



Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 12:33 am BST

PDB ID : 2MWI
Title : The structure of the carboxy-terminal domain of DNTTIP1
Authors : Schwabe, J.W.R.; Muskett, F.W.; Itoh, T.
Deposited on : 2014-11-11

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 following versions of software and data (see [references ⓘ](#)) 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

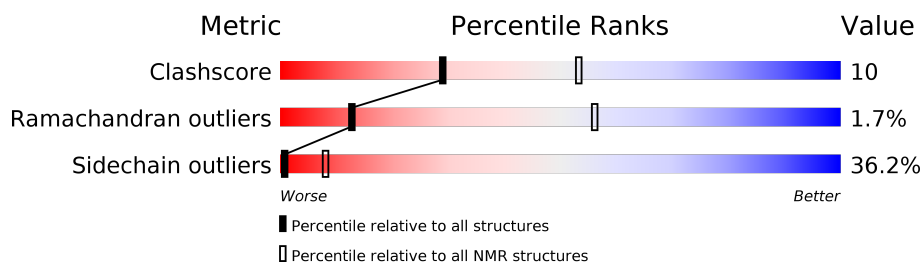
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 80%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	122	

2 Ensemble composition and analysis

This entry contains 65 models. Model 2 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:199-A:215, A:222-A:223, A:231-A:253, A:266-A:315 (92)	0.18	2

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1967 atoms, of which 982 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Deoxynucleotidyltransferase terminal-interacting protein 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	122	1967	623	982	179	176	7	0

There are 2 discrepancies between the modelled and reference sequences:

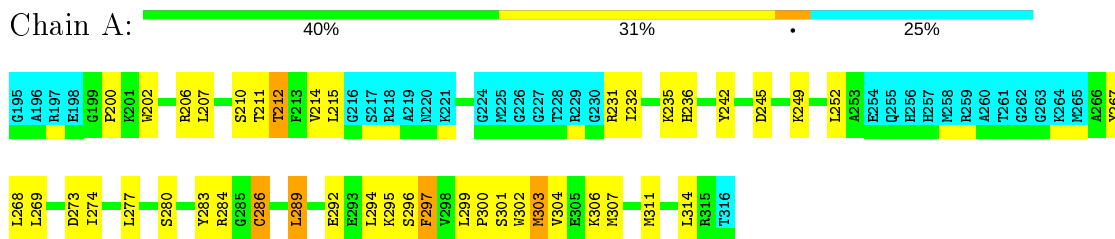
Chain	Residue	Modelled	Actual	Comment	Reference
A	195	GLY	-	EXPRESSION TAG	UNP Q9H147
A	196	ALA	-	EXPRESSION TAG	UNP Q9H147

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: Deoxynucleotidyltransferase terminal-interacting protein 1

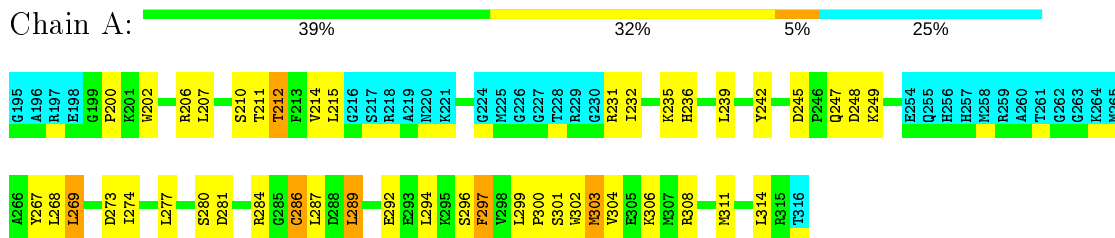


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

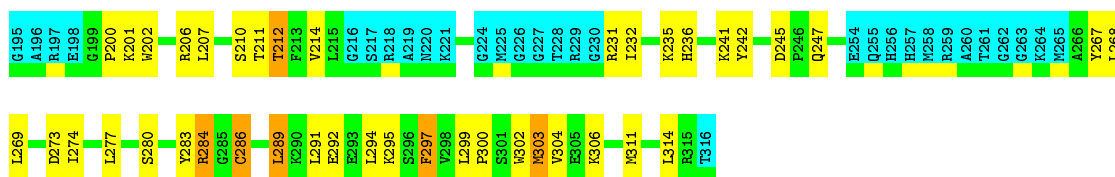
- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1

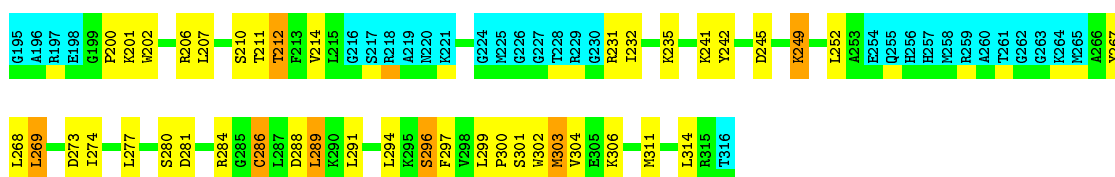




4.2.3 Score per residue for model 3

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1

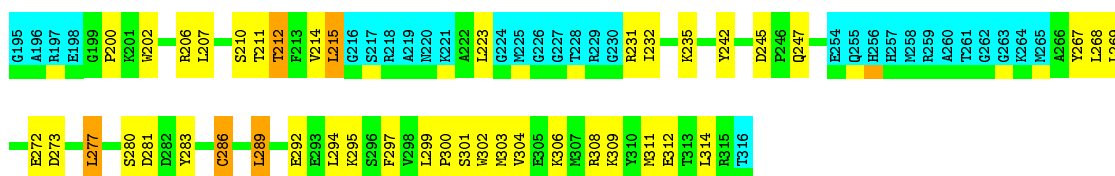
Chain A: 41% 29% 6% 25%



4.2.4 Score per residue for model 4

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1

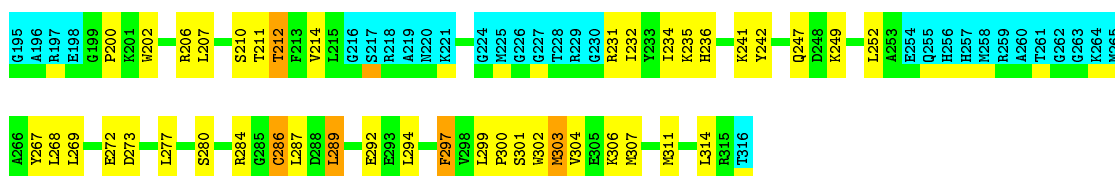
Chain A: 40% 31% 25%



4.2.5 Score per residue for model 5

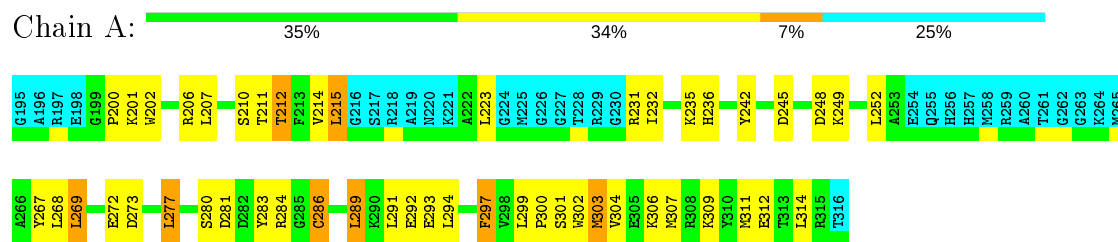
- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1

Chain A: 41% 30% 25%



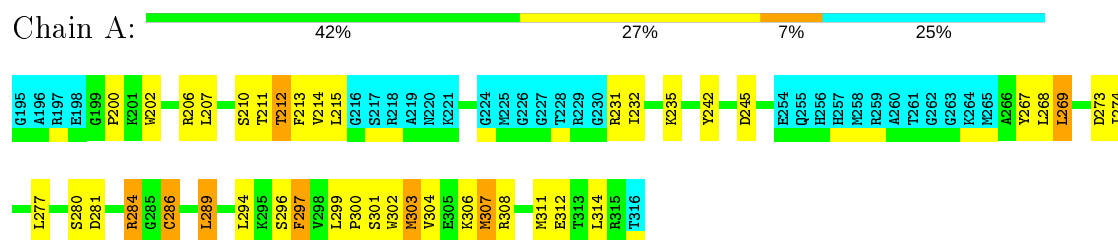
4.2.6 Score per residue for model 6

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



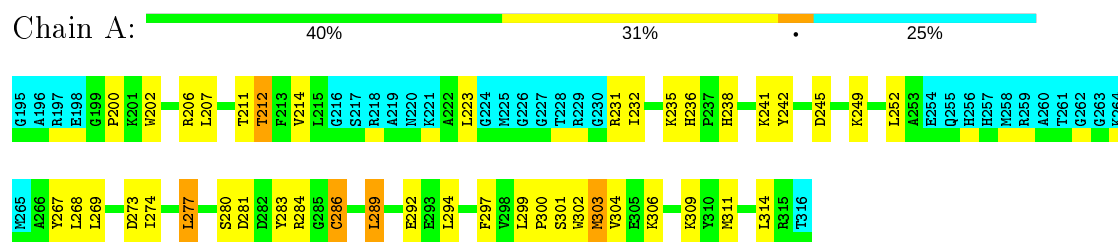
4.2.7 Score per residue for model 7

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



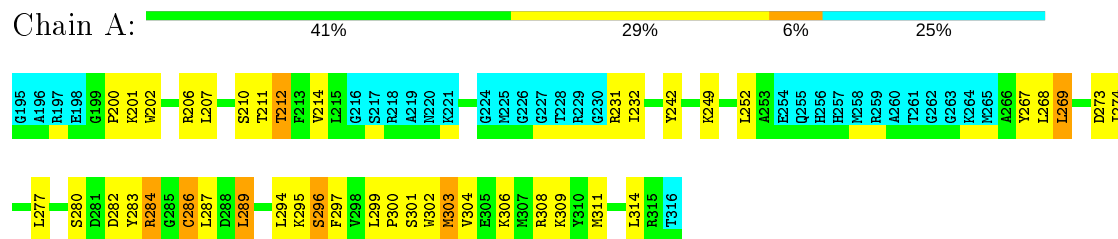
4.2.8 Score per residue for model 8

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



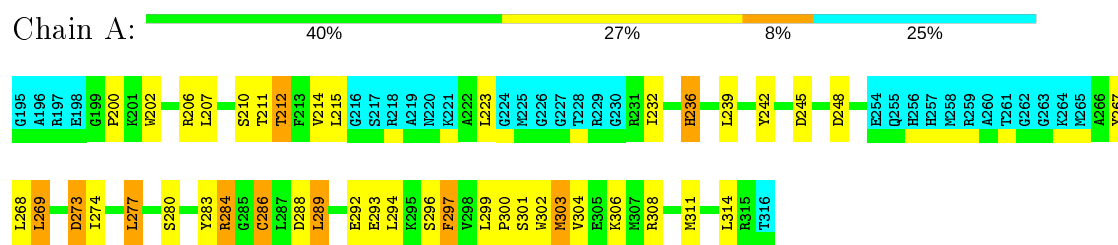
4.2.9 Score per residue for model 9

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



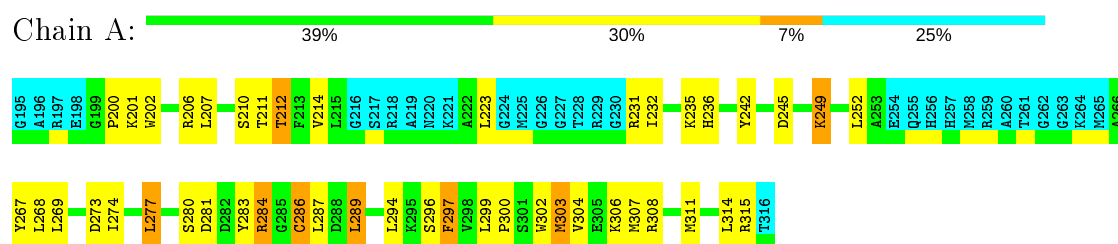
4.2.10 Score per residue for model 10

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



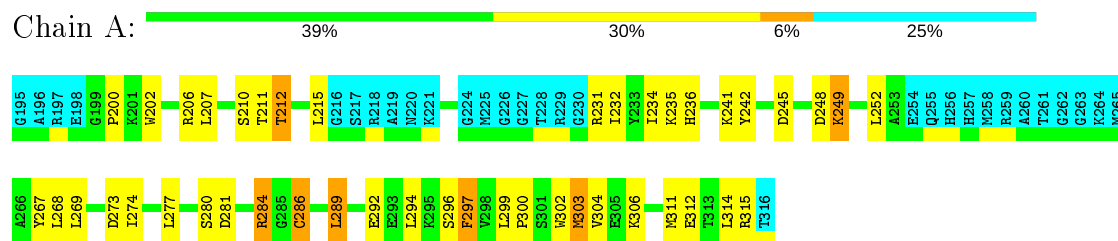
4.2.11 Score per residue for model 11

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



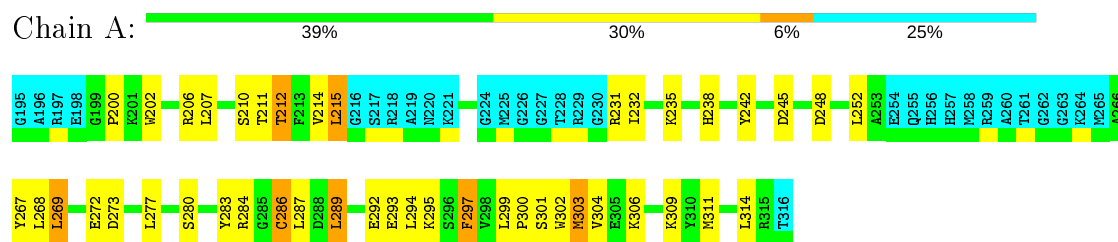
4.2.12 Score per residue for model 12

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



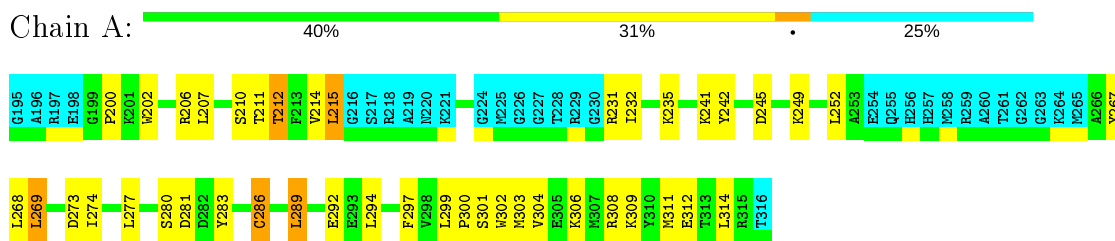
4.2.13 Score per residue for model 13

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



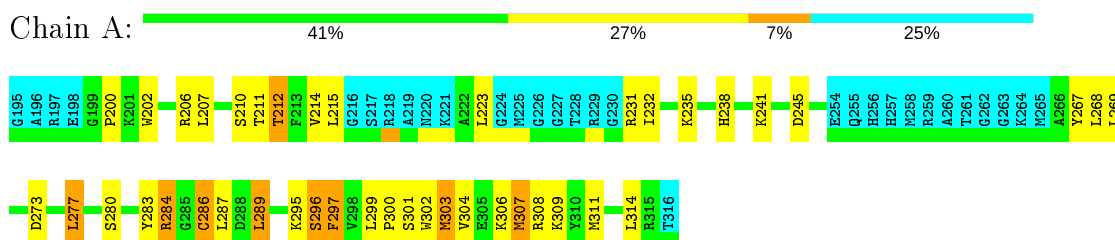
4.2.14 Score per residue for model 14

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



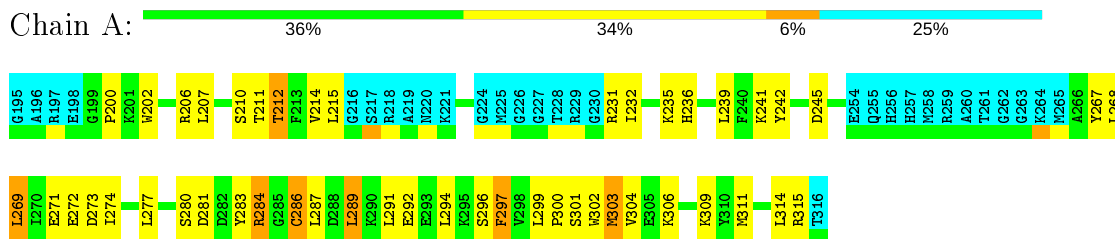
4.2.15 Score per residue for model 15

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



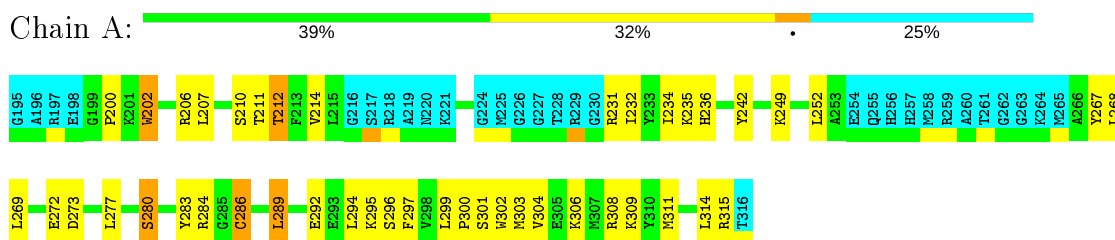
4.2.16 Score per residue for model 16

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



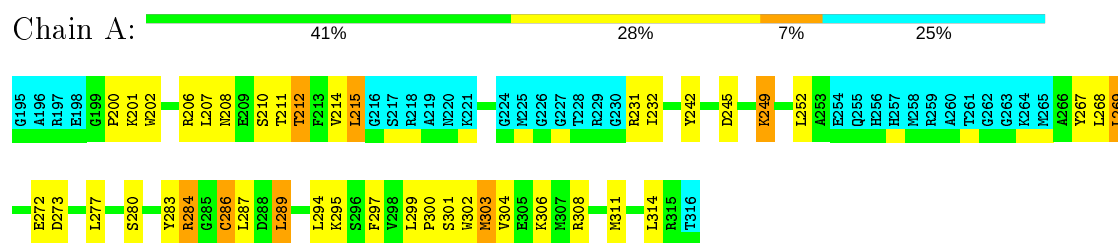
4.2.17 Score per residue for model 17

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



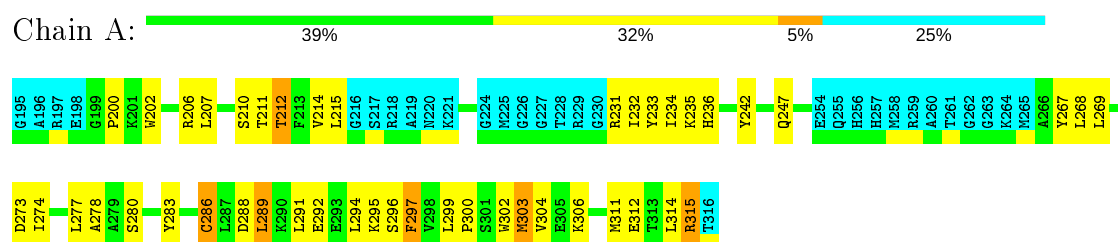
4.2.18 Score per residue for model 18

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



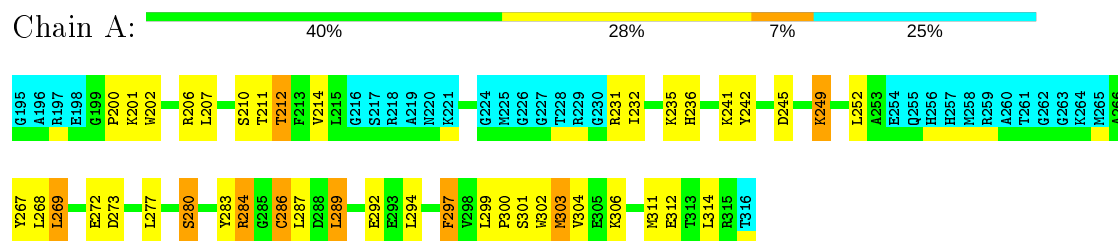
4.2.19 Score per residue for model 19

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



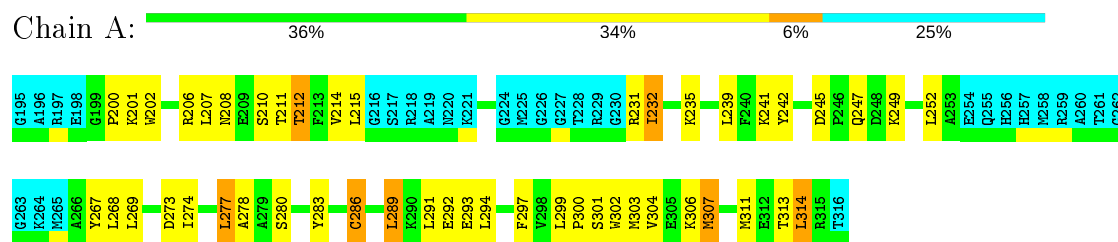
4.2.20 Score per residue for model 20

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



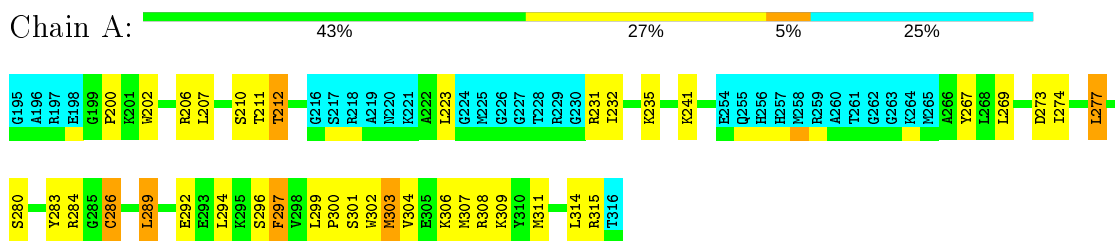
4.2.21 Score per residue for model 21

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



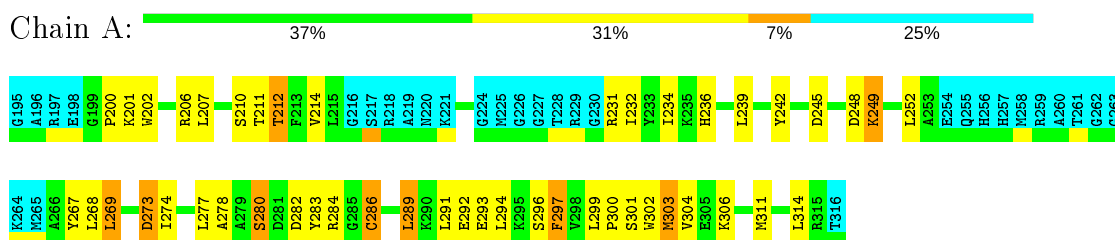
4.2.22 Score per residue for model 22

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



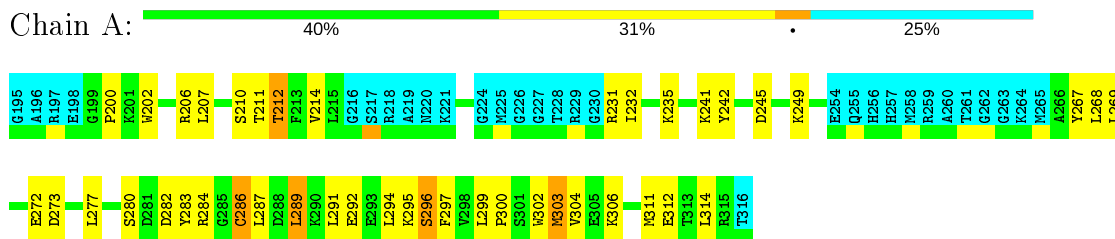
4.2.23 Score per residue for model 23

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



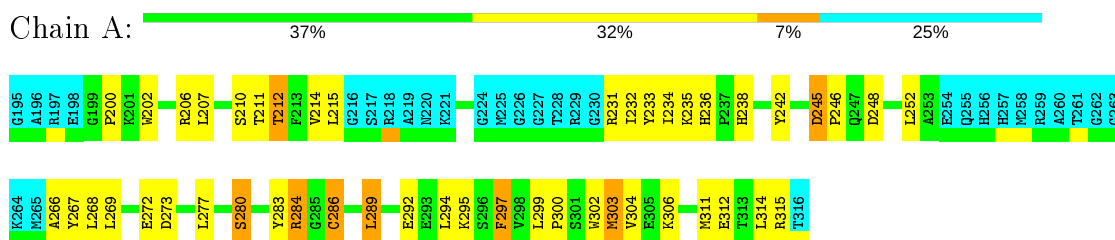
4.2.24 Score per residue for model 24

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



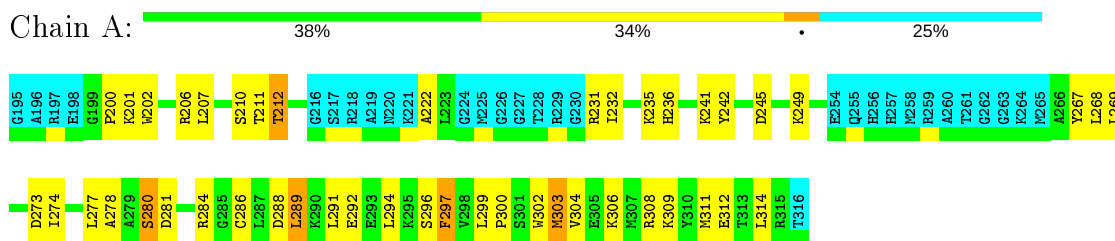
4.2.25 Score per residue for model 25

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



4.2.26 Score per residue for model 26

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



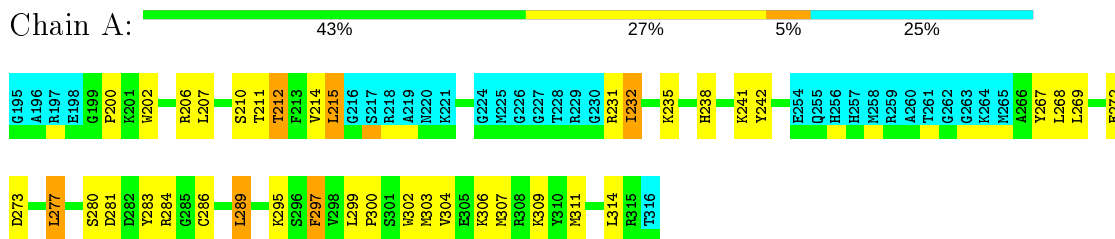
4.2.27 Score per residue for model 27

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



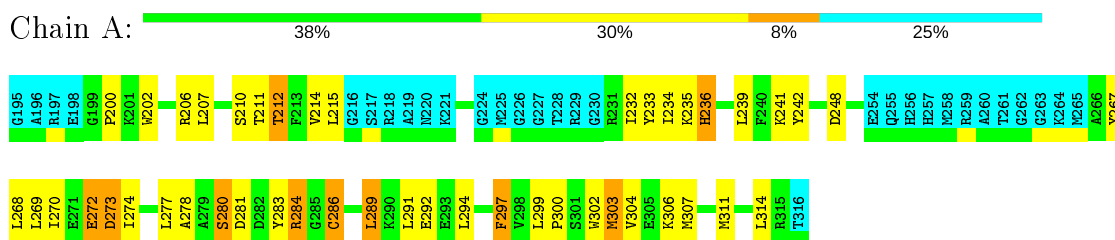
4.2.28 Score per residue for model 28

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



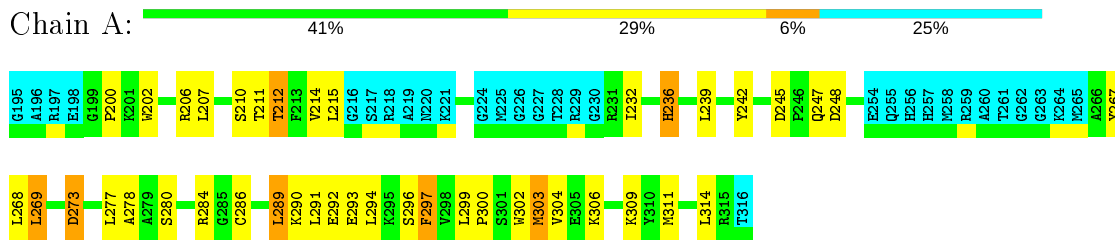
4.2.29 Score per residue for model 29

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



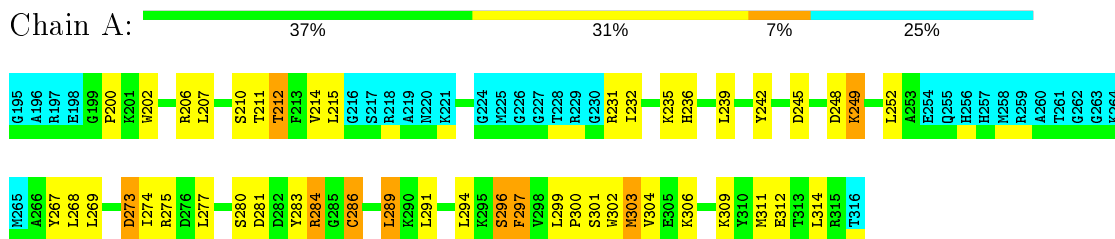
4.2.30 Score per residue for model 30

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



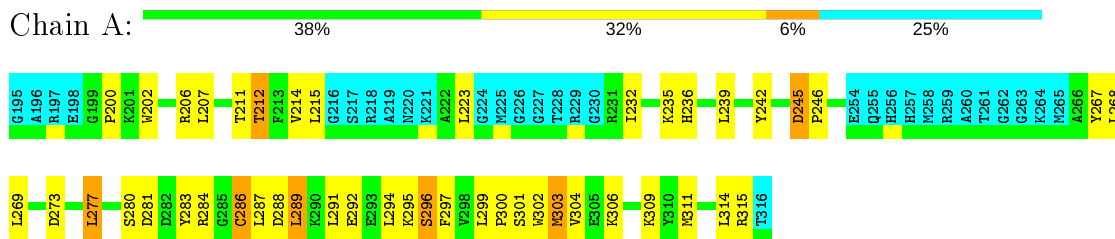
4.2.31 Score per residue for model 31

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



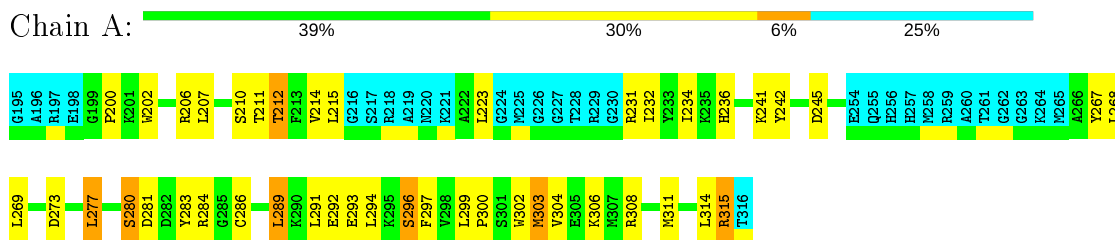
4.2.32 Score per residue for model 32

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



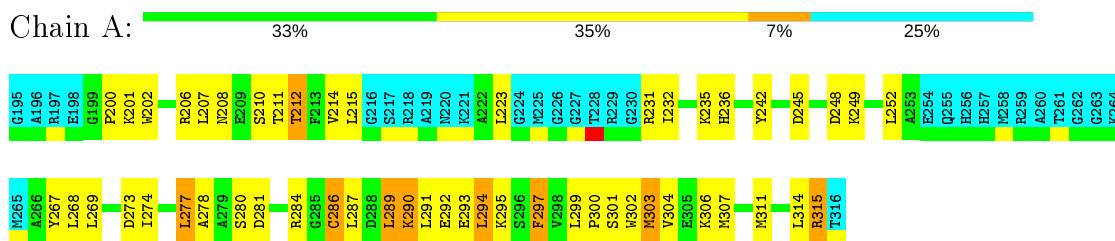
4.2.33 Score per residue for model 33

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



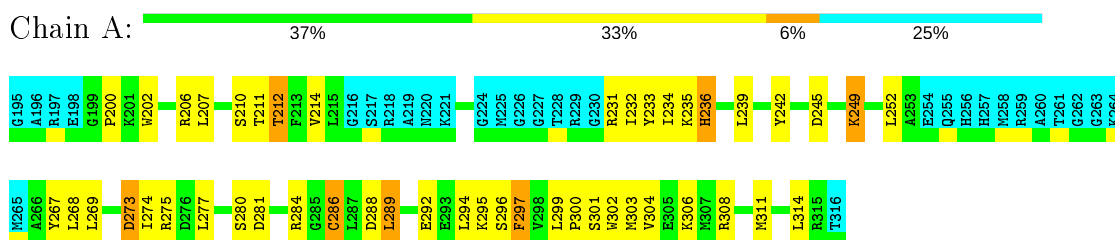
4.2.34 Score per residue for model 34

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



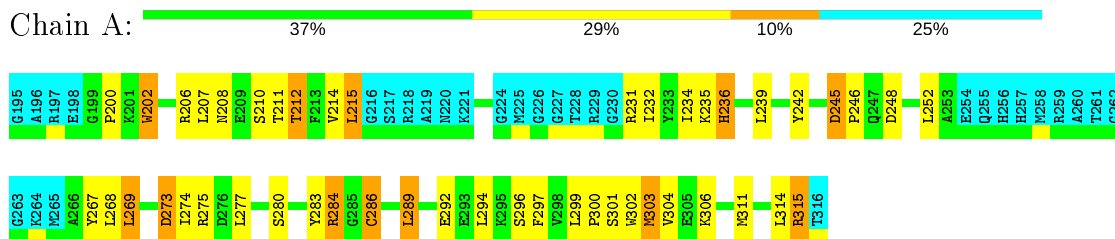
4.2.35 Score per residue for model 35

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



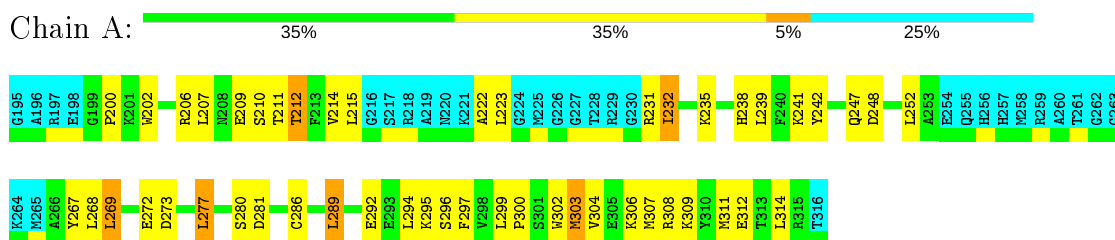
4.2.36 Score per residue for model 36

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



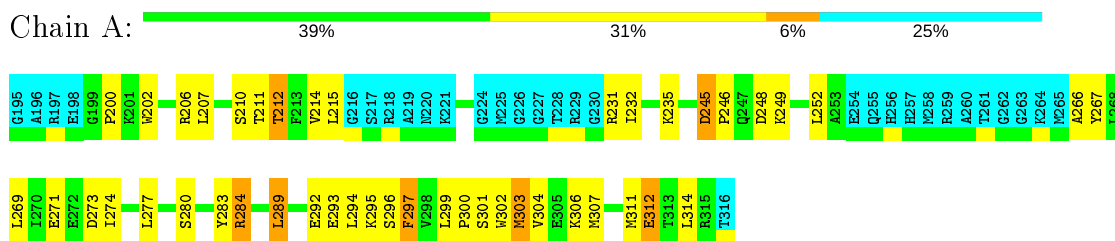
4.2.37 Score per residue for model 37

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



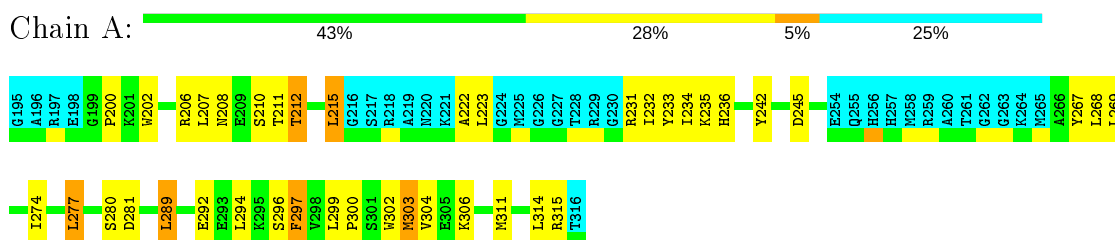
4.2.38 Score per residue for model 38

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



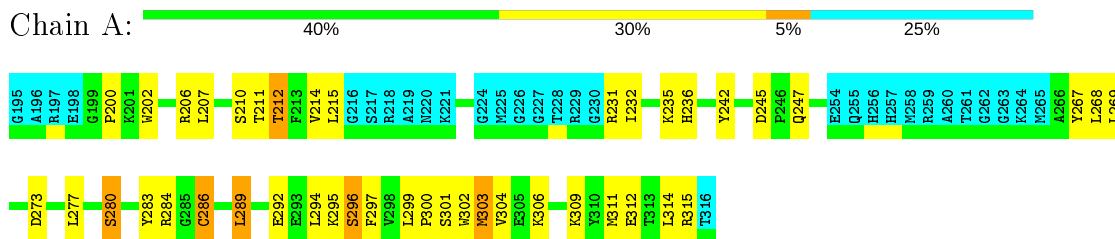
4.2.39 Score per residue for model 39

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



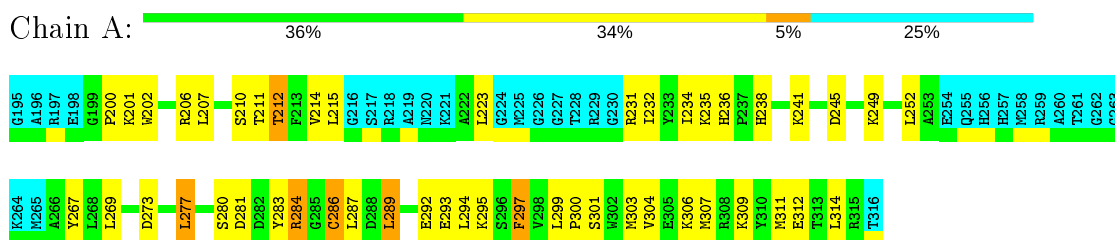
4.2.40 Score per residue for model 40

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



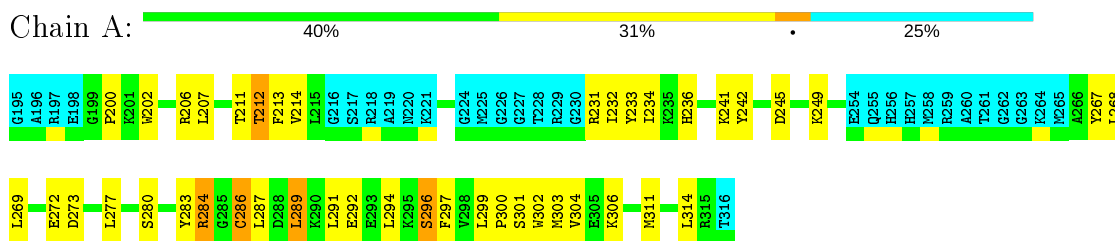
4.2.41 Score per residue for model 41

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



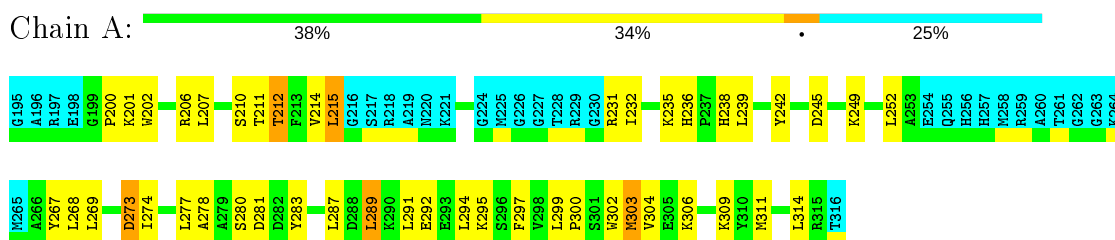
4.2.42 Score per residue for model 42

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



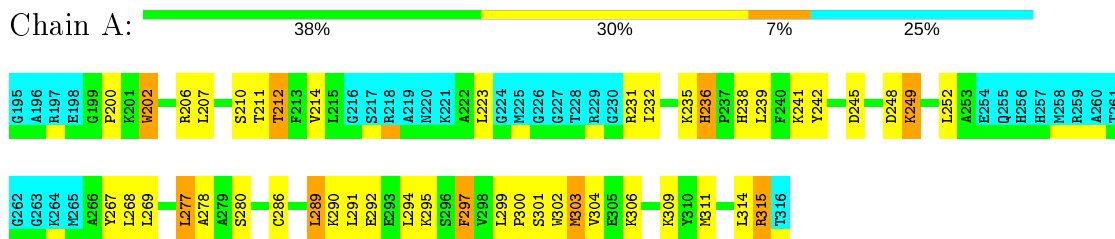
4.2.43 Score per residue for model 43

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



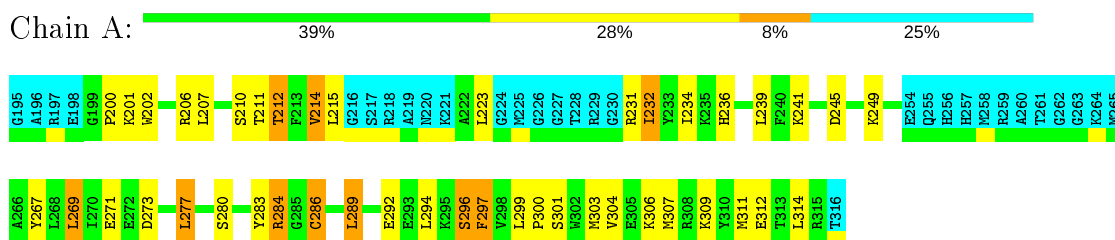
4.2.44 Score per residue for model 44

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



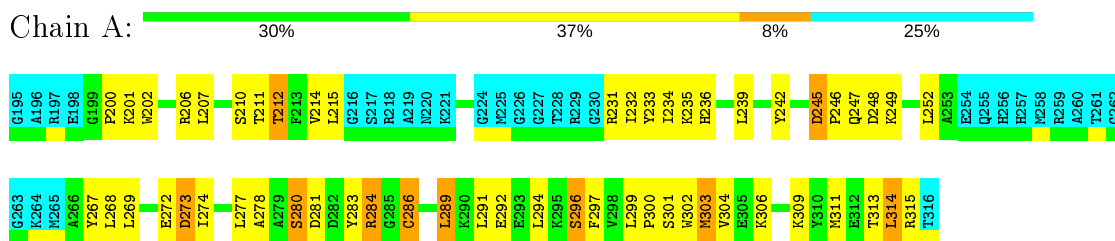
4.2.45 Score per residue for model 45

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



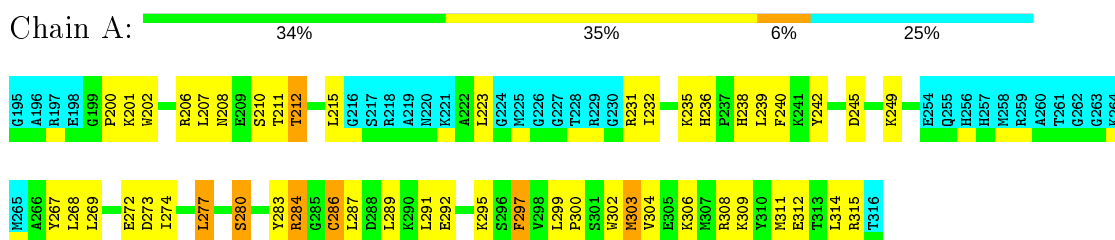
4.2.46 Score per residue for model 46

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



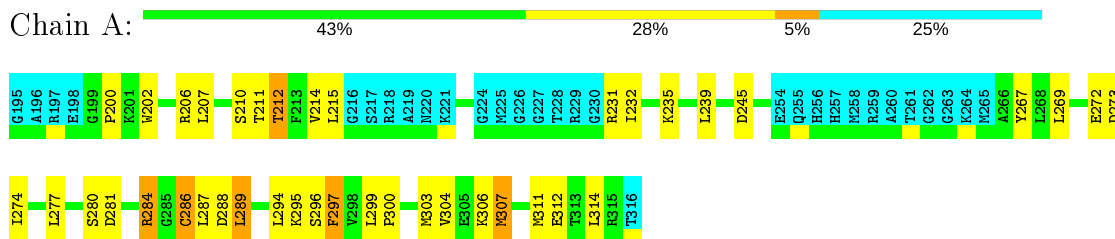
4.2.47 Score per residue for model 47

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



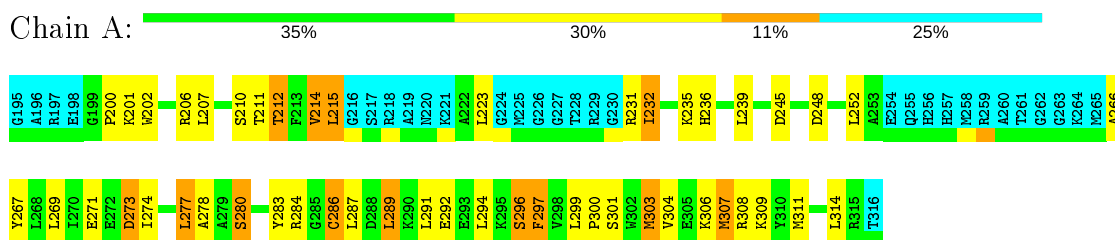
4.2.48 Score per residue for model 48

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



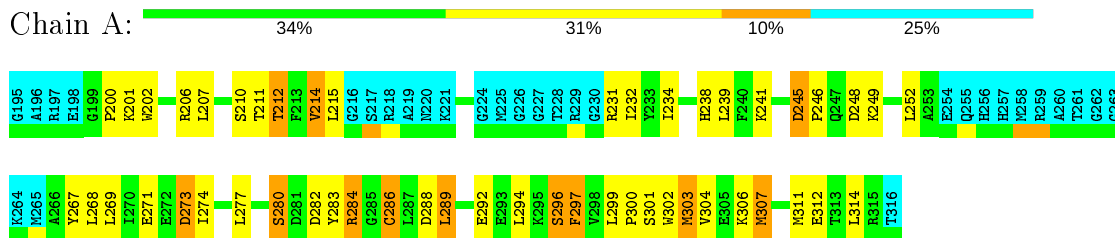
4.2.49 Score per residue for model 49

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



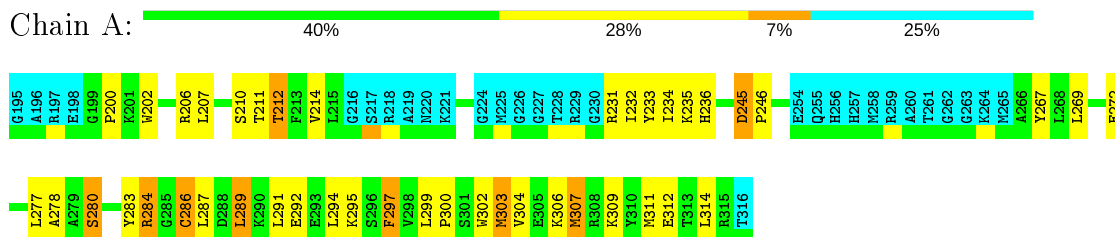
4.2.50 Score per residue for model 50

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



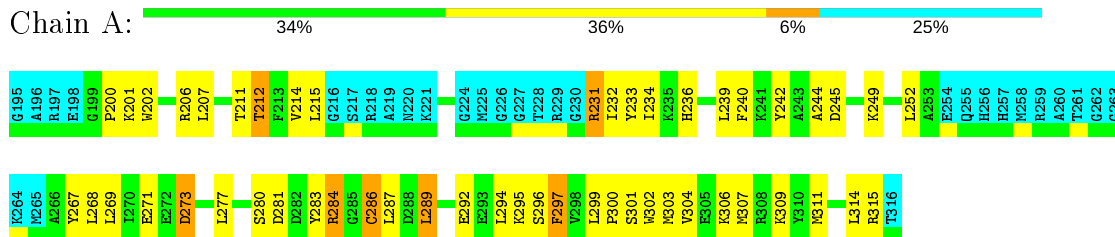
4.2.51 Score per residue for model 51

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



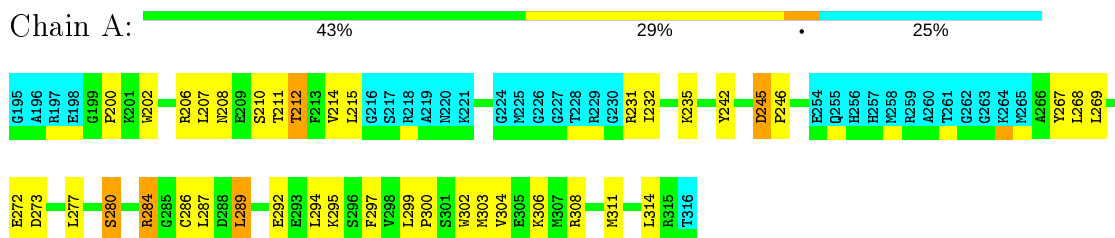
4.2.52 Score per residue for model 52

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



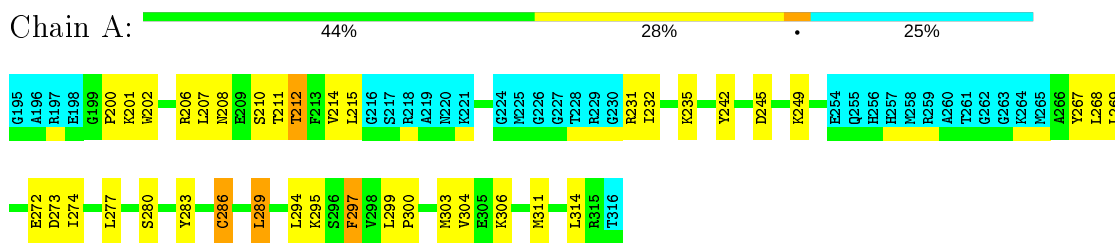
4.2.53 Score per residue for model 53

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1

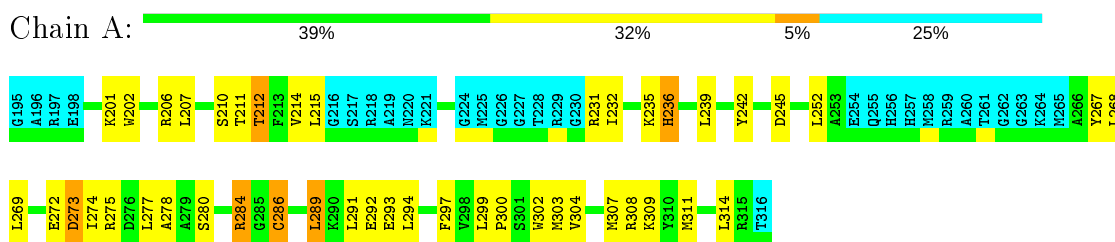


4.2.54 Score per residue for model 54

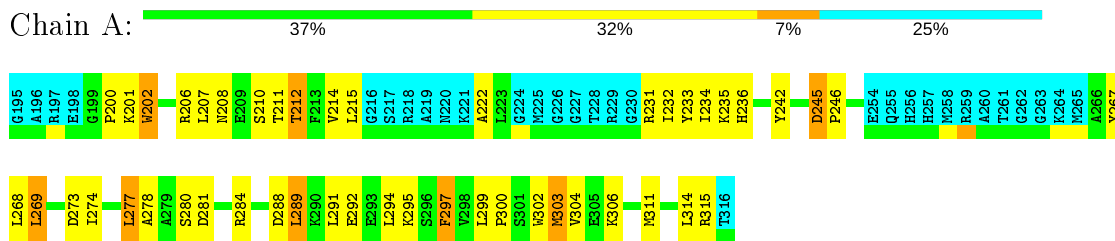
- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



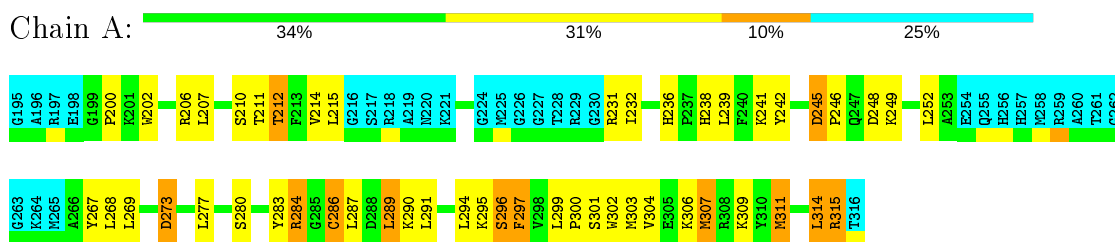
- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1

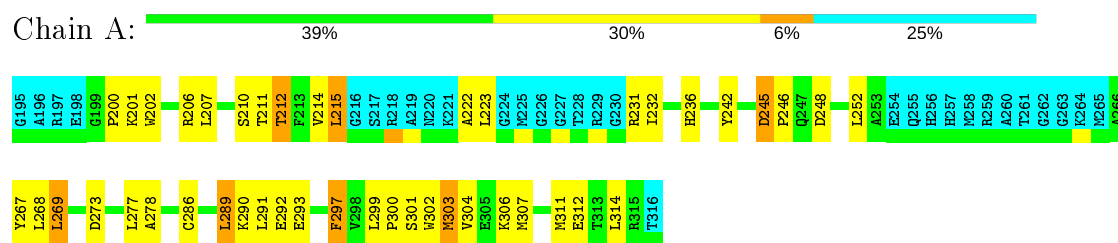


- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



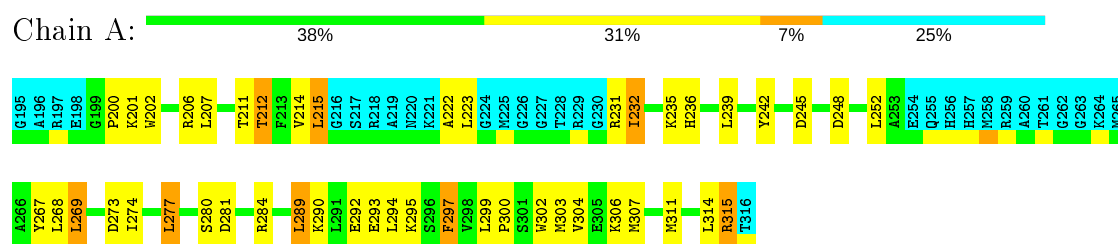
4.2.58 Score per residue for model 58

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



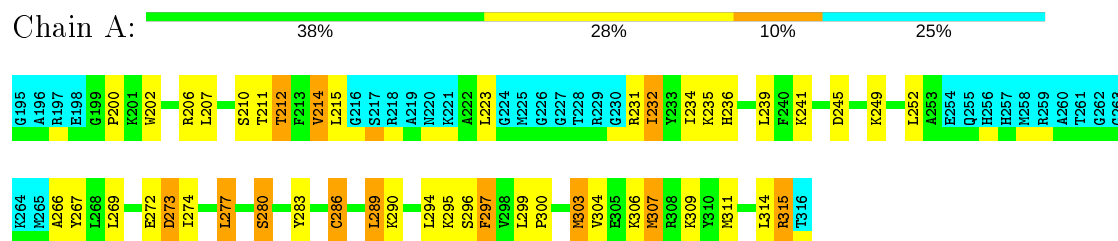
4.2.59 Score per residue for model 59

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



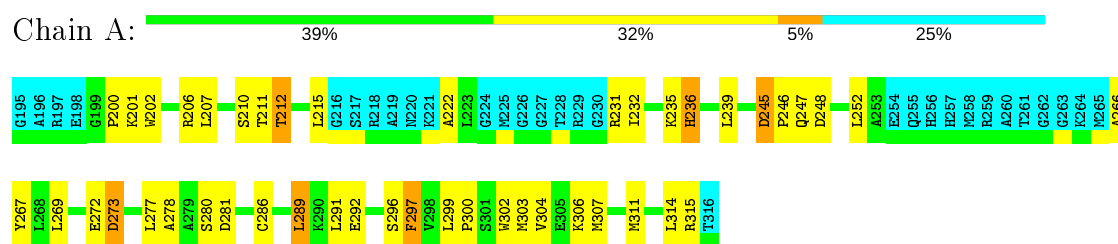
4.2.60 Score per residue for model 60

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



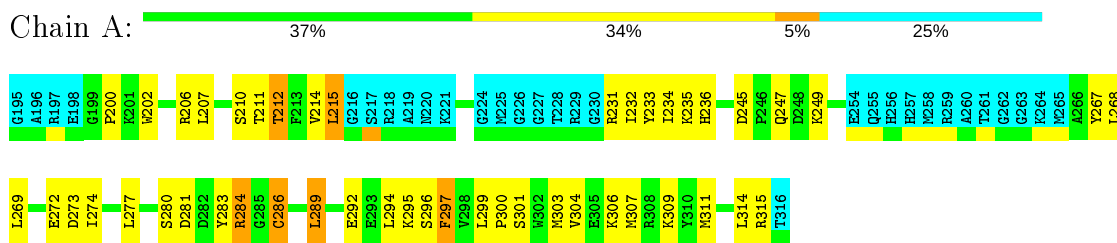
4.2.61 Score per residue for model 61

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



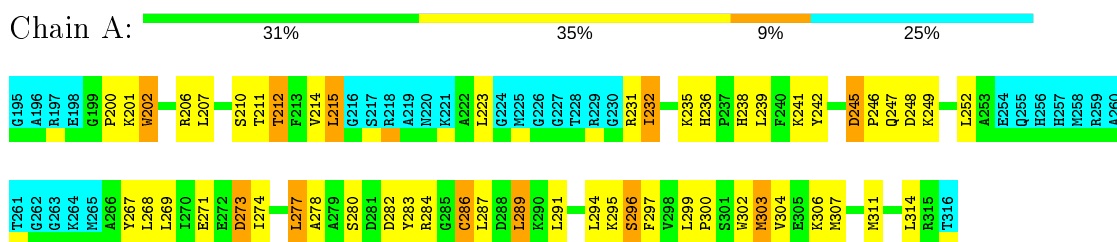
4.2.62 Score per residue for model 62

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



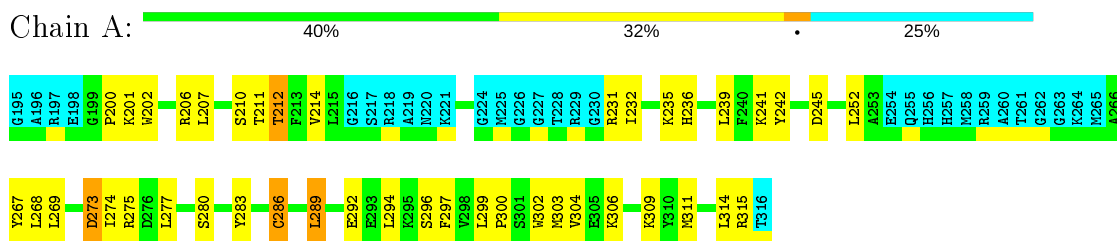
4.2.63 Score per residue for model 63

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



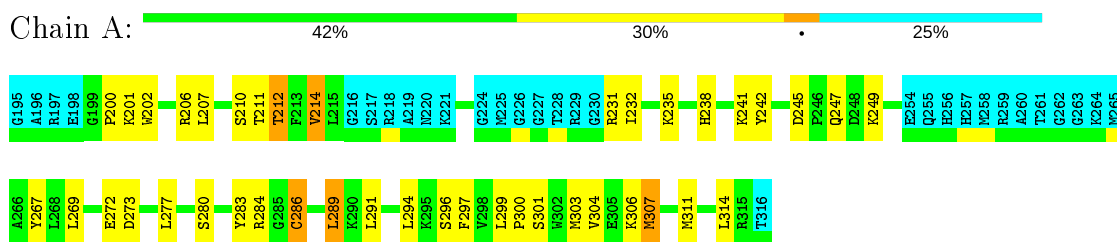
4.2.64 Score per residue for model 64

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



4.2.65 Score per residue for model 65

- Molecule 1: Deoxynucleotidyltransferase terminal-interacting protein 1



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 65 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	refinement	2.1

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

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1224
Number of shifts mapped to atoms	1224
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

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

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	770	772	772	16±3
All	All	50050	50180	50180	1029

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:215:LEU:HD21	1:A:252:LEU:HD22	0.85	1.44	61	7
1:A:232:ILE:HD11	1:A:239:LEU:HD22	0.84	1.48	59	3
1:A:215:LEU:HD22	1:A:268:LEU:HD22	0.74	1.58	62	1
1:A:215:LEU:HD22	1:A:252:LEU:HD22	0.72	1.59	14	10
1:A:274:ILE:HG21	1:A:294:LEU:HD11	0.70	1.63	12	15
1:A:274:ILE:HG21	1:A:294:LEU:HD21	0.70	1.64	2	17
1:A:232:ILE:CD1	1:A:239:LEU:HD22	0.67	2.19	60	3
1:A:239:LEU:HD21	1:A:273:ASP:OD1	0.67	1.90	55	16
1:A:214:VAL:HG11	1:A:294:LEU:HD22	0.67	1.65	62	47
1:A:242:TYR:CD1	1:A:268:LEU:HD12	0.66	2.25	33	52
1:A:286:CYS:HB2	1:A:289:LEU:HD13	0.65	1.69	27	51
1:A:252:LEU:HD22	1:A:268:LEU:HD21	0.64	1.68	27	3
1:A:299:LEU:HD13	1:A:303:MET:HG2	0.64	1.68	55	61
1:A:233:TYR:O	1:A:234:ILE:HD13	0.64	1.93	62	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:236:HIS:CE1	1:A:239:LEU:HD23	0.63	2.28	35	9
1:A:215:LEU:HD23	1:A:268:LEU:CD2	0.63	2.23	50	7
1:A:215:LEU:CD2	1:A:252:LEU:HD22	0.62	2.24	50	2
1:A:278:ALA:HB2	1:A:291:LEU:HD21	0.62	1.72	43	9
1:A:223:LEU:CD1	1:A:277:LEU:HD11	0.61	2.25	47	18
1:A:248:ASP:OD2	1:A:252:LEU:HD11	0.61	1.96	63	9
1:A:232:ILE:CG1	1:A:239:LEU:HD13	0.61	2.26	59	3
1:A:223:LEU:HD13	1:A:277:LEU:HD11	0.60	1.72	47	8
1:A:214:VAL:HG13	1:A:296:SER:OG	0.60	1.96	15	15
1:A:286:CYS:CB	1:A:289:LEU:HD23	0.59	2.27	61	4
1:A:300:PRO:O	1:A:304:VAL:HG13	0.59	1.97	54	65
1:A:207:LEU:HD22	1:A:211:THR:OG1	0.59	1.98	55	14
1:A:249:LYS:HA	1:A:252:LEU:HD12	0.59	1.74	41	19
1:A:211:THR:O	1:A:212:THR:HG23	0.59	1.97	49	65
1:A:299:LEU:HD11	1:A:307:MET:HE3	0.58	1.76	21	1
1:A:278:ALA:CB	1:A:291:LEU:HD11	0.58	2.29	56	9
1:A:299:LEU:HD22	1:A:303:MET:CE	0.57	2.29	48	57
1:A:299:LEU:HD22	1:A:303:MET:SD	0.56	2.41	42	7
1:A:299:LEU:HD22	1:A:303:MET:HE3	0.55	1.77	57	6
1:A:299:LEU:HD11	1:A:307:MET:HE2	0.54	1.78	50	4
1:A:215:LEU:HD23	1:A:268:LEU:HD21	0.54	1.76	50	1
1:A:215:LEU:HD22	1:A:252:LEU:CD2	0.54	2.32	14	3
1:A:232:ILE:CG1	1:A:239:LEU:HD22	0.53	2.33	49	2
1:A:286:CYS:HB3	1:A:289:LEU:HD23	0.52	1.80	37	3
1:A:222:ALA:O	1:A:289:LEU:HD13	0.52	2.04	58	7
1:A:232:ILE:HG13	1:A:239:LEU:HD13	0.51	1.80	59	3
1:A:274:ILE:HG22	1:A:291:LEU:CD2	0.51	2.36	55	4
1:A:278:ALA:HB1	1:A:291:LEU:HD11	0.50	1.83	34	4
1:A:274:ILE:CG2	1:A:294:LEU:HD11	0.49	2.35	23	7
1:A:212:THR:HG22	1:A:297:PHE:C	0.49	2.28	45	43
1:A:200:PRO:HG3	1:A:207:LEU:HD21	0.49	1.85	44	54
1:A:286:CYS:CB	1:A:289:LEU:HD13	0.49	2.37	24	35
1:A:214:VAL:O	1:A:269:LEU:HD12	0.49	2.08	14	12
1:A:239:LEU:HD11	1:A:273:ASP:OD1	0.48	2.07	60	2
1:A:200:PRO:HG3	1:A:207:LEU:HD11	0.48	1.85	59	60
1:A:299:LEU:HD11	1:A:307:MET:CE	0.47	2.39	57	3
1:A:289:LEU:CD1	1:A:291:LEU:HD12	0.47	2.38	61	4
1:A:273:ASP:OD1	1:A:273:ASP:C	0.47	2.52	46	10
1:A:299:LEU:HD22	1:A:303:MET:HE2	0.47	1.86	35	1
1:A:223:LEU:HD22	1:A:277:LEU:HD11	0.47	1.87	37	2
1:A:274:ILE:HA	1:A:277:LEU:HD23	0.47	1.87	49	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:283:TYR:O	1:A:289:LEU:HD22	0.46	2.10	32	46
1:A:291:LEU:O	1:A:294:LEU:HD12	0.46	2.10	32	13
1:A:273:ASP:C	1:A:273:ASP:OD1	0.46	2.54	36	4
1:A:232:ILE:HD11	1:A:269:LEU:CD2	0.45	2.40	45	2
1:A:239:LEU:HD12	1:A:269:LEU:HD23	0.45	1.88	45	4
1:A:252:LEU:HD21	1:A:303:MET:CE	0.45	2.42	55	2
1:A:223:LEU:CD2	1:A:277:LEU:HD11	0.45	2.42	39	2
1:A:252:LEU:CD2	1:A:268:LEU:HD21	0.44	2.40	27	1
1:A:215:LEU:CD2	1:A:268:LEU:HD22	0.44	2.37	62	1
1:A:286:CYS:HB2	1:A:289:LEU:HD23	0.44	1.89	61	3
1:A:232:ILE:HG13	1:A:277:LEU:HD22	0.44	1.88	63	1
1:A:270:ILE:HG21	1:A:272:GLU:OE1	0.44	2.13	29	1
1:A:214:VAL:HG22	1:A:269:LEU:O	0.43	2.13	20	6
1:A:274:ILE:HG22	1:A:291:LEU:HD23	0.43	1.89	43	2
1:A:232:ILE:HG12	1:A:239:LEU:HD13	0.43	1.88	49	3
1:A:313:THR:OG1	1:A:314:LEU:HD23	0.43	2.13	27	3
1:A:299:LEU:HD22	1:A:303:MET:HG2	0.43	1.89	45	2
1:A:239:LEU:HD21	1:A:273:ASP:HB3	0.43	1.90	63	1
1:A:213:PHE:CD2	1:A:307:MET:HE3	0.43	2.48	7	1
1:A:245:ASP:CB	1:A:246:PRO:HD2	0.43	2.44	63	12
1:A:297:PHE:CZ	1:A:299:LEU:HD23	0.42	2.50	47	2
1:A:278:ALA:CB	1:A:291:LEU:HD21	0.42	2.45	21	1
1:A:215:LEU:HD22	1:A:266:ALA:HB1	0.42	1.91	25	1
1:A:300:PRO:O	1:A:304:VAL:HG22	0.42	2.14	24	2
1:A:245:ASP:HB3	1:A:246:PRO:HD2	0.42	1.91	53	1
1:A:232:ILE:HD13	1:A:232:ILE:O	0.42	2.15	60	1
1:A:215:LEU:CB	1:A:268:LEU:HD23	0.41	2.46	47	1
1:A:244:ALA:HB1	1:A:252:LEU:CD1	0.41	2.46	52	1
1:A:239:LEU:HD13	1:A:240:PHE:O	0.41	2.16	47	2
1:A:236:HIS:ND1	1:A:239:LEU:HD23	0.41	2.30	55	1
1:A:311:MET:HA	1:A:314:LEU:HD21	0.41	1.93	57	1
1:A:242:TYR:CZ	1:A:307:MET:CE	0.41	3.04	65	1
1:A:252:LEU:HD21	1:A:303:MET:SD	0.41	2.56	64	1
1:A:213:PHE:CD1	1:A:213:PHE:N	0.40	2.89	42	1
1:A:211:THR:HG23	1:A:212:THR:N	0.40	2.31	46	1
1:A:242:TYR:CE1	1:A:268:LEU:HD12	0.40	2.52	4	1
1:A:232:ILE:HB	1:A:277:LEU:HD13	0.40	1.94	28	2
1:A:242:TYR:HD1	1:A:268:LEU:HD12	0.40	1.71	46	1
1:A:289:LEU:HD12	1:A:291:LEU:HD12	0.40	1.93	56	1
1:A:289:LEU:O	1:A:290:LYS:HG2	0.40	2.16	34	2
1:A:215:LEU:HD23	1:A:268:LEU:HD23	0.40	1.93	54	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	92/122 (75%)	83±1 (90±1%)	8±2 (8±2%)	2±1 (2±1%)	13	56
All	All	5980/7930 (75%)	5380 (90%)	499 (8%)	101 (2%)	13	56

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	280	SER	44
1	A	284	ARG	44
1	A	234	ILE	8
1	A	202	TRP	5

6.3.2 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	82/101 (81%)	52±3 (64±3%)	30±3 (36±3%)	1	8
All	All	5330/6565 (81%)	3403 (64%)	1927 (36%)	1	8

All 53 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	311	MET	65
1	A	277	LEU	65
1	A	202	TRP	65
1	A	232	ILE	65
1	A	206	ARG	65
1	A	267	TYR	65

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Mol	Chain	Res	Type	Models (Total)
1	A	212	THR	65
1	A	297	PHE	65
1	A	269	LEU	65
1	A	314	LEU	65
1	A	289	LEU	64
1	A	306	LYS	64
1	A	273	ASP	62
1	A	231	ARG	61
1	A	210	SER	60
1	A	245	ASP	56
1	A	302	TRP	56
1	A	286	CYS	55
1	A	235	LYS	52
1	A	292	GLU	50
1	A	236	HIS	46
1	A	303	MET	44
1	A	296	SER	40
1	A	301	SER	38
1	A	284	ARG	37
1	A	280	SER	35
1	A	295	LYS	33
1	A	309	LYS	31
1	A	281	ASP	30
1	A	201	LYS	29
1	A	215	LEU	29
1	A	241	LYS	28
1	A	307	MET	28
1	A	249	LYS	27
1	A	272	GLU	26
1	A	287	LEU	24
1	A	315	ARG	23
1	A	312	GLU	20
1	A	308	ARG	19
1	A	247	GLN	15
1	A	238	HIS	14
1	A	248	ASP	14
1	A	293	GLU	13
1	A	208	ASN	10
1	A	288	ASP	9
1	A	271	GLU	7
1	A	214	VAL	7
1	A	290	LYS	6

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Mol	Chain	Res	Type	Models (Total)
1	A	282	ASP	5
1	A	275	ARG	5
1	A	239	LEU	3
1	A	294	LEU	1
1	A	209	GLU	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 carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 80% for the well-defined parts and 70% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1224
Number of shifts mapped to atoms	1224
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	112	-0.14 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	106	0.20 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	101	0.31 ± 0.38	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 80%, i.e. 976 atoms were assigned a chemical shift out of a possible 1218. 16 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	358/450 (80%)	179/179 (100%)	92/184 (50%)	87/87 (100%)
Sidechain	517/644 (80%)	315/380 (83%)	198/236 (84%)	4/28 (14%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	101/124 (81%)	55/65 (85%)	43/53 (81%)	3/6 (50%)
Overall	976/1218 (80%)	549/624 (88%)	333/473 (70%)	94/121 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 70%, i.e. 1093 atoms were assigned a chemical shift out of a possible 1562. 16 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	421/600 (70%)	208/239 (87%)	112/244 (46%)	101/117 (86%)
Sidechain	567/824 (69%)	344/488 (70%)	219/292 (75%)	4/44 (9%)
Aromatic	105/138 (76%)	57/73 (78%)	45/57 (79%)	3/8 (38%)
Overall	1093/1562 (70%)	609/800 (76%)	376/593 (63%)	108/169 (64%)

7.1.4 Statistically unusual chemical shifts [i](#)

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

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	300	PRO	HG2	-0.23	3.48 – 0.38	-7.0
1	A	256	HIS	HB3	0.49	5.00 – 1.10	-6.6

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.

Random coil index (RCI) for chain A:

