refinement protocol and experimental data overview

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

Of the 78 calculated structures, 78 were deposited, based on the following criterion: *Total, Tensor and NOE xplor energies simultaneously below thresholds (6000, 1500 and 2 kcal.mol-1 respectively).*

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

Software name	Classification	Version
X-PLOR NIH	structure solution	2.28
X-PLOR NIH	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	3
Total number of shifts	1564
Number of shifts mapped to atoms	1564
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	29%

No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

5.1 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	1456	1443	1443	46±5
2	B	924	506	505	46±4
All	All	185796	152022	151942	6667

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 20.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:3:DT:N3	2:B:4:DG:C5	1.23	2.07	2	78
2:B:3:DT:C2	2:B:4:DG:C5	1.10	2.39	2	78
2:B:3:DT:C2	2:B:4:DG:C8	1.07	2.43	2	3
1:A:24:CYS:O	1:A:25:SER:OG	1.03	1.75	72	2
2:B:3:DT:C2	2:B:4:DG:N7	1.00	2.29	2	5
2:B:3:DT:N3	2:B:4:DG:C6	1.00	2.30	2	78
2:B:12:DA:C6	2:B:13:DA:N1	1.00	2.29	55	1
2:B:41:DC:C4	2:B:42:DC:N4	0.98	2.31	36	78
2:B:3:DT:O2	2:B:4:DG:C4	0.95	2.20	2	1
1:A:39:VAL:HG22	1:A:48:VAL:O	0.94	1.62	58	39
1:A:154:ILE:HD11	2:B:45:DG:C8	0.93	1.97	72	66
1:A:151:LEU:HD11	2:B:45:DG:N1	0.92	1.79	15	16
1:A:151:LEU:HD21	2:B:45:DG:C6	0.92	2.00	45	15
2:B:4:DG:H2"	2:B:5:DG:C8	0.91	2.01	60	8
1:A:110:LEU:HD21	1:A:176:TYR:CE1	0.91	2.00	67	22
2:B:12:DA:C5	2:B:13:DA:C6	0.88	2.62	55	78
1:A:110:LEU:HD11	1:A:176:TYR:CE1	0.88	2.03	3	5
1:A:151:LEU:HD11	2:B:45:DG:C6	0.88	2.04	76	36
1:A:36:ALA:HB2	1:A:51:TRP:CE3	0.87	2.05	36	78
1:A:39:VAL:HG13	1:A:149:PRO:HG2	0.86	1.46	2	32
1:A:48:VAL:HG11	2:B:23:DT:C7	0.85	2.00	57	5
2:B:12:DA:C6	2:B:13:DA:C6	0.85	2.64	55	78
1:A:39:VAL:HG13	1:A:149:PRO:CG	0.85	2.01	41	36
1:A:22:LYS:CB	1:A:52:TYR:CE2	0.85	2.59	47	77
1:A:143:MET:O	1:A:154:ILE:HG22	0.84	1.72	69	72
2:B:40:DA:H2"	2:B:41:DC:C5	0.84	2.08	59	2
2:B:3:DT:C2	2:B:4:DG:C4	0.83	2.65	2	1
2:B:42:DC:OP2	2:B:42:DC:H2'	0.83	1.74	44	1
1:A:39:VAL:HG21	1:A:50:HIS:CD2	0.83	2.08	41	37
2:B:14:DG:H2"	2:B:15:DA:C5'	0.83	2.04	3	1
1:A:110:LEU:HD23	1:A:113:PHE:CD1	0.82	2.10	28	3
1:A:151:LEU:HD11	2:B:45:DG:C2	0.81	2.11	64	11
1:A:39:VAL:HG11	1:A:50:HIS:NE2	0.80	1.90	38	29
2:B:14:DG:H2"	2:B:15:DA:O5'	0.80	1.74	3	1
1:A:151:LEU:HD21	2:B:45:DG:C2	0.80	2.11	4	5
2:B:25:DG:C5	2:B:26:DC:C5	0.80	2.70	38	76
1:A:151:LEU:CD2	1:A:154:ILE:HD12	0.79	2.06	22	26
2:B:25:DG:C4	2:B:26:DC:C5	0.79	2.71	38	76
1:A:9:TYR:CE1	1:A:37:ILE:HD12	0.79	2.13	2	5
1:A:9:TYR:CE1	1:A:37:ILE:HD13	0.79	2.13	6	9
2:B:31:DA:H2"	2:B:32:DG:O5'	0.79	1.77	8	78

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:CYS:O	1:A:25:SER:CB	0.78	2.28	72	76
1:A:39:VAL:HG12	1:A:48:VAL:O	0.78	1.78	68	2
1:A:39:VAL:HG23	1:A:149:PRO:CG	0.78	2.09	68	1
1:A:110:LEU:HD23	1:A:113:PHE:CD2	0.78	2.12	26	2
2:B:3:DT:O2	2:B:4:DG:N9	0.78	2.16	2	1
2:B:23:DT:O2	2:B:23:DT:H2'	0.77	1.79	62	2
2:B:41:DC:C6	2:B:41:DC:P	0.77	2.77	43	2
2:B:41:DC:C5	2:B:42:DC:N4	0.77	2.53	67	78
1:A:39:VAL:HG11	1:A:50:HIS:CD2	0.76	2.14	58	39
1:A:39:VAL:HG21	1:A:50:HIS:NE2	0.76	1.94	30	70
1:A:39:VAL:HG12	1:A:149:PRO:HB2	0.76	1.55	36	18
2:B:13:DA:C2'	2:B:14:DG:O5'	0.76	2.32	10	78
2:B:1:DG:H3'	2:B:1:DG:OP3	0.76	1.79	6	5
1:A:22:LYS:HB2	1:A:52:TYR:CE2	0.76	2.13	47	76
1:A:39:VAL:HG13	1:A:149:PRO:HG3	0.75	1.58	72	9
2:B:3:DT:N3	2:B:4:DG:N7	0.75	2.31	2	1
1:A:48:VAL:HG11	2:B:23:DT:H72	0.74	1.59	57	4
1:A:39:VAL:HG22	1:A:149:PRO:HB2	0.74	1.57	64	32
2:B:21:DG:H2"	2:B:22:DC:O5'	0.74	1.82	42	8
1:A:39:VAL:HG22	1:A:149:PRO:CB	0.73	2.13	72	1
1:A:57:PHE:CE2	1:A:62:HIS:CG	0.71	2.78	41	3
1:A:62:HIS:CD2	1:A:63:SER:N	0.70	2.59	49	3
1:A:41:SER:OG	1:A:48:VAL:HG23	0.70	1.86	74	5
2:B:23:DT:H2'	2:B:23:DT:O2	0.70	1.85	40	3
1:A:22:LYS:HB3	1:A:52:TYR:CE2	0.69	2.20	47	7
1:A:8:LEU:HD21	1:A:144:VAL:HG11	0.69	1.63	9	2
2:B:41:DC:C6	2:B:41:DC:O5'	0.69	2.46	43	1
1:A:39:VAL:HG23	1:A:48:VAL:HG12	0.69	1.64	63	2
1:A:148:LYS:CB	1:A:151:LEU:HD21	0.69	2.18	39	1
2:B:25:DG:C4	2:B:26:DC:C6	0.68	2.81	38	73
1:A:22:LYS:CB	1:A:52:TYR:CZ	0.68	2.77	47	16
1:A:110:LEU:HD21	1:A:176:TYR:CZ	0.68	2.23	49	31
1:A:39:VAL:HG13	1:A:48:VAL:CG1	0.68	2.19	38	1
1:A:151:LEU:HD13	1:A:154:ILE:HD12	0.67	1.65	48	15
1:A:57:PHE:HE2	1:A:62:HIS:CD2	0.67	2.08	41	3
1:A:57:PHE:CE2	1:A:62:HIS:CD2	0.67	2.82	49	3
2:B:2:DC:C2'	2:B:3:DT:H72	0.67	2.18	69	3
1:A:151:LEU:HD21	2:B:45:DG:O6	0.67	1.89	64	5
2:B:3:DT:H1'	2:B:4:DG:H5'	0.67	1.64	2	1
2:B:3:DT:C4	2:B:4:DG:C6	0.67	2.82	2	1
2:B:41:DC:H2"	2:B:42:DC:H5'	0.66	1.64	55	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:SER:CB	1:A:44:PHE:CE1	0.66	2.77	42	1
2:B:15:DA:H2"	2:B:16:DA:OP2	0.66	1.90	10	56
1:A:148:LYS:HG2	1:A:151:LEU:HD13	0.66	1.67	18	1
1:A:48:VAL:HG21	2:B:23:DT:O4	0.66	1.89	58	2
1:A:39:VAL:HG13	1:A:149:PRO:CB	0.66	2.21	31	27
2:B:2:DC:H6	2:B:2:DC:O5'	0.65	1.73	55	1
1:A:151:LEU:HD21	2:B:45:DG:N1	0.65	2.06	18	11
1:A:36:ALA:HB2	1:A:51:TRP:CD2	0.65	2.27	22	78
1:A:148:LYS:HB3	1:A:151:LEU:HD21	0.65	1.68	39	1
1:A:22:LYS:HB2	1:A:52:TYR:CZ	0.65	2.27	15	75
2:B:3:DT:C2'	2:B:4:DG:C8	0.65	2.79	57	5
1:A:60:VAL:HG11	1:A:62:HIS:CE1	0.65	2.27	75	5
2:B:3:DT:N1	2:B:4:DG:C8	0.64	2.64	2	1
1:A:8:LEU:HD11	1:A:144:VAL:HG11	0.64	1.68	58	4
2:B:25:DG:C5	2:B:26:DC:C4	0.64	2.85	9	76
2:B:22:DC:H2"	2:B:23:DT:OP1	0.64	1.91	35	2
1:A:148:LYS:CG	1:A:151:LEU:HD21	0.64	2.22	39	1
1:A:48:VAL:HG11	2:B:23:DT:H71	0.64	1.68	21	2
2:B:29:DT:C6	2:B:30:DC:C5	0.64	2.86	47	78
1:A:110:LEU:HD13	1:A:180:GLN:HB3	0.64	1.70	78	5
2:B:41:DC:C6	2:B:42:DC:C5	0.63	2.86	55	3
2:B:2:DC:C6	2:B:2:DC:O5'	0.63	2.52	55	1
1:A:48:VAL:HG21	2:B:23:DT:C7	0.62	2.24	53	1
1:A:151:LEU:HD23	1:A:154:ILE:CG2	0.62	2.25	32	2
1:A:39:VAL:HB	1:A:149:PRO:CB	0.62	2.24	42	1
2:B:23:DT:O2	2:B:23:DT:C2'	0.62	2.48	62	2
1:A:39:VAL:HG13	1:A:48:VAL:HG12	0.62	1.70	38	1
1:A:110:LEU:HD23	1:A:180:GLN:HB3	0.61	1.72	56	7
1:A:150:GLN:OE1	2:B:23:DT:H2"	0.61	1.95	21	1
1:A:151:LEU:HD11	1:A:154:ILE:HD12	0.61	1.73	35	1
1:A:39:VAL:HG12	1:A:149:PRO:CB	0.61	2.24	36	1
1:A:20:SER:OG	2:B:22:DC:OP1	0.61	2.19	40	1
1:A:62:HIS:CG	1:A:63:SER:N	0.61	2.69	49	3
1:A:148:LYS:HG2	1:A:151:LEU:HD12	0.61	1.72	59	1
1:A:48:VAL:HG21	2:B:23:DT:H71	0.61	1.71	40	2
1:A:64:ILE:HD11	1:A:70:GLU:HB3	0.61	1.70	49	3
2:B:41:DC:H2"	2:B:42:DC:C6	0.61	2.30	44	2
2:B:2:DC:P	2:B:2:DC:H6	0.60	2.19	55	1
1:A:117:TYR:CE2	1:A:187:LEU:HD23	0.60	2.32	77	78
2:B:40:DA:O3'	2:B:41:DC:C6	0.60	2.54	39	77
2:B:41:DC:H6	2:B:41:DC:O5'	0.60	1.78	43	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:TYR:CD2	1:A:64:ILE:HD11	0.60	2.31	1	13
1:A:21:CYS:HB3	1:A:24:CYS:SG	0.60	2.37	15	2
1:A:50:HIS:NE2	2:B:23:DT:H73	0.60	2.12	62	1
2:B:3:DT:C4	2:B:4:DG:O6	0.59	2.55	2	2
2:B:3:DT:C4	2:B:4:DG:C5	0.59	2.90	2	1
2:B:13:DA:H2'	2:B:14:DG:O5'	0.59	1.96	12	77
1:A:151:LEU:HD23	1:A:154:ILE:HG21	0.59	1.75	32	2
2:B:4:DG:H2'	2:B:4:DG:O5'	0.59	1.98	39	2
1:A:39:VAL:HG13	1:A:149:PRO:HB2	0.59	1.74	70	21
2:B:5:DG:C5	2:B:6:DC:C4	0.59	2.91	59	78
2:B:3:DT:H2"	2:B:4:DG:OP2	0.58	1.97	64	2
2:B:41:DC:C5	2:B:42:DC:C4	0.58	2.91	67	1
1:A:39:VAL:HG23	1:A:149:PRO:CB	0.58	2.28	68	1
2:B:21:DG:H2"	2:B:22:DC:C5'	0.58	2.28	42	1
2:B:17:DG:C5	2:B:18:DC:C4	0.58	2.92	78	78
1:A:160:PRO:O	1:A:164:VAL:HG23	0.58	1.99	67	78
1:A:151:LEU:CD1	1:A:154:ILE:HD12	0.58	2.27	35	7
1:A:152:GLY:O	1:A:153:MET:C	0.58	2.42	69	2
1:A:9:TYR:CE2	1:A:64:ILE:HD11	0.58	2.34	37	13
2:B:24:DC:H2"	2:B:25:DG:C8	0.58	2.34	24	4
1:A:63:SER:C	1:A:64:ILE:HD12	0.57	2.19	27	22
1:A:44:PHE:CZ	2:B:1:DG:C6	0.57	2.93	64	1
1:A:39:VAL:CG1	1:A:48:VAL:O	0.57	2.50	68	2
1:A:50:HIS:CD2	2:B:23:DT:C7	0.57	2.88	62	1
1:A:60:VAL:HG11	1:A:62:HIS:CD2	0.57	2.35	66	15
2:B:43:DG:C6	2:B:44:DC:N4	0.56	2.73	36	77
2:B:1:DG:H2'	2:B:2:DC:C6	0.56	2.35	13	3
1:A:117:TYR:CE1	1:A:137:VAL:HG22	0.56	2.35	47	78
1:A:110:LEU:HD13	1:A:113:PHE:CD1	0.56	2.35	7	3
2:B:5:DG:H2"	2:B:6:DC:OP2	0.56	1.99	59	1
1:A:8:LEU:CD2	1:A:144:VAL:HG11	0.56	2.30	9	2
2:B:23:DT:H2"	2:B:24:DC:OP1	0.56	2.00	42	1
2:B:3:DT:H5'	2:B:3:DT:C6	0.56	2.35	43	2
1:A:39:VAL:CG2	1:A:149:PRO:HG3	0.56	2.30	38	1
1:A:39:VAL:HG23	1:A:149:PRO:HG3	0.56	1.76	68	2
2:B:24:DC:O2	2:B:25:DG:C5	0.56	2.59	7	2
2:B:30:DC:H2"	2:B:31:DA:O5'	0.55	2.01	8	1
1:A:63:SER:O	1:A:64:ILE:HD13	0.55	2.01	55	4
1:A:148:LYS:HG2	1:A:151:LEU:HD21	0.55	1.76	39	1
1:A:151:LEU:HD21	1:A:154:ILE:HD12	0.55	1.78	16	14
1:A:39:VAL:CB	1:A:149:PRO:HB2	0.55	2.31	8	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:12:DA:N1	2:B:13:DA:N1	0.55	2.55	55	1
2:B:4:DG:C2	2:B:20:DA:C2	0.55	2.95	60	78
1:A:48:VAL:HG11	2:B:23:DT:H73	0.55	1.75	21	1
1:A:21:CYS:HB2	1:A:53:HIS:CE1	0.55	2.37	47	78
1:A:41:SER:HG	1:A:48:VAL:HG23	0.55	1.62	74	5
1:A:151:LEU:HD11	2:B:24:DC:N3	0.55	2.17	38	7
2:B:2:DC:H2"	2:B:3:DT:C7	0.55	2.32	69	2
2:B:19:DC:N4	2:B:20:DA:N6	0.54	2.55	55	78
2:B:25:DG:C6	2:B:26:DC:C4	0.54	2.94	38	75
1:A:39:VAL:HG23	1:A:48:VAL:CG1	0.54	2.32	30	2
2:B:41:DC:C4	2:B:42:DC:C4	0.54	2.95	55	2
1:A:110:LEU:HD11	1:A:176:TYR:CD1	0.54	2.38	3	12
1:A:110:LEU:HD13	1:A:113:PHE:CD2	0.54	2.38	40	8
2:B:12:DA:C2	2:B:13:DA:C2	0.54	2.95	55	1
1:A:141:LYS:HG3	1:A:156:ARG:HB3	0.54	1.77	76	1
2:B:2:DC:C2'	2:B:3:DT:C7	0.53	2.86	69	2
1:A:150:GLN:HG2	2:B:24:DC:OP2	0.53	2.03	72	1
1:A:110:LEU:HD22	1:A:113:PHE:CD2	0.53	2.39	24	1
2:B:43:DG:C6	2:B:44:DC:C4	0.53	2.97	36	77
1:A:37:ILE:HG23	1:A:37:ILE:O	0.53	2.04	56	21
1:A:151:LEU:HD11	2:B:45:DG:C5	0.53	2.39	77	22
1:A:39:VAL:CG2	1:A:50:HIS:NE2	0.53	2.72	46	1
1:A:148:LYS:CG	1:A:151:LEU:HD12	0.53	2.34	59	1
1:A:140:SER:HB3	1:A:157:TRP:CE3	0.53	2.39	47	78
2:B:12:DA:N1	2:B:13:DA:C2	0.53	2.77	55	1
1:A:37:ILE:O	1:A:37:ILE:HG23	0.52	2.03	65	21
1:A:30:LYS:O	1:A:31:ASP:HB2	0.52	2.04	47	78
2:B:3:DT:C4	2:B:4:DG:N7	0.52	2.77	2	1
1:A:38:MET:O	1:A:39:VAL:HG23	0.52	2.04	40	21
1:A:39:VAL:CG1	1:A:149:PRO:HB2	0.52	2.35	43	15
1:A:39:VAL:CG2	1:A:50:HIS:CD2	0.52	2.91	2	34
1:A:110:LEU:CD2	1:A:176:TYR:CE1	0.52	2.92	8	4
2:B:25:DG:C8	2:B:26:DC:C5	0.52	2.97	9	6
1:A:39:VAL:CG2	1:A:48:VAL:CG1	0.52	2.88	63	3
1:A:9:TYR:CE1	1:A:62:HIS:ND1	0.52	2.78	46	3
1:A:151:LEU:HD23	1:A:154:ILE:HD12	0.52	1.78	41	6
2:B:9:DC:H2"	2:B:10:DG:O5'	0.52	2.04	47	78
1:A:50:HIS:CD2	2:B:23:DT:H73	0.52	2.40	62	1
2:B:29:DT:H2"	2:B:30:DC:O5'	0.51	2.05	47	78
1:A:138:ARG:CD	1:A:157:TRP:CE3	0.51	2.93	46	78
2:B:3:DT:H2"	2:B:4:DG:C8	0.51	2.39	57	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:ILE:HD13	1:A:62:HIS:CE1	0.51	2.41	76	1
1:A:39:VAL:CG1	1:A:50:HIS:CD2	0.51	2.90	58	34
2:B:12:DA:N6	2:B:13:DA:N1	0.51	2.56	55	1
2:B:12:DA:N6	2:B:13:DA:N6	0.51	2.59	55	78
2:B:41:DC:H6	2:B:41:DC:P	0.51	2.23	43	1
2:B:23:DT:C2'	2:B:24:DC:OP1	0.51	2.59	42	3
1:A:39:VAL:HG21	2:B:23:DT:C7	0.51	2.36	32	1
2:B:4:DG:C2'	2:B:4:DG:O5'	0.51	2.56	39	3
1:A:151:LEU:N	1:A:151:LEU:HD23	0.51	2.21	39	1
1:A:9:TYR:CZ	1:A:62:HIS:CE1	0.51	2.99	46	3
1:A:39:VAL:HG22	1:A:149:PRO:HG2	0.51	1.83	76	2
2:B:23:DT:H3'	2:B:23:DT:O2	0.51	2.06	66	1
1:A:151:LEU:HD22	1:A:154:ILE:HB	0.50	1.84	11	6
1:A:113:PHE:O	1:A:182:LYS:HB3	0.50	2.07	55	1
2:B:4:DG:H2"	2:B:5:DG:N7	0.50	2.21	60	1
2:B:24:DC:H2"	2:B:25:DG:O5'	0.50	2.06	76	1
1:A:8:LEU:HD23	1:A:9:TYR:CE2	0.50	2.42	76	3
1:A:151:LEU:HD21	2:B:45:DG:C5	0.50	2.39	45	7
2:B:42:DC:H1'	2:B:43:DG:C8	0.50	2.41	44	2
2:B:2:DC:OP2	2:B:2:DC:C6	0.50	2.64	55	1
1:A:39:VAL:CG1	1:A:149:PRO:CB	0.50	2.89	33	1
2:B:42:DC:H2'	2:B:42:DC:OP2	0.50	2.07	59	1
2:B:43:DG:C4	2:B:44:DC:C5	0.50	3.00	78	77
1:A:8:LEU:HD11	1:A:144:VAL:HG21	0.50	1.83	62	2
1:A:62:HIS:CD2	1:A:62:HIS:C	0.50	2.85	41	1
1:A:21:CYS:CB	1:A:24:CYS:SG	0.50	2.98	15	1
1:A:39:VAL:CG1	1:A:149:PRO:HG2	0.50	2.35	76	1
2:B:3:DT:C6	2:B:3:DT:H5'	0.49	2.42	64	1
2:B:4:DG:O5'	2:B:4:DG:H2'	0.49	2.07	64	1
1:A:44:PHE:CD1	1:A:44:PHE:N	0.49	2.81	42	1
2:B:3:DT:O2	2:B:4:DG:C8	0.49	2.56	2	1
1:A:154:ILE:HD11	2:B:45:DG:N9	0.49	2.23	59	23
1:A:34:ARG:HD3	1:A:51:TRP:CE3	0.49	2.43	47	78
1:A:39:VAL:HG11	1:A:149:PRO:CB	0.49	2.38	33	1
1:A:41:SER:HB2	1:A:44:PHE:CE1	0.49	2.41	42	1
1:A:39:VAL:CG2	1:A:149:PRO:HB2	0.49	2.37	72	1
1:A:9:TYR:CE1	1:A:37:ILE:CD1	0.49	2.94	46	9
1:A:151:LEU:HD11	1:A:154:ILE:HB	0.49	1.85	35	1
1:A:57:PHE:CZ	1:A:62:HIS:ND1	0.49	2.81	41	3
2:B:23:DT:O5'	2:B:23:DT:C6	0.49	2.66	41	1
1:A:39:VAL:HA	1:A:149:PRO:HB2	0.49	1.84	69	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:PHE:CD2	2:B:1:DG:C4	0.49	3.01	64	8
2:B:3:DT:O4	2:B:4:DG:O6	0.48	2.30	2	1
2:B:14:DG:C2'	2:B:15:DA:C5'	0.48	2.87	3	1
1:A:41:SER:HB3	1:A:44:PHE:CE1	0.48	2.42	42	1
2:B:41:DC:C6	2:B:42:DC:C4	0.48	3.02	67	1
1:A:148:LYS:O	1:A:151:LEU:HG	0.48	2.09	39	1
2:B:25:DG:N1	2:B:45:DG:N2	0.48	2.61	30	1
2:B:2:DC:H2"	2:B:3:DT:O5'	0.48	2.08	57	1
1:A:148:LYS:HB3	1:A:151:LEU:HD12	0.48	1.85	1	1
1:A:151:LEU:HD21	2:B:24:DC:N3	0.48	2.23	69	3
1:A:153:MET:O	1:A:153:MET:CG	0.48	2.62	8	1
1:A:50:HIS:O	1:A:52:TYR:CE1	0.48	2.67	40	1
2:B:40:DA:H2"	2:B:41:DC:C4	0.48	2.43	59	1
2:B:14:DG:H2"	2:B:15:DA:H5'	0.48	1.82	3	1
2:B:33:DC:H2"	2:B:34:DT:O5'	0.48	2.09	3	1
2:B:23:DT:P	2:B:23:DT:O4'	0.48	2.72	35	1
1:A:44:PHE:CB	2:B:1:DG:C8	0.47	2.97	45	9
1:A:62:HIS:C	1:A:62:HIS:CD2	0.47	2.85	46	2
1:A:151:LEU:CD1	2:B:45:DG:C6	0.47	2.97	48	14
2:B:40:DA:O3'	2:B:41:DC:C5	0.47	2.67	43	3
2:B:24:DC:H4'	2:B:24:DC:OP1	0.47	2.00	40	1
2:B:15:DA:C2'	2:B:16:DA:OP2	0.47	2.59	10	1
2:B:5:DG:C5	2:B:6:DC:N4	0.47	2.83	2	77
1:A:34:ARG:CD	1:A:51:TRP:CE3	0.47	2.98	25	78
2:B:3:DT:H2"	2:B:4:DG:H8	0.47	1.70	57	1
2:B:23:DT:C2'	2:B:23:DT:O2	0.47	2.63	66	3
1:A:141:LYS:CE	1:A:170:LEU:HD23	0.47	2.39	69	3
1:A:142:LYS:CG	1:A:153:MET:HB2	0.47	2.39	24	4
2:B:34:DT:O2	2:B:36:DG:N2	0.47	2.48	3	73
1:A:151:LEU:O	1:A:151:LEU:HD23	0.47	2.10	48	5
2:B:25:DG:C2	2:B:45:DG:N2	0.47	2.82	30	1
1:A:64:ILE:CD1	1:A:70:GLU:HB3	0.47	2.40	41	1
2:B:2:DC:OP2	2:B:2:DC:H6	0.47	1.92	55	1
2:B:22:DC:H2"	2:B:23:DT:H71	0.47	1.86	57	1
1:A:68:ASP:OD2	1:A:69:VAL:HG13	0.47	2.10	55	78
1:A:151:LEU:C	1:A:151:LEU:HD23	0.47	2.30	12	5
2:B:23:DT:H1'	2:B:24:DC:OP1	0.47	2.10	42	1
1:A:122:ARG:NH2	2:B:27:DG:H21	0.47	2.08	25	78
1:A:8:LEU:HD13	1:A:8:LEU:O	0.47	2.09	33	1
1:A:62:HIS:CE1	1:A:64:ILE:HG12	0.47	2.44	41	1
1:A:144:VAL:HG12	1:A:152:GLY:C	0.47	2.30	55	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:LYS:O	1:A:31:ASP:CB	0.47	2.63	47	78
1:A:153:MET:SD	1:A:153:MET:N	0.47	2.87	8	1
2:B:3:DT:C1'	2:B:4:DG:H5'	0.46	2.40	2	1
1:A:145:ASP:OD2	1:A:154:ILE:HG21	0.46	2.10	37	2
1:A:39:VAL:CB	1:A:50:HIS:NE2	0.46	2.78	46	1
2:B:23:DT:H2"	2:B:24:DC:O5'	0.46	2.10	62	1
2:B:31:DA:C2'	2:B:32:DG:O5'	0.46	2.56	8	1
2:B:41:DC:N4	2:B:42:DC:N4	0.46	2.62	36	1
1:A:108:LYS:O	1:A:109:THR:HG23	0.46	2.10	52	1
1:A:39:VAL:CA	1:A:149:PRO:HB2	0.46	2.40	69	1
2:B:5:DG:C2'	2:B:6:DC:OP2	0.46	2.63	59	1
2:B:43:DG:C5	2:B:44:DC:C5	0.46	3.03	36	76
1:A:151:LEU:HD23	1:A:151:LEU:C	0.46	2.31	11	5
2:B:3:DT:C2'	2:B:4:DG:OP2	0.46	2.62	39	2
1:A:62:HIS:NE2	1:A:64:ILE:HB	0.46	2.25	46	2
1:A:48:VAL:HG11	2:B:23:DT:C4	0.46	2.45	63	1
2:B:12:DA:O5'	2:B:12:DA:H8	0.46	1.94	71	37
2:B:23:DT:C3'	2:B:23:DT:O2	0.46	2.64	66	1
2:B:41:DC:H2"	2:B:42:DC:OP2	0.46	2.11	59	1
1:A:39:VAL:CG2	1:A:149:PRO:CG	0.46	2.87	68	1
2:B:12:DA:H8	2:B:12:DA:O5'	0.46	1.94	8	41
1:A:39:VAL:HB	1:A:149:PRO:HB2	0.46	1.88	8	1
1:A:60:VAL:CG1	1:A:62:HIS:CD2	0.46	2.99	1	7
1:A:54:PHE:CE2	1:A:84:LYS:CD	0.46	2.99	47	78
2:B:43:DG:C5	2:B:44:DC:C4	0.46	3.03	36	76
2:B:23:DT:OP2	2:B:23:DT:C6	0.46	2.69	3	1
1:A:113:PHE:CE2	1:A:141:LYS:CD	0.46	2.98	7	4
1:A:110:LEU:HD12	1:A:180:GLN:HB3	0.46	1.88	63	2
1:A:113:PHE:CE1	1:A:141:LYS:CG	0.45	3.00	40	1
1:A:81:ASP:O	1:A:85:VAL:HG23	0.45	2.12	71	78
1:A:151:LEU:CD1	2:B:45:DG:C2	0.45	2.98	15	5
2:B:23:DT:OP2	2:B:23:DT:C2	0.45	2.69	36	3
1:A:122:ARG:NH2	2:B:27:DG:N2	0.45	2.65	6	78
1:A:113:PHE:N	1:A:113:PHE:CD1	0.45	2.84	7	3
1:A:50:HIS:CE1	1:A:150:GLN:NE2	0.45	2.85	23	1
2:B:25:DG:H2"	2:B:26:DC:O5'	0.45	2.10	38	1
2:B:41:DC:O5'	2:B:41:DC:C6	0.45	2.69	44	1
2:B:41:DC:P	2:B:41:DC:C6	0.45	3.10	44	1
2:B:23:DT:C6	2:B:23:DT:OP2	0.45	2.70	12	1
1:A:39:VAL:CG1	1:A:48:VAL:CG1	0.45	2.94	38	1
1:A:150:GLN:HA	2:B:23:DT:H72	0.45	1.89	62	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:110:LEU:HD12	1:A:112:ASP:OD1	0.45	2.11	27	1
1:A:65:ARG:HG3	1:A:66:HIS:CD2	0.45	2.47	41	4
2:B:12:DA:N6	2:B:13:DA:H61	0.45	2.09	55	1
1:A:57:PHE:O	1:A:60:VAL:HG22	0.45	2.12	64	1
2:B:27:DG:C6	2:B:28:DG:C6	0.45	3.05	36	78
1:A:57:PHE:O	1:A:60:VAL:HG12	0.44	2.13	43	10
1:A:113:PHE:CE1	1:A:141:LYS:HD3	0.44	2.47	10	1
2:B:3:DT:C1'	2:B:4:DG:C8	0.44	2.99	57	2
1:A:48:VAL:HG21	2:B:23:DT:H72	0.44	1.90	53	1
1:A:155:ASP:CB	1:A:157:TRP:CZ2	0.44	3.01	70	78
1:A:153:MET:HG2	1:A:153:MET:O	0.44	2.11	8	3
2:B:16:DA:H2"	2:B:17:DG:OP2	0.44	2.13	8	78
1:A:138:ARG:HD3	1:A:157:TRP:CE3	0.44	2.47	46	78
1:A:145:ASP:OD1	1:A:148:LYS:CB	0.44	2.65	73	2
2:B:2:DC:H1'	2:B:3:DT:H5'	0.44	1.90	37	3
1:A:23:LYS:CD	1:A:56:CYS:HB3	0.44	2.43	67	1
2:B:17:DG:C8	2:B:18:DC:C5	0.44	3.06	76	78
1:A:151:LEU:CD1	2:B:24:DC:N4	0.44	2.81	30	1
1:A:8:LEU:HA	1:A:38:MET:CG	0.44	2.42	36	1
1:A:65:ARG:HG3	1:A:66:HIS:N	0.44	2.28	67	3
1:A:8:LEU:CD1	1:A:144:VAL:HG21	0.44	2.43	62	2
1:A:8:LEU:HD23	1:A:38:MET:CE	0.43	2.42	36	1
1:A:43:MET:CE	2:B:1:DG:N3	0.43	2.81	44	1
1:A:36:ALA:CB	1:A:51:TRP:CE3	0.43	2.93	55	70
1:A:9:TYR:CE1	1:A:62:HIS:CE1	0.43	3.05	46	3
1:A:64:ILE:O	1:A:64:ILE:CG2	0.43	2.65	46	1
1:A:44:PHE:CE2	2:B:1:DG:C2	0.43	3.07	64	1
2:B:1:DG:OP3	2:B:1:DG:H8	0.43	1.96	5	1
1:A:110:LEU:HD22	1:A:113:PHE:CE2	0.43	2.48	24	1
2:B:40:DA:H4'	2:B:41:DC:OP1	0.43	2.14	55	1
2:B:2:DC:H2'	2:B:3:DT:H72	0.43	1.88	69	1
1:A:48:VAL:O	1:A:48:VAL:HG13	0.43	2.13	62	1
2:B:40:DA:H1'	2:B:41:DC:C4	0.43	2.48	43	1
1:A:110:LEU:HD21	1:A:176:TYR:CD1	0.43	2.46	57	1
1:A:62:HIS:NE2	1:A:64:ILE:CG1	0.43	2.82	41	1
1:A:41:SER:HB2	1:A:44:PHE:CZ	0.43	2.48	42	1
1:A:143:MET:O	1:A:154:ILE:CG2	0.43	2.62	76	1
1:A:150:GLN:NE2	2:B:24:DC:O4'	0.43	2.52	8	2
2:B:12:DA:N6	2:B:13:DA:C6	0.43	2.86	55	1
1:A:151:LEU:HD22	1:A:154:ILE:HD12	0.43	1.90	66	1
1:A:39:VAL:CG1	1:A:48:VAL:HG13	0.42	2.44	38	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:VAL:HB	1:A:149:PRO:CG	0.42	2.43	42	2
2:B:3:DT:C2'	2:B:4:DG:H8	0.42	2.25	57	1
1:A:39:VAL:CG1	1:A:149:PRO:HG3	0.42	2.39	72	1
1:A:151:LEU:HD23	1:A:151:LEU:O	0.42	2.14	9	3
1:A:112:ASP:OD2	1:A:113:PHE:CE2	0.42	2.72	29	4
1:A:154:ILE:HD11	2:B:45:DG:H2'	0.42	1.90	76	2
1:A:39:VAL:CG2	1:A:48:VAL:HG13	0.42	2.44	30	1
2:B:44:DC:C4	2:B:45:DG:C6	0.42	3.08	30	1
1:A:44:PHE:CE1	2:B:1:DG:C6	0.42	3.07	64	1
1:A:22:LYS:HB3	1:A:52:TYR:CZ	0.42	2.49	42	2
1:A:153:MET:SD	1:A:153:MET:O	0.42	2.78	36	1
2:B:6:DC:H2"	2:B:7:DT:C5	0.42	2.48	59	1
1:A:64:ILE:CD1	1:A:70:GLU:CB	0.42	2.97	41	1
2:B:3:DT:H2"	2:B:4:DG:O5'	0.42	2.14	37	1
2:B:23:DT:O2	2:B:23:DT:O4'	0.42	2.36	58	1
1:A:54:PHE:CE2	1:A:84:LYS:HD3	0.42	2.50	47	77
1:A:154:ILE:HD11	2:B:45:DG:C2'	0.42	2.45	35	1
1:A:138:ARG:HD2	1:A:157:TRP:CE3	0.42	2.50	33	78
2:B:22:DC:H2"	2:B:23:DT:H72	0.42	1.91	6	1
1:A:113:PHE:CE2	1:A:141:LYS:HD3	0.42	2.50	34	4
1:A:151:LEU:CD2	2:B:45:DG:C6	0.42	3.00	59	1
1:A:8:LEU:HD12	1:A:37:ILE:HD11	0.42	1.90	6	1
1:A:64:ILE:CG2	1:A:64:ILE:O	0.42	2.67	49	1
1:A:142:LYS:CD	1:A:155:ASP:OD1	0.42	2.68	55	2
1:A:110:LEU:HD22	1:A:113:PHE:CD1	0.42	2.50	47	2
1:A:113:PHE:CD1	1:A:113:PHE:N	0.42	2.88	47	1
1:A:39:VAL:HG22	1:A:149:PRO:O	0.42	2.14	62	1
1:A:141:LYS:CG	1:A:141:LYS:O	0.42	2.67	76	1
2:B:3:DT:N1	2:B:4:DG:N7	0.41	2.67	2	1
1:A:39:VAL:HA	1:A:149:PRO:CG	0.41	2.45	76	1
1:A:64:ILE:HD13	1:A:71:VAL:CG2	0.41	2.45	9	2
1:A:50:HIS:CD2	2:B:23:DT:H71	0.41	2.50	62	1
2:B:19:DC:C4	2:B:20:DA:C6	0.41	3.09	6	76
1:A:68:ASP:N	1:A:68:ASP:OD1	0.41	2.54	67	31
1:A:109:THR:HG23	1:A:109:THR:O	0.41	2.15	32	2
1:A:58:TRP:CH2	1:A:64:ILE:HG12	0.41	2.51	32	2
1:A:110:LEU:HD13	1:A:113:PHE:HD2	0.41	1.73	40	1
1:A:108:LYS:O	1:A:109:THR:O	0.41	2.38	44	2
2:B:2:DC:H2"	2:B:3:DT:C5'	0.41	2.45	60	1
2:B:12:DA:O5'	2:B:12:DA:C8	0.41	2.74	47	38
1:A:37:ILE:CD1	1:A:62:HIS:NE2	0.41	2.84	37	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:TRP:C	1:A:52:TYR:CD1	0.41	2.94	40	1
2:B:12:DA:C8	2:B:12:DA:O5'	0.41	2.74	67	40
1:A:151:LEU:HD11	1:A:154:ILE:CD1	0.41	2.44	35	1
1:A:113:PHE:CE1	1:A:141:LYS:HG2	0.41	2.51	40	1
1:A:68:ASP:OD1	1:A:68:ASP:N	0.41	2.53	47	18
1:A:38:MET:C	1:A:39:VAL:HG23	0.41	2.35	41	1
1:A:153:MET:O	1:A:153:MET:HG2	0.41	2.16	2	1
2:B:24:DC:OP1	2:B:24:DC:H4'	0.41	2.16	15	1
2:B:41:DC:C2	2:B:42:DC:C4	0.41	3.08	36	1
1:A:64:ILE:HG22	1:A:64:ILE:O	0.41	2.16	41	1
1:A:112:ASP:HA	1:A:142:LYS:HB3	0.41	1.93	67	1
2:B:25:DG:N9	2:B:26:DC:C5	0.41	2.89	38	1
1:A:148:LYS:HB3	1:A:151:LEU:HD11	0.41	1.93	39	1
1:A:65:ARG:NH2	1:A:66:HIS:NE2	0.41	2.69	65	1
1:A:112:ASP:OD1	1:A:113:PHE:CD2	0.40	2.74	46	1
2:B:41:DC:N1	2:B:42:DC:C5	0.40	2.89	36	1
1:A:23:LYS:HD3	1:A:56:CYS:HB3	0.40	1.94	67	1
1:A:141:LYS:HG2	1:A:170:LEU:HD22	0.40	1.92	76	1
1:A:113:PHE:CZ	1:A:141:LYS:HD3	0.40	2.51	10	1
1:A:41:SER:CB	1:A:44:PHE:CZ	0.40	3.05	42	1
2:B:19:DC:N3	2:B:20:DA:C5	0.40	2.90	35	9
1:A:9:TYR:CE1	1:A:37:ILE:CG1	0.40	3.04	22	1
1:A:172:PHE:CE1	1:A:199:LEU:HD22	0.40	2.51	24	4
1:A:11:VAL:CG1	1:A:77:LEU:HD11	0.40	2.46	47	1
1:A:150:GLN:OE1	2:B:24:DC:O4'	0.40	2.40	8	1

5.2 Torsion angles (i)

5.2.1 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	181/214 (85%)	168±1 (93±1%)	13±1 (7±1%)	0±1 (0±0%)	50	82
All	All	14118/16692 (85%)	13112 (93%)	976 (7%)	30 (0%)	50	82

All 5 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	91	ALA	18
1	A	108	LYS	7
1	A	109	THR	2
1	A	153	MET	2
1	A	5	SER	1

5.2.2 Protein sidechains (i)

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	158/181 (87%)	145±3 (92±2%)	13±3 (8±2%)	16 63
All	All	12324/14118 (87%)	11337 (92%)	987 (8%)	16 63

All 35 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	10	ARG	78
1	A	167	ARG	78
1	A	34	ARG	78
1	A	138	ARG	78
1	A	122	ARG	78
1	A	153	MET	73
1	A	8	LEU	45
1	A	141	LYS	38
1	A	108	LYS	35
1	A	41	SER	34
1	A	47	LYS	30
1	A	65	ARG	30
1	A	7	LYS	30
1	A	142	LYS	29
1	A	151	LEU	25
1	A	38	MET	22
1	A	148	LYS	22
1	A	143	MET	21
1	A	145	ASP	18
1	A	63	SER	17
1	A	5	SER	16

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Mol	Chain	Res	Type	Models (Total)
1	A	40	GLN	15
1	A	150	GLN	13
1	A	90	GLU	13
1	A	112	ASP	10
1	A	147	GLU	10
1	A	154	ILE	9
1	A	43	MET	8
1	A	37	ILE	8
1	A	6	ASP	8
1	A	45	ASP	7
1	A	25	SER	3
1	A	60	VAL	3
1	A	64	ILE	3
1	A	110	LEU	2

5.2.3 RNA

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains

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

5.4 Carbohydrates

There are no carbohydrates in this entry.

5.5 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

5.6 Other polymers

There are no such molecules in this entry.

5.7 Polymer linkage issues

There are no chain breaks in this entry.

6 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 29% for the well-defined parts and 29% for the entire structure.

6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *CS_bound_F1F2*

6.1.1 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	877
Number of shifts mapped to atoms	877
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

6.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	210	-0.05 ± 0.21	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	0	—	None (insufficient data)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	200	0.99 ± 0.20	Should be applied

6.1.3 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 20%, i.e. 650 atoms were assigned a chemical shift out of a possible 3207. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	523/887 (59%)	174/353 (49%)	179/362 (49%)	170/172 (99%)
Sidechain	123/1220 (10%)	68/730 (9%)	55/428 (13%)	0/62 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	4/203 (2%)	4/108 (4%)	0/86 (0%)	0/9 (0%)
Overall	650/3207 (20%)	246/1728 (14%)	234/1176 (20%)	170/303 (56%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 21%, i.e. 756 atoms were assigned a chemical shift out of a possible 3557. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	614/1052 (58%)	204/419 (49%)	210/428 (49%)	200/205 (98%)
Sidechain	138/1405 (10%)	76/838 (9%)	62/496 (12%)	0/71 (0%)
Aromatic	4/203 (2%)	4/108 (4%)	0/86 (0%)	0/9 (0%)
Overall	756/3557 (21%)	284/1902 (15%)	272/1310 (21%)	200/345 (58%)

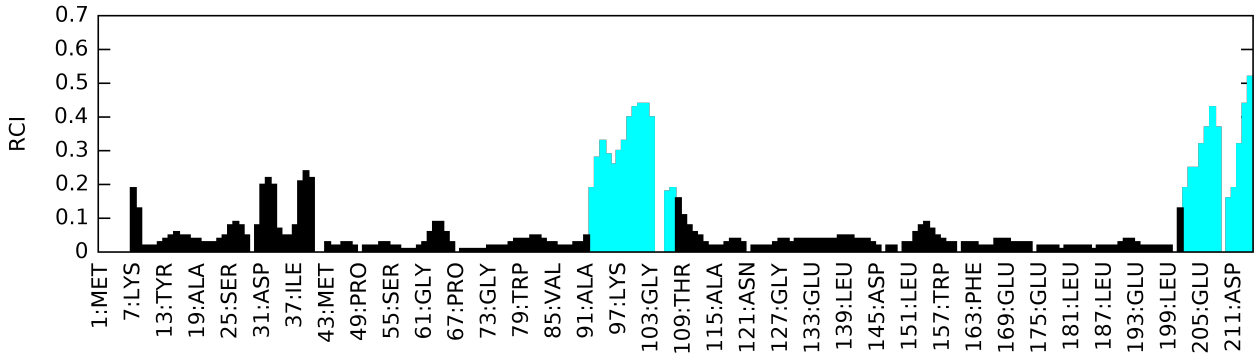
6.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

6.1.5 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.

Random coil index (RCI) for chain A:



6.2 Chemical shift list 2

File name: input_cs.cif

Chemical shift list name: *CS_bound_F1F2_high_salt*

6.2.1 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	392
Number of shifts mapped to atoms	392
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

6.2.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	0	—	None (insufficient data)
$^{13}C_{\beta}$	0	—	None (insufficient data)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	194	0.85 ± 0.23	Should be applied

6.2.3 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 11%, i.e. 340 atoms were assigned a chemical shift out of a possible 3207. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	336/887 (38%)	168/353 (48%)	0/362 (0%)	168/172 (98%)
Sidechain	0/1220 (0%)	0/730 (0%)	0/428 (0%)	0/62 (0%)
Aromatic	4/203 (2%)	2/108 (2%)	0/86 (0%)	2/9 (22%)
Overall	340/3207 (11%)	170/1728 (10%)	0/1176 (0%)	170/303 (56%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 11%, i.e. 392 atoms were assigned a chemical shift out of a possible 3557. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	388/1052 (37%)	194/419 (46%)	0/428 (0%)	194/205 (95%)

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	Total	^{1}H	^{13}C	^{15}N
Sidechain	0/1405 (0%)	0/838 (0%)	0/496 (0%)	0/71 (0%)
Aromatic	4/203 (2%)	2/108 (2%)	0/86 (0%)	2/9 (22%)
Overall	392/3557 (11%)	196/1902 (10%)	0/1310 (0%)	196/345 (57%)

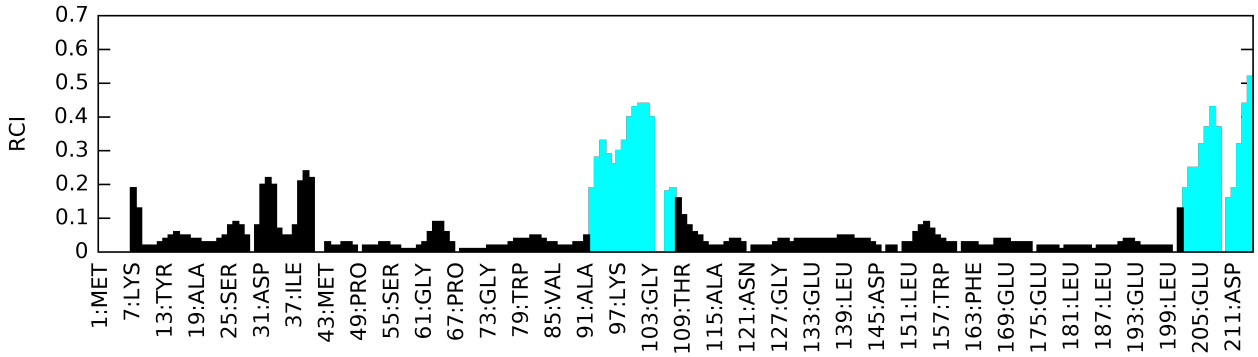
6.2.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

6.2.5 Random Coil Index (RCI) plots

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:



6.3 Chemical shift list 3

File name: input_cs.cif

Chemical shift list name: *bound_DNA*

6.3.1 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	295
Number of shifts mapped to atoms	295

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

6.3.2 Chemical shift referencing

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

6.3.3 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 8%, i.e. 270 atoms were assigned a chemical shift out of a possible 3207. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/887 (0%)	0/353 (0%)	0/362 (0%)	0/172 (0%)
Sidechain	0/1220 (0%)	0/730 (0%)	0/428 (0%)	0/62 (0%)
Aromatic	0/203 (0%)	0/108 (0%)	0/86 (0%)	0/9 (0%)
Overall	270/3207 (8%)	270/1728 (16%)	0/1176 (0%)	0/303 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 8%, i.e. 270 atoms were assigned a chemical shift out of a possible 3557. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/1052 (0%)	0/419 (0%)	0/428 (0%)	0/205 (0%)
Sidechain	0/1405 (0%)	0/838 (0%)	0/496 (0%)	0/71 (0%)
Aromatic	0/203 (0%)	0/108 (0%)	0/86 (0%)	0/9 (0%)
Overall	270/3557 (8%)	270/1902 (14%)	0/1310 (0%)	0/345 (0%)

6.3.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

6.3.5 Random Coil Index (RCI) plots

No *random coil index* (RCI) plot could be generated from the current chemical shift list (bound_DNA). RCI is only applicable to proteins.