



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 8, 2022 – 01:10 PM EST

PDB ID : 1BNP  
Title : NMR SOLUTION STRUCTURE OF THE N-TERMINAL DOMAIN OF  
DNA POLYMERASE BETA, 55 STRUCTURES  
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Deposited on : 1996-04-25

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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 : 2.26  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.26

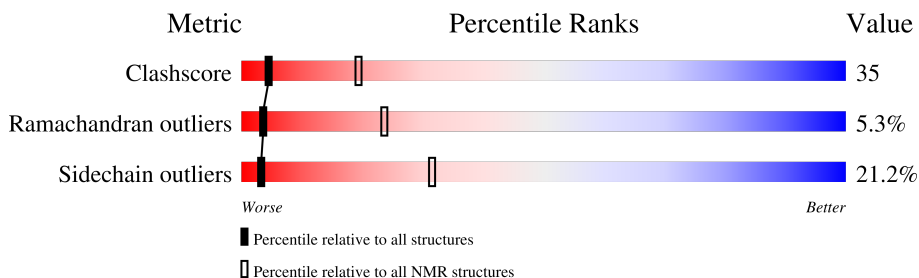
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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  $\geq 3$ , 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	87	

## 2 Ensemble composition and analysis i

This entry contains 55 models. Model 33 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:13-A:29, A:33-A:78 (63)	0.59	33

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 7 clusters and 8 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1400 atoms, of which 724 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA POLYMERASE BETA.

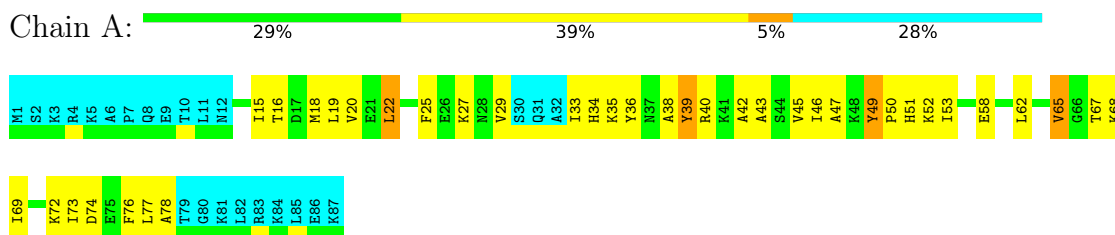
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	87	1400	430	724	121	123	2	0

## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: DNA POLYMERASE BETA

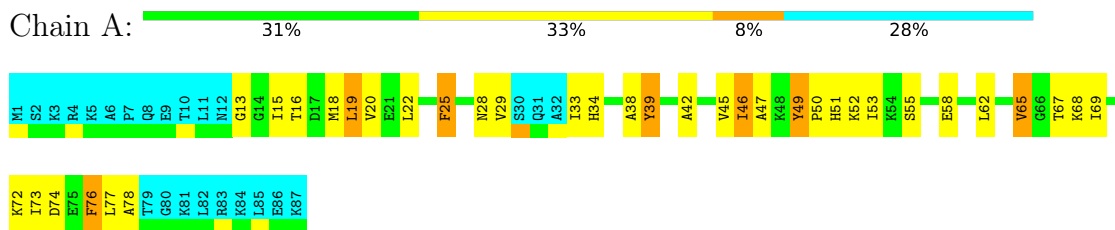


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

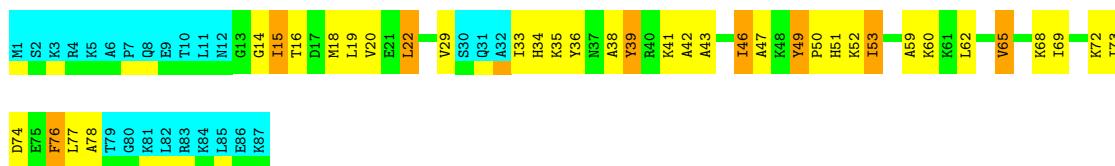
- Molecule 1: DNA POLYMERASE BETA



#### 4.2.2 Score per residue for model 2

- Molecule 1: DNA POLYMERASE BETA





### 4.2.3 Score per residue for model 3

- Molecule 1: DNA POLYMERASE BETA

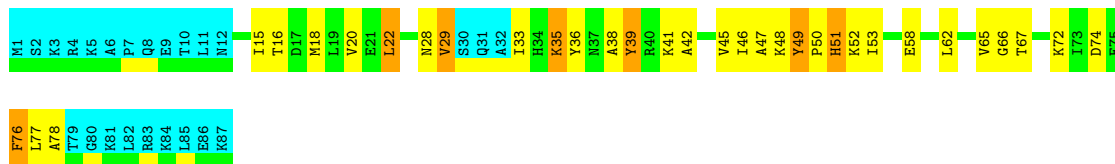
Chain A: 40% 29% 28%



### 4.2.4 Score per residue for model 4

- Molecule 1: DNA POLYMERASE BETA

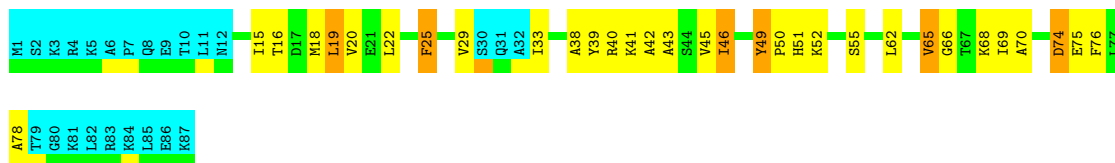
Chain A: 34% 30% 8% 28%



### 4.2.5 Score per residue for model 5

- Molecule 1: DNA POLYMERASE BETA

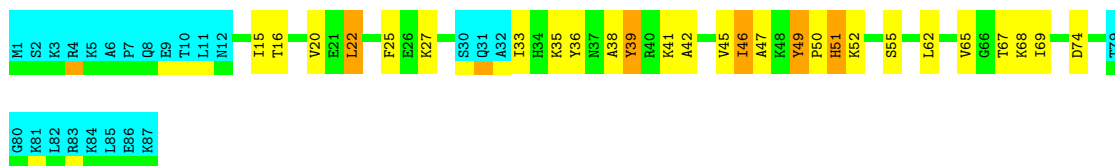
Chain A: 36% 30% 7% 28%



### 4.2.6 Score per residue for model 6

- Molecule 1: DNA POLYMERASE BETA

Chain A: 41% 25% 6% 28%



#### 4.2.7 Score per residue for model 7

- Molecule 1: DNA POLYMERASE BETA

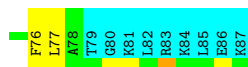
Chain A: 30% 38% 5% 28%



#### 4.2.8 Score per residue for model 8

- Molecule 1: DNA POLYMERASE BETA

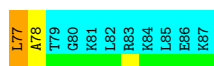
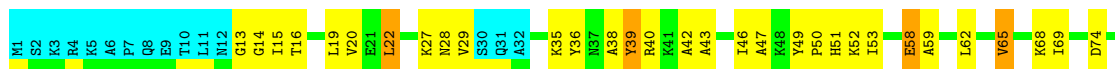
Chain A: 34% 34% 28%



#### 4.2.9 Score per residue for model 9

- Molecule 1: DNA POLYMERASE BETA

Chain A: 34% 32% 6% 28%



#### 4.2.10 Score per residue for model 10

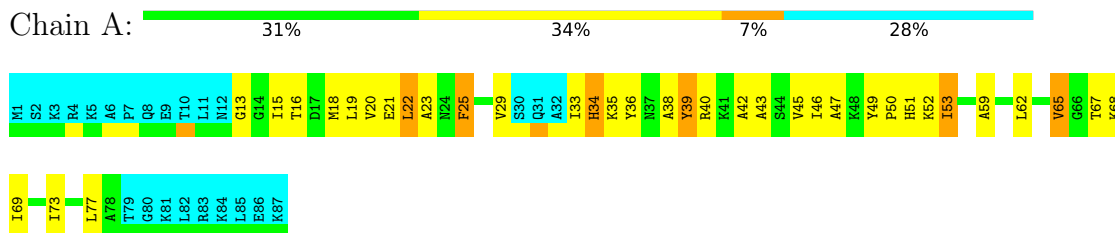
- Molecule 1: DNA POLYMERASE BETA

Chain A: 31% 33% 8% 28%



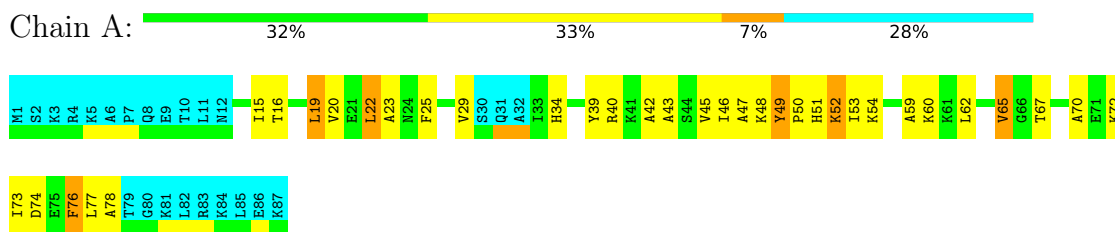
#### 4.2.11 Score per residue for model 11

- Molecule 1: DNA POLYMERASE BETA



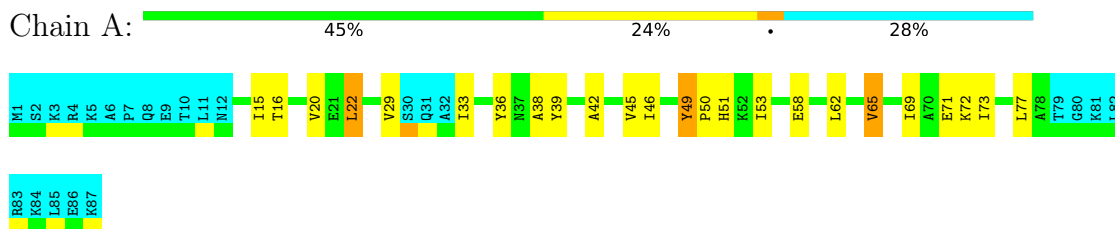
#### 4.2.12 Score per residue for model 12

- Molecule 1: DNA POLYMERASE BETA



#### 4.2.13 Score per residue for model 13

- Molecule 1: DNA POLYMERASE BETA

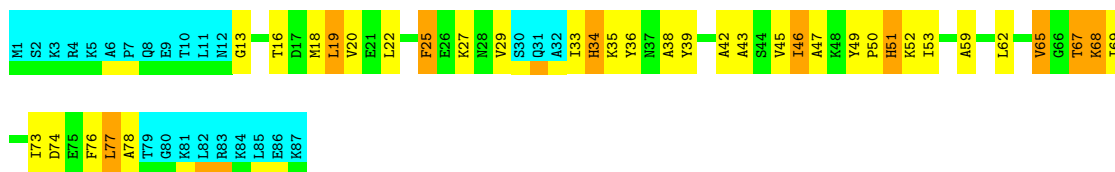


#### 4.2.14 Score per residue for model 14

- Molecule 1: DNA POLYMERASE BETA

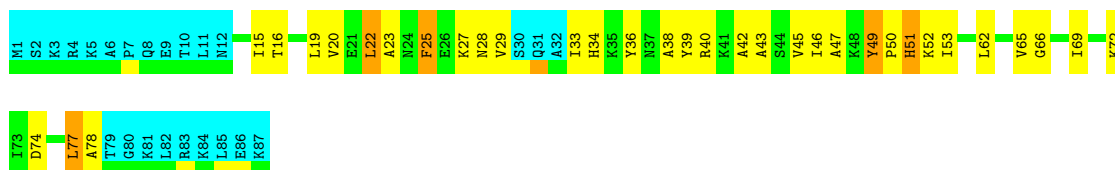
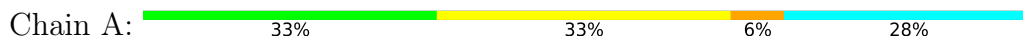






#### 4.2.15 Score per residue for model 15

- Molecule 1: DNA POLYMERASE BETA



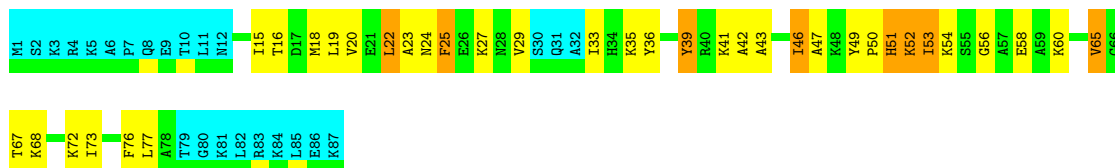
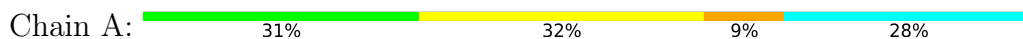
#### 4.2.16 Score per residue for model 16

- Molecule 1: DNA POLYMERASE BETA



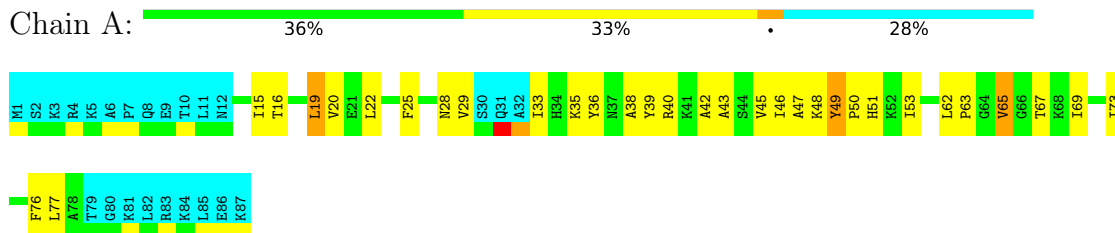
#### 4.2.17 Score per residue for model 17

- Molecule 1: DNA POLYMERASE BETA



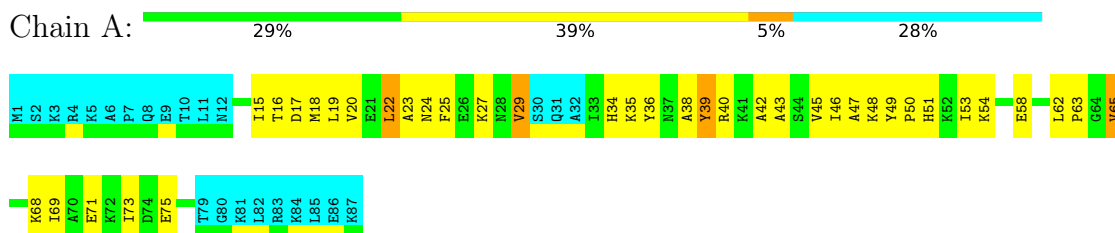
#### 4.2.18 Score per residue for model 18

- Molecule 1: DNA POLYMERASE BETA



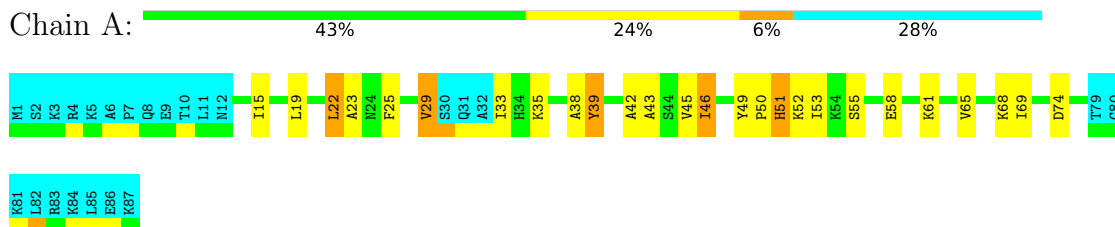
#### 4.2.19 Score per residue for model 19

- Molecule 1: DNA POLYMERASE BETA



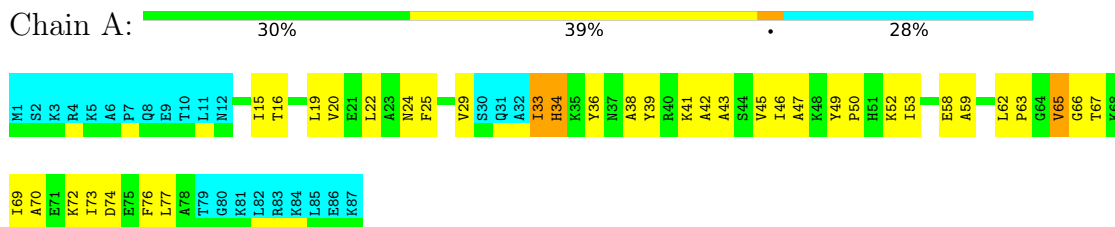
#### 4.2.20 Score per residue for model 20

- Molecule 1: DNA POLYMERASE BETA



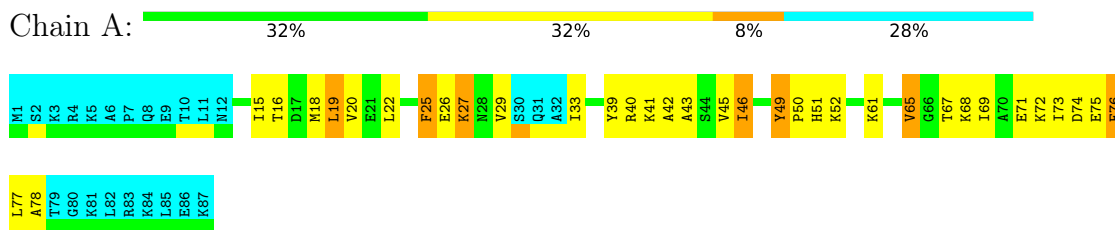
#### 4.2.21 Score per residue for model 21

- Molecule 1: DNA POLYMERASE BETA



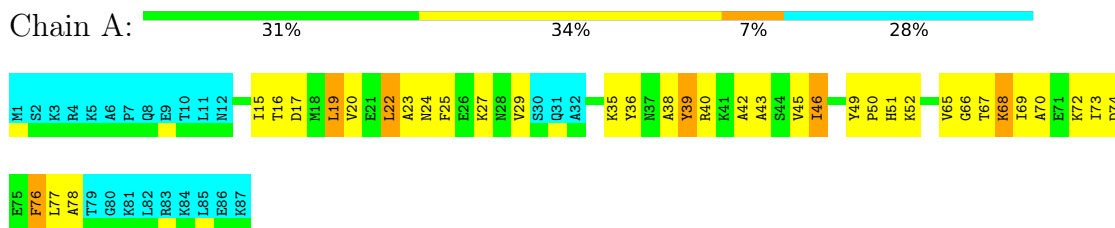
#### 4.2.22 Score per residue for model 22

- Molecule 1: DNA POLYMERASE BETA



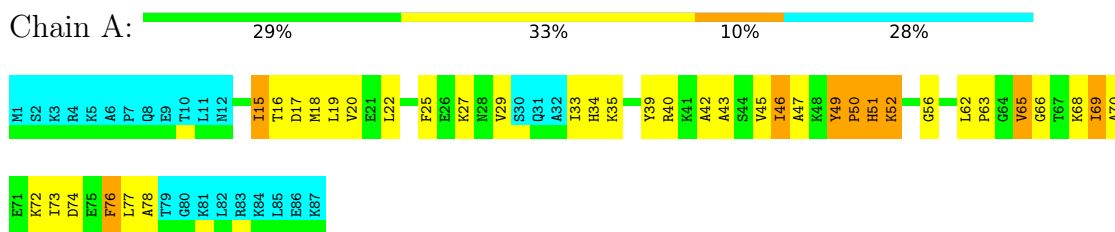
#### 4.2.23 Score per residue for model 23

- Molecule 1: DNA POLYMERASE BETA



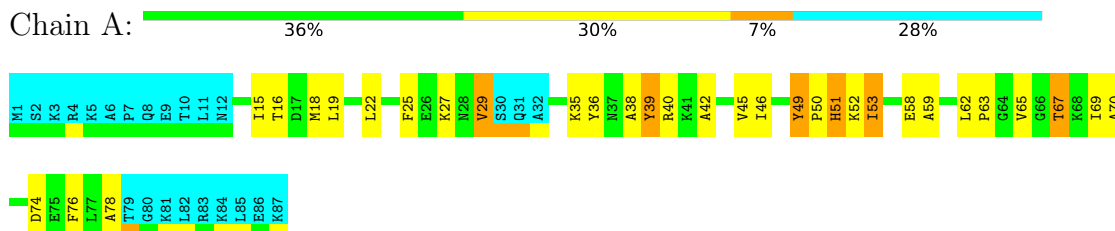
#### 4.2.24 Score per residue for model 24

- Molecule 1: DNA POLYMERASE BETA



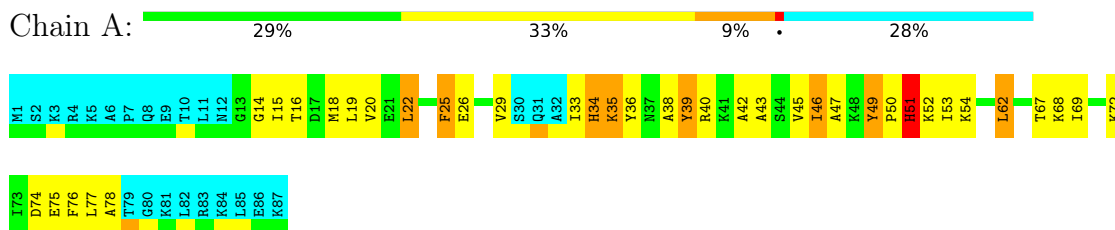
#### 4.2.25 Score per residue for model 25

- Molecule 1: DNA POLYMERASE BETA



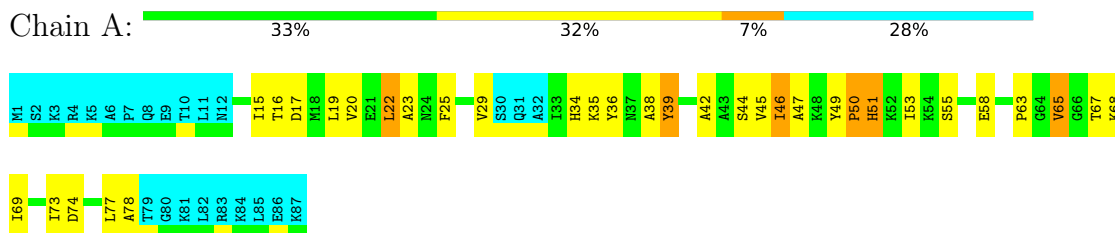
#### 4.2.26 Score per residue for model 26

- Molecule 1: DNA POLYMERASE BETA



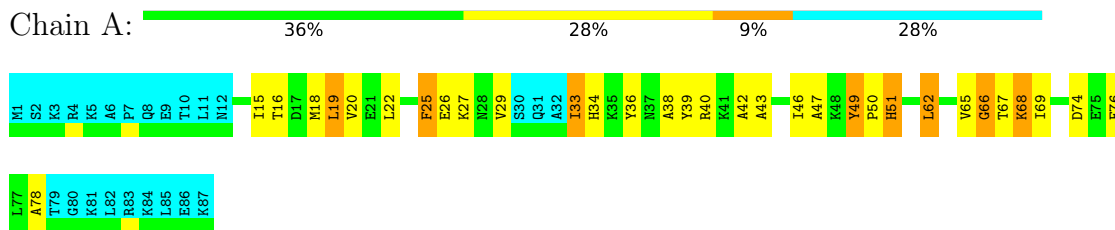
#### 4.2.27 Score per residue for model 27

- Molecule 1: DNA POLYMERASE BETA



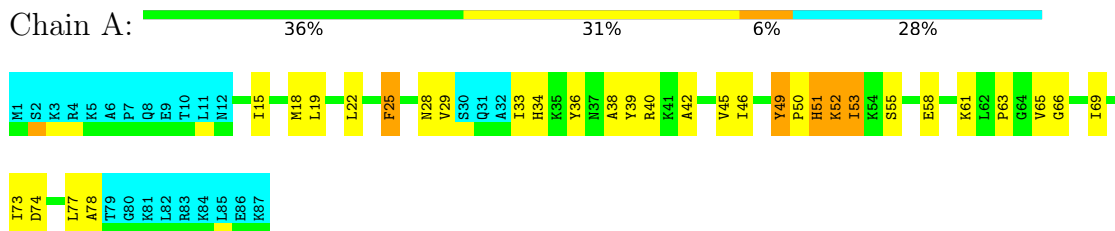
#### 4.2.28 Score per residue for model 28

- Molecule 1: DNA POLYMERASE BETA



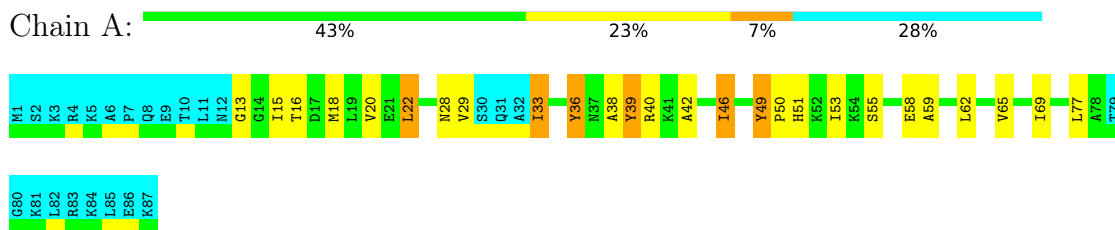
#### 4.2.29 Score per residue for model 29

- Molecule 1: DNA POLYMERASE BETA



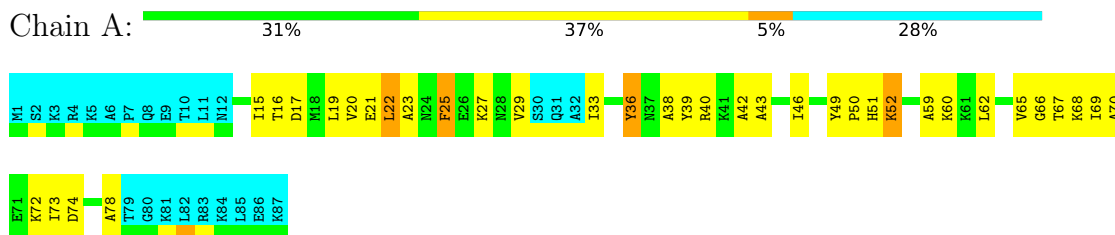
#### 4.2.30 Score per residue for model 30

- Molecule 1: DNA POLYMERASE BETA



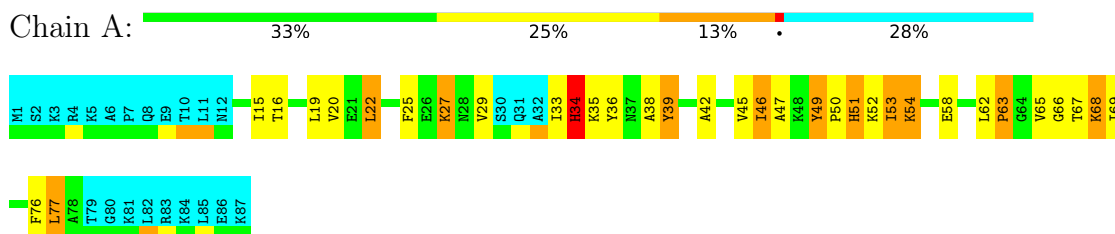
#### 4.2.31 Score per residue for model 31

- Molecule 1: DNA POLYMERASE BETA



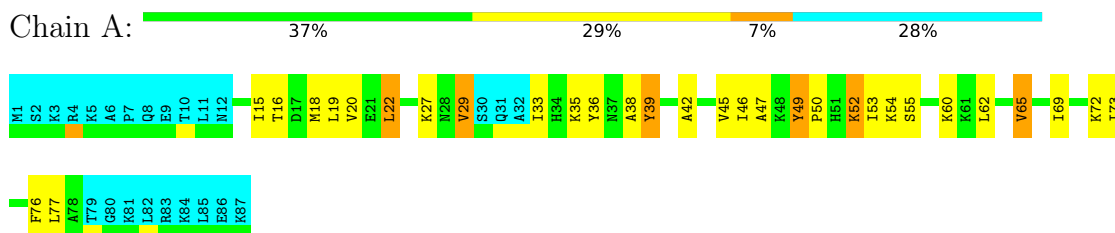
#### 4.2.32 Score per residue for model 32

- Molecule 1: DNA POLYMERASE BETA



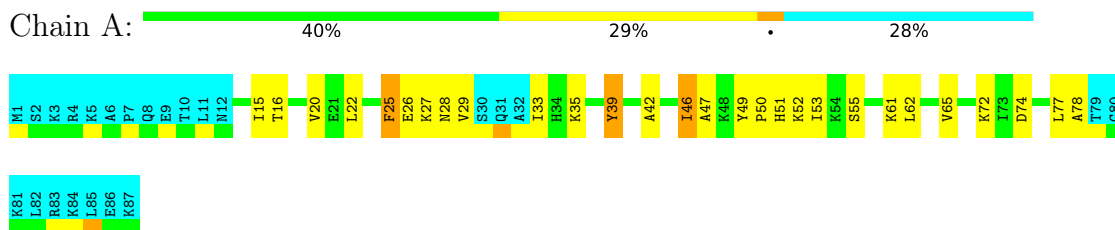
#### 4.2.33 Score per residue for model 33 (medoid)

- Molecule 1: DNA POLYMERASE BETA



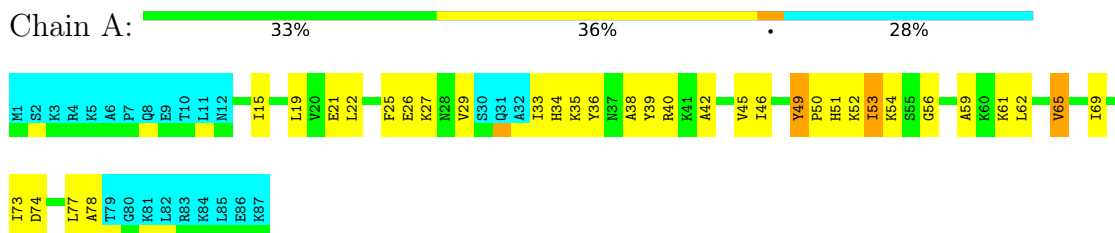
#### 4.2.34 Score per residue for model 34

- Molecule 1: DNA POLYMERASE BETA



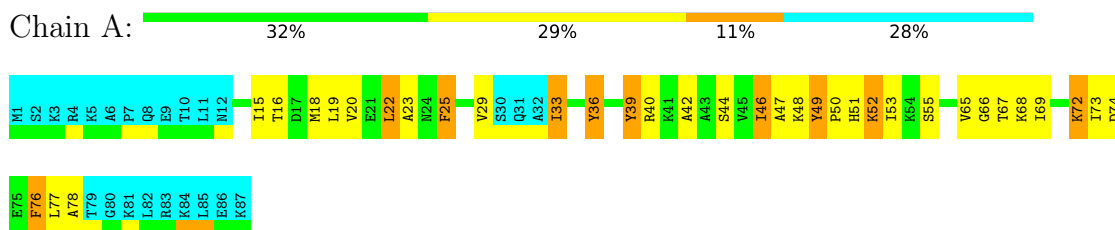
#### 4.2.35 Score per residue for model 35

- Molecule 1: DNA POLYMERASE BETA



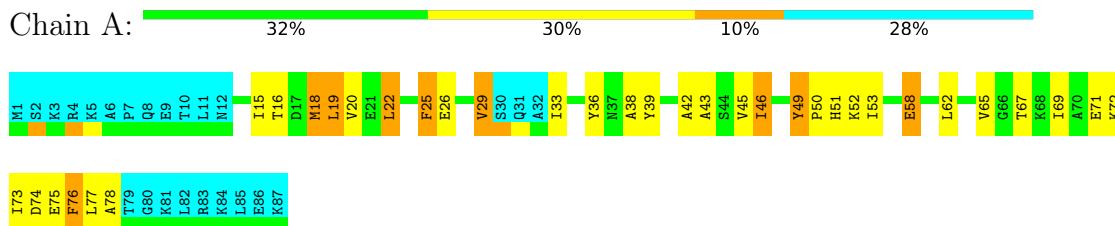
#### 4.2.36 Score per residue for model 36

- Molecule 1: DNA POLYMERASE BETA



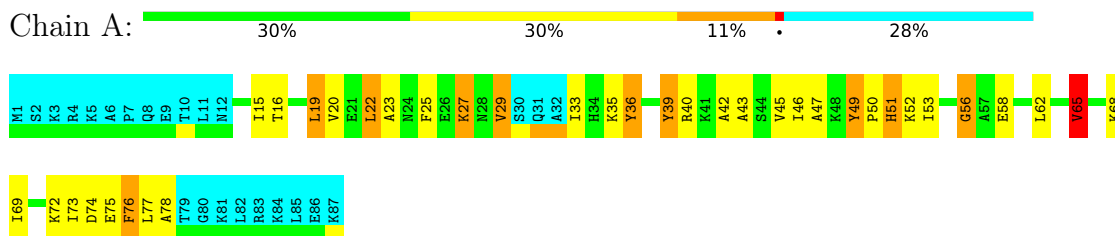
#### 4.2.37 Score per residue for model 37

- Molecule 1: DNA POLYMERASE BETA



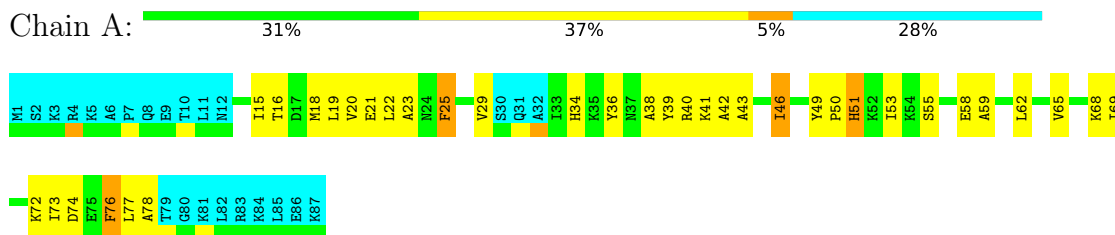
### 4.2.38 Score per residue for model 38

- Molecule 1: DNA POLYMERASE BETA



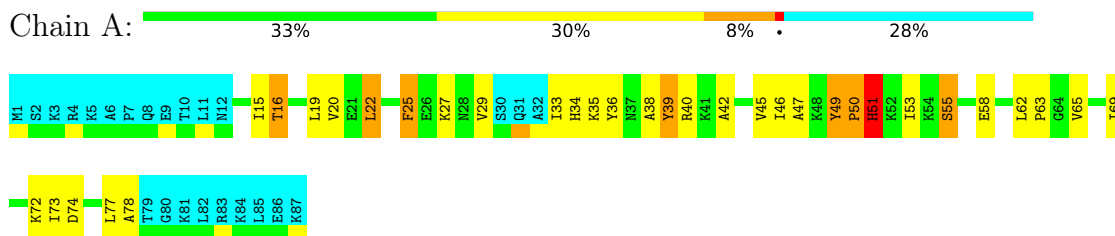
### 4.2.39 Score per residue for model 39

- Molecule 1: DNA POLYMERASE BETA



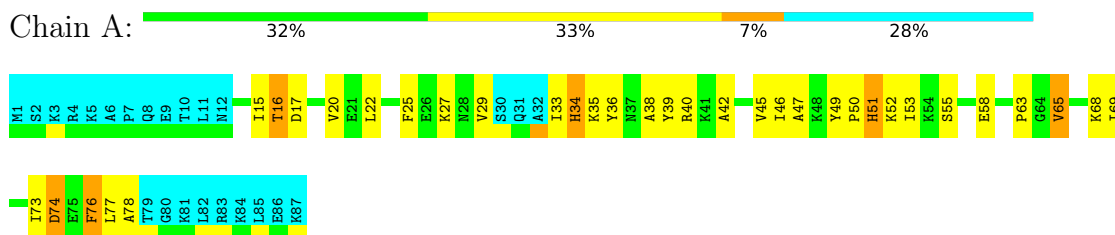
### 4.2.40 Score per residue for model 40

- Molecule 1: DNA POLYMERASE BETA



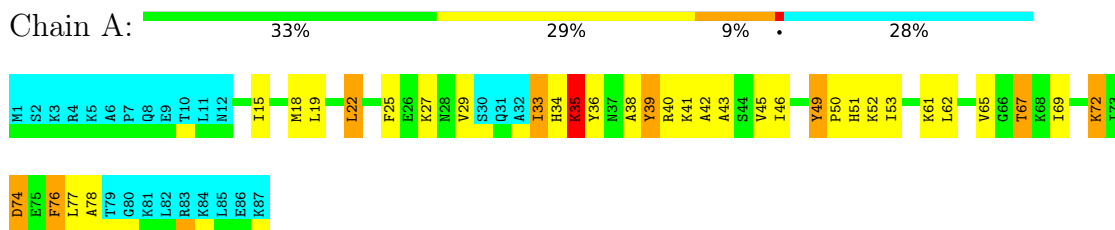
### 4.2.41 Score per residue for model 41

- Molecule 1: DNA POLYMERASE BETA



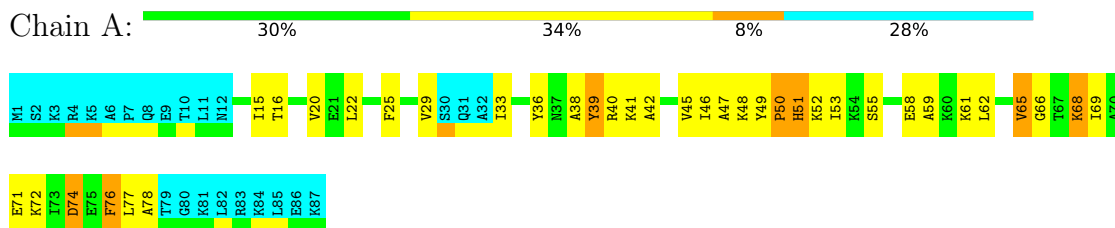
#### 4.2.42 Score per residue for model 42

- Molecule 1: DNA POLYMERASE BETA



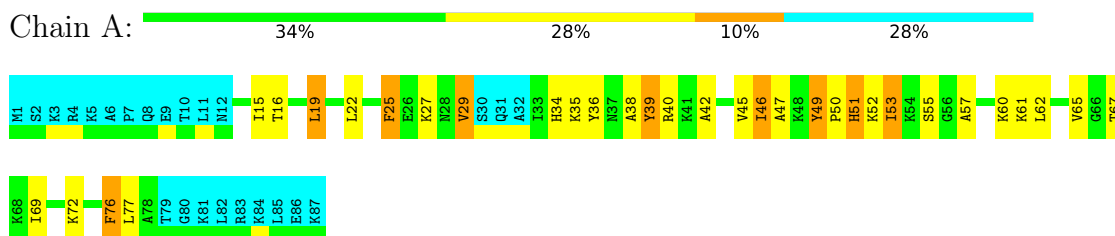
#### 4.2.43 Score per residue for model 43

- Molecule 1: DNA POLYMERASE BETA



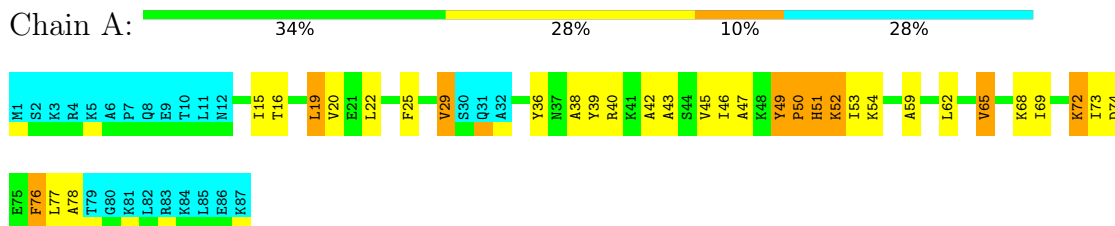
#### 4.2.44 Score per residue for model 44

- Molecule 1: DNA POLYMERASE BETA



#### 4.2.45 Score per residue for model 45

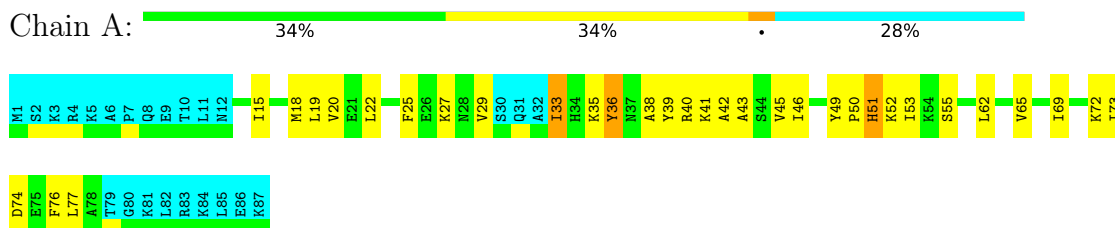
- Molecule 1: DNA POLYMERASE BETA





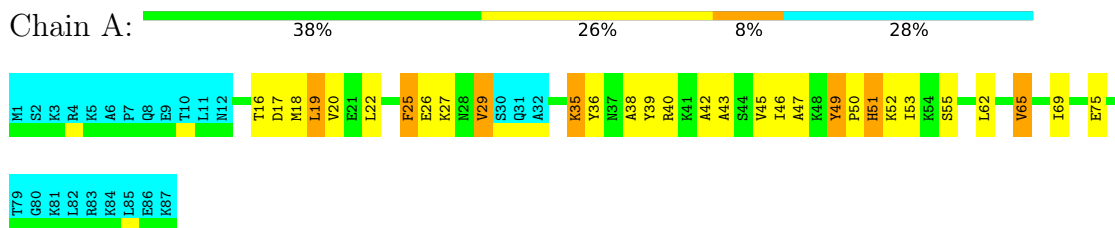
## 4.2.46 Score per residue for model 46

## • Molecule 1: DNA POLYMERASE BETA



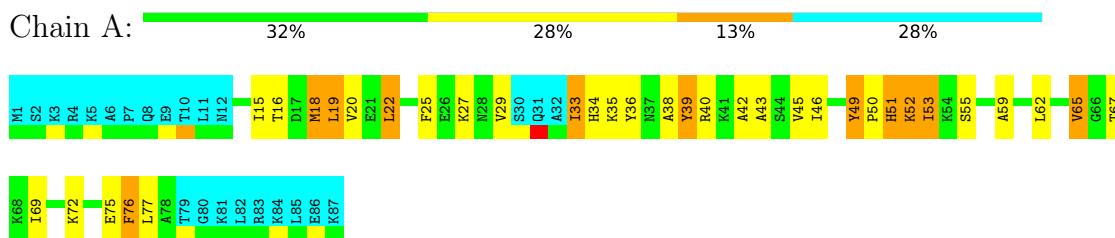
## 4.2.47 Score per residue for model 47

## • Molecule 1: DNA POLYMERASE BETA



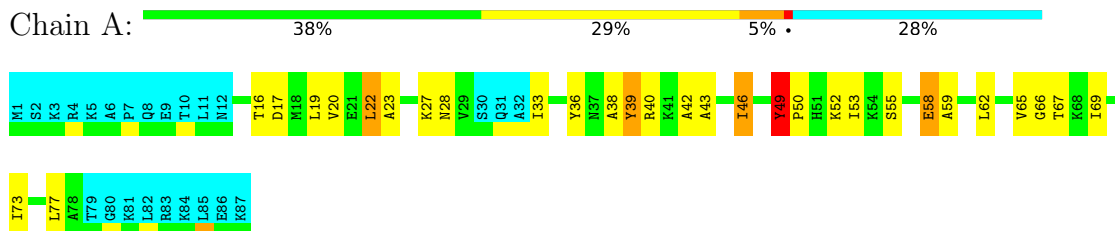
## 4.2.48 Score per residue for model 48

## • Molecule 1: DNA POLYMERASE BETA



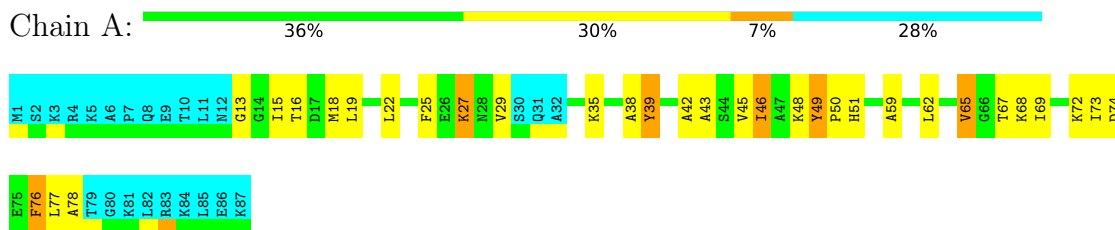
## 4.2.49 Score per residue for model 49

## • Molecule 1: DNA POLYMERASE BETA



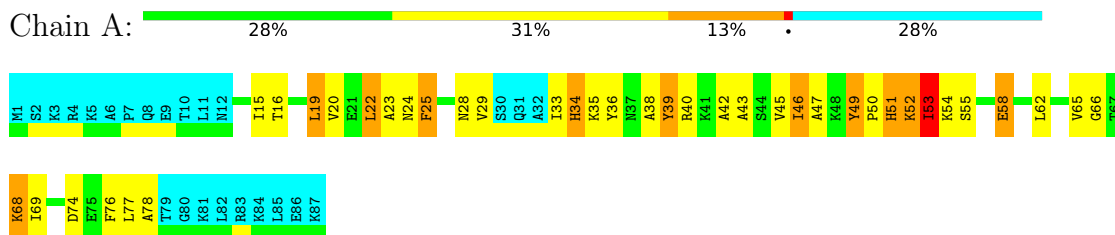
#### 4.2.50 Score per residue for model 50

- Molecule 1: DNA POLYMERASE BETA



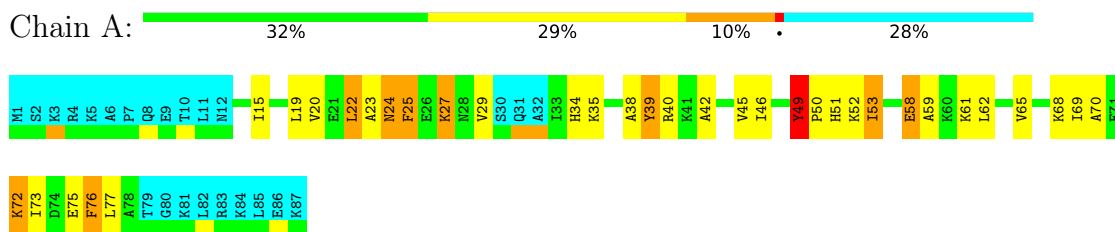
#### 4.2.51 Score per residue for model 51

- Molecule 1: DNA POLYMERASE BETA



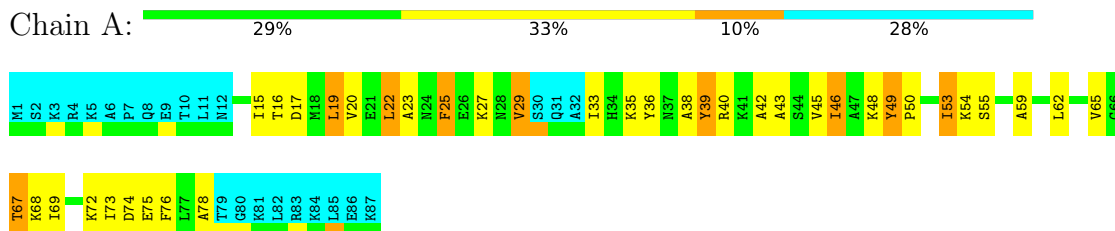
#### 4.2.52 Score per residue for model 52

- Molecule 1: DNA POLYMERASE BETA



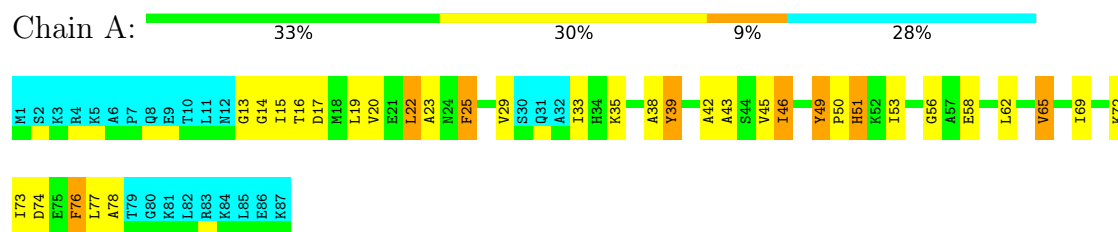
#### 4.2.53 Score per residue for model 53

- Molecule 1: DNA POLYMERASE BETA



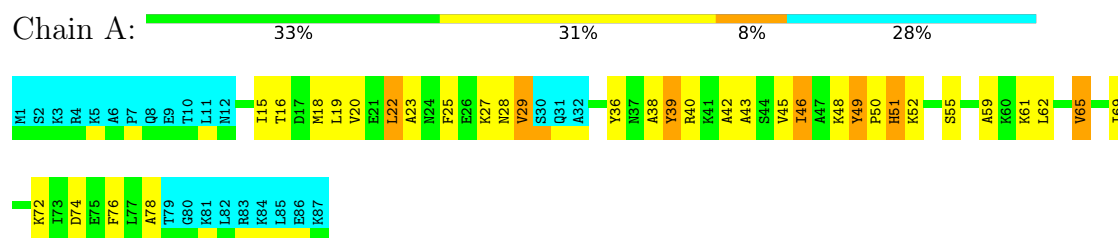
#### 4.2.54 Score per residue for model 54

- Molecule 1: DNA POLYMERASE BETA



#### 4.2.55 Score per residue for model 55

- Molecule 1: DNA POLYMERASE BETA



## 5 Refinement protocol and experimental data overview

Of the 55 calculated structures, 55 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
X-PLOR	refinement	3.1
X-PLOR	structure solution	3.1

No chemical shift data was provided.

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.02±0.01	0±0/494 ( 0.0± 0.0%)	0.85±0.01	0±0/663 ( 0.0± 0.0%)
All	All	1.02	0/27170 ( 0.0%)	0.85	2/36465 ( 0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	49	TYR	CB-CG-CD2	-5.33	117.80	121.00	52	2

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	485	511	511	35±6
All	All	26675	28105	28105	1902

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 35.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:ALA:HB1	1:A:69:ILE:HD11	1.10	1.18	53	38

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:ILE:HG21	1:A:46:ILE:HG21	1.08	1.20	16	16
1:A:42:ALA:HB2	1:A:65:VAL:HG11	1.02	1.28	22	12
1:A:22:LEU:HD21	1:A:29:VAL:HG21	0.99	1.33	18	13
1:A:22:LEU:HD13	1:A:39:TYR:CZ	0.88	2.03	41	21
1:A:49:TYR:CE2	1:A:62:LEU:HD11	0.87	2.04	18	18
1:A:22:LEU:HD21	1:A:39:TYR:CG	0.86	2.06	19	3
1:A:15:ILE:HG22	1:A:46:ILE:HD13	0.85	1.47	48	5
1:A:22:LEU:HD11	1:A:39:TYR:CG	0.85	2.07	11	11
1:A:15:ILE:CG2	1:A:46:ILE:HG21	0.85	2.02	45	20
1:A:42:ALA:HB1	1:A:65:VAL:HG13	0.84	1.49	10	28
1:A:49:TYR:CE2	1:A:53:ILE:HG21	0.83	2.09	53	3
1:A:49:TYR:CD2	1:A:62:LEU:HD11	0.82	2.09	1	7
1:A:38:ALA:HB1	1:A:69:ILE:CD1	0.82	2.03	48	21
1:A:22:LEU:HD22	1:A:39:TYR:CE2	0.82	2.08	26	26
1:A:22:LEU:HD13	1:A:23:ALA:N	0.82	1.90	17	11
1:A:46:ILE:CD1	1:A:62:LEU:HD13	0.82	2.05	11	5
1:A:42:ALA:HB2	1:A:65:VAL:CG1	0.81	2.05	22	10
1:A:16:THR:HG22	1:A:51:HIS:CE1	0.81	2.10	50	1
1:A:25:PHE:CD2	1:A:29:VAL:HG23	0.80	2.11	10	15
1:A:16:THR:OG1	1:A:47:ALA:HB2	0.79	1.78	28	29
1:A:22:LEU:CD2	1:A:29:VAL:HG21	0.79	2.07	43	18
1:A:15:ILE:CG2	1:A:46:ILE:HD12	0.79	2.07	54	7
1:A:45:VAL:HG13	1:A:46:ILE:HD12	0.78	1.56	46	2
1:A:22:LEU:O	1:A:22:LEU:HD22	0.78	1.79	11	11
1:A:22:LEU:HD13	1:A:39:TYR:CE1	0.77	2.13	43	28
1:A:49:TYR:CE2	1:A:62:LEU:HD21	0.77	2.15	15	3
1:A:19:LEU:HB3	1:A:43:ALA:HB2	0.76	1.55	21	14
1:A:15:ILE:HG22	1:A:46:ILE:HG21	0.75	1.57	17	25
1:A:45:VAL:HG21	1:A:63:PRO:HD2	0.75	1.58	24	4
1:A:51:HIS:O	1:A:53:ILE:HG23	0.75	1.82	29	2
1:A:46:ILE:HD11	1:A:65:VAL:HG21	0.75	1.58	11	7
1:A:53:ILE:HG21	1:A:58:GLU:CB	0.75	2.12	25	4
1:A:42:ALA:CB	1:A:65:VAL:HG11	0.74	2.12	6	11
1:A:16:THR:O	1:A:20:VAL:HG23	0.74	1.83	37	45
1:A:45:VAL:CG2	1:A:62:LEU:HD22	0.74	2.12	52	10
1:A:38:ALA:CB	1:A:69:ILE:HD11	0.74	2.13	54	24
1:A:22:LEU:HD23	1:A:23:ALA:N	0.74	1.96	19	3
1:A:59:ALA:HA	1:A:62:LEU:HD12	0.73	1.61	43	15
1:A:42:ALA:CB	1:A:69:ILE:HG21	0.73	2.13	16	14
1:A:22:LEU:HD11	1:A:39:TYR:CE1	0.73	2.18	20	3
1:A:39:TYR:CD1	1:A:69:ILE:HD12	0.72	2.19	54	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:ALA:HB2	1:A:73:ILE:HG21	0.72	1.59	53	4
1:A:29:VAL:HG11	1:A:36:TYR:CD1	0.72	2.19	10	3
1:A:22:LEU:HD23	1:A:22:LEU:O	0.72	1.84	44	27
1:A:22:LEU:HD12	1:A:39:TYR:CD2	0.72	2.19	48	7
1:A:15:ILE:HD13	1:A:51:HIS:CD2	0.72	2.20	17	1
1:A:15:ILE:HG21	1:A:46:ILE:CG2	0.71	2.13	53	5
1:A:33:ILE:HG22	1:A:36:TYR:HB2	0.71	1.61	21	1
1:A:46:ILE:HG22	1:A:51:HIS:HB3	0.71	1.63	19	4
1:A:22:LEU:HD12	1:A:39:TYR:CE2	0.71	2.20	36	12
1:A:53:ILE:O	1:A:77:LEU:HD22	0.70	1.87	15	4
1:A:19:LEU:CB	1:A:43:ALA:HB2	0.70	2.16	46	5
1:A:19:LEU:HD11	1:A:73:ILE:CD1	0.70	2.16	33	3
1:A:42:ALA:CB	1:A:65:VAL:HG13	0.70	2.17	40	21
1:A:15:ILE:HD13	1:A:51:HIS:CG	0.70	2.21	17	2
1:A:53:ILE:O	1:A:77:LEU:HD12	0.70	1.86	1	2
1:A:53:ILE:O	1:A:77:LEU:HD13	0.69	1.87	26	8
1:A:42:ALA:HA	1:A:65:VAL:HG11	0.69	1.64	42	10
1:A:52:LYS:O	1:A:53:ILE:HD13	0.69	1.87	33	1
1:A:53:ILE:HD12	1:A:55:SER:O	0.69	1.87	40	8
1:A:19:LEU:HD22	1:A:43:ALA:HB2	0.69	1.63	20	7
1:A:15:ILE:HD12	1:A:51:HIS:HA	0.69	1.65	1	21
1:A:42:ALA:CA	1:A:65:VAL:HG11	0.69	2.18	42	10
1:A:22:LEU:HD21	1:A:39:TYR:CD2	0.69	2.23	19	3
1:A:49:TYR:CZ	1:A:62:LEU:HD21	0.68	2.23	48	12
1:A:42:ALA:HA	1:A:65:VAL:HG22	0.68	1.65	46	10
1:A:49:TYR:CE1	1:A:62:LEU:HD21	0.68	2.23	48	5
1:A:38:ALA:HB1	1:A:69:ILE:CG1	0.68	2.17	28	12
1:A:15:ILE:HG22	1:A:46:ILE:HD12	0.68	1.64	5	4
1:A:29:VAL:HG13	1:A:36:TYR:HB2	0.67	1.66	28	5
1:A:33:ILE:HG21	1:A:36:TYR:HB2	0.67	1.66	31	3
1:A:15:ILE:HG12	1:A:73:ILE:HG23	0.67	1.65	46	4
1:A:42:ALA:O	1:A:45:VAL:HG12	0.66	1.90	12	13
1:A:20:VAL:HG23	1:A:43:ALA:HB1	0.66	1.66	46	2
1:A:42:ALA:O	1:A:46:ILE:HD13	0.66	1.90	25	6
1:A:45:VAL:HG21	1:A:62:LEU:HB3	0.66	1.67	7	8
1:A:22:LEU:HD21	1:A:39:TYR:CB	0.66	2.21	16	3
1:A:23:ALA:HB2	1:A:39:TYR:HB2	0.66	1.68	17	2
1:A:46:ILE:HG22	1:A:51:HIS:CB	0.65	2.21	19	1
1:A:13:GLY:HA2	1:A:77:LEU:HD11	0.65	1.69	50	1
1:A:29:VAL:HG12	1:A:36:TYR:CD1	0.65	2.27	44	12
1:A:29:VAL:O	1:A:33:ILE:HG23	0.65	1.90	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:ILE:CB	1:A:46:ILE:HG21	0.65	2.21	29	3
1:A:16:THR:CB	1:A:47:ALA:HB2	0.64	2.22	40	15
1:A:15:ILE:HD13	1:A:51:HIS:HB2	0.64	1.69	17	1
1:A:29:VAL:HG12	1:A:36:TYR:CD2	0.64	2.28	11	8
1:A:45:VAL:HG22	1:A:62:LEU:HD22	0.64	1.68	13	10
1:A:22:LEU:HD22	1:A:39:TYR:CD2	0.64	2.28	28	10
1:A:29:VAL:HA	1:A:33:ILE:HD12	0.64	1.70	4	4
1:A:15:ILE:HD11	1:A:51:HIS:C	0.64	2.13	7	1
1:A:19:LEU:HB2	1:A:43:ALA:HB2	0.64	1.68	46	1
1:A:19:LEU:O	1:A:19:LEU:HD23	0.63	1.93	55	3
1:A:19:LEU:HD11	1:A:42:ALA:CB	0.63	2.24	20	1
1:A:49:TYR:CG	1:A:62:LEU:HD21	0.63	2.27	11	5
1:A:15:ILE:CG2	1:A:46:ILE:HD13	0.63	2.21	48	4
1:A:19:LEU:O	1:A:19:LEU:HD13	0.63	1.93	53	1
1:A:59:ALA:HB1	1:A:65:VAL:O	0.63	1.94	8	1
1:A:33:ILE:HG23	1:A:36:TYR:HB3	0.63	1.70	41	9
1:A:15:ILE:HD11	1:A:53:ILE:CD1	0.62	2.24	2	2
1:A:52:LYS:O	1:A:77:LEU:HD11	0.62	1.94	32	1
1:A:22:LEU:HD11	1:A:39:TYR:CZ	0.62	2.28	19	3
1:A:19:LEU:HD11	1:A:73:ILE:HD11	0.62	1.70	27	7
1:A:22:LEU:HD11	1:A:39:TYR:CD1	0.62	2.30	53	10
1:A:46:ILE:HG23	1:A:62:LEU:HD11	0.62	1.71	24	1
1:A:16:THR:HG22	1:A:51:HIS:NE2	0.61	2.10	5	2
1:A:49:TYR:CE1	1:A:62:LEU:HD11	0.61	2.30	16	1
1:A:53:ILE:HD11	1:A:56:GLY:HA2	0.61	1.72	35	1
1:A:46:ILE:HG23	1:A:62:LEU:CD1	0.61	2.26	5	2
1:A:19:LEU:CD1	1:A:73:ILE:HD11	0.61	2.25	18	1
1:A:22:LEU:HD11	1:A:39:TYR:CD2	0.61	2.30	54	5
1:A:15:ILE:HD12	1:A:15:ILE:N	0.61	2.10	32	4
1:A:19:LEU:HD23	1:A:43:ALA:HB2	0.61	1.73	23	3
1:A:53:ILE:HD13	1:A:58:GLU:HB2	0.61	1.72	40	4
1:A:52:LYS:HG2	1:A:77:LEU:HD21	0.61	1.70	17	1
1:A:45:VAL:HG13	1:A:46:ILE:HD13	0.60	1.72	53	1
1:A:42:ALA:HB3	1:A:69:ILE:HG21	0.60	1.74	38	3
1:A:15:ILE:HD13	1:A:51:HIS:CB	0.60	2.25	17	1
1:A:33:ILE:HD12	1:A:33:ILE:N	0.60	2.12	32	4
1:A:33:ILE:N	1:A:33:ILE:HD13	0.60	2.11	21	2
1:A:33:ILE:HG22	1:A:36:TYR:CB	0.60	2.26	21	1
1:A:53:ILE:HG23	1:A:58:GLU:OE1	0.60	1.96	51	2
1:A:38:ALA:HB1	1:A:69:ILE:HG13	0.60	1.72	28	4
1:A:74:ASP:O	1:A:78:ALA:HB2	0.60	1.97	43	32

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:ILE:N	1:A:53:ILE:HD13	0.60	2.11	25	3
1:A:15:ILE:HG21	1:A:46:ILE:HD12	0.60	1.73	13	9
1:A:49:TYR:CD2	1:A:62:LEU:HD21	0.60	2.32	11	4
1:A:59:ALA:HB3	1:A:70:ALA:HB2	0.60	1.74	25	1
1:A:23:ALA:HB1	1:A:36:TYR:CE1	0.60	2.30	27	2
1:A:66:GLY:HA2	1:A:70:ALA:HB2	0.60	1.72	31	3
1:A:15:ILE:HD13	1:A:51:HIS:HB3	0.60	1.72	32	2
1:A:22:LEU:HD13	1:A:39:TYR:CE2	0.60	2.31	29	7
1:A:74:ASP:O	1:A:78:ALA:HB3	0.59	1.97	22	2
1:A:13:GLY:HA2	1:A:77:LEU:HD21	0.59	1.73	30	1
1:A:33:ILE:HG23	1:A:36:TYR:CB	0.59	2.28	11	5
1:A:23:ALA:HA	1:A:29:VAL:HG11	0.59	1.73	36	2
1:A:29:VAL:HG12	1:A:29:VAL:O	0.59	1.97	46	15
1:A:45:VAL:HG11	1:A:65:VAL:CG2	0.59	2.28	20	3
1:A:45:VAL:CG1	1:A:62:LEU:HD13	0.59	2.26	25	1
1:A:52:LYS:O	1:A:53:ILE:HG22	0.59	1.97	51	1
1:A:46:ILE:HD13	1:A:62:LEU:HD13	0.59	1.73	45	4
1:A:53:ILE:HD11	1:A:58:GLU:CB	0.59	2.27	21	1
1:A:33:ILE:HG21	1:A:36:TYR:CB	0.58	2.28	31	3
1:A:19:LEU:HD12	1:A:43:ALA:HB2	0.58	1.76	28	6
1:A:53:ILE:HG21	1:A:58:GLU:HB2	0.58	1.76	54	3
1:A:65:VAL:CG1	1:A:73:ILE:HD12	0.58	2.29	18	1
1:A:22:LEU:HD13	1:A:22:LEU:C	0.57	2.19	12	9
1:A:22:LEU:C	1:A:22:LEU:HD13	0.57	2.19	31	2
1:A:49:TYR:CG	1:A:50:PRO:HD2	0.57	2.34	50	32
1:A:53:ILE:HD13	1:A:58:GLU:CG	0.57	2.29	17	1
1:A:58:GLU:OE2	1:A:73:ILE:HG21	0.57	1.98	52	1
1:A:53:ILE:HG13	1:A:77:LEU:HD13	0.57	1.74	9	4
1:A:45:VAL:CG2	1:A:62:LEU:HD13	0.57	2.30	52	1
1:A:22:LEU:HD22	1:A:22:LEU:C	0.57	2.20	54	11
1:A:65:VAL:HG11	1:A:73:ILE:CD1	0.57	2.30	10	4
1:A:45:VAL:HG11	1:A:63:PRO:O	0.57	1.98	19	1
1:A:29:VAL:HG13	1:A:39:TYR:CE2	0.57	2.34	53	1
1:A:35:LYS:O	1:A:38:ALA:HB3	0.56	1.99	41	13
1:A:49:TYR:CD2	1:A:53:ILE:HD11	0.56	2.36	32	2
1:A:65:VAL:HG11	1:A:73:ILE:HD11	0.56	1.77	3	2
1:A:49:TYR:CD1	1:A:50:PRO:HD2	0.56	2.36	25	47
1:A:15:ILE:HG23	1:A:73:ILE:HG23	0.56	1.76	40	4
1:A:53:ILE:HD13	1:A:53:ILE:H	0.56	1.61	11	2
1:A:19:LEU:HD11	1:A:42:ALA:HB1	0.56	1.77	20	1
1:A:15:ILE:HD12	1:A:15:ILE:H	0.55	1.61	17	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:LEU:CD2	1:A:29:VAL:HG11	0.55	2.30	47	2
1:A:46:ILE:HD13	1:A:73:ILE:HD12	0.55	1.77	36	2
1:A:49:TYR:CE2	1:A:53:ILE:HD11	0.55	2.35	43	1
1:A:77:LEU:N	1:A:77:LEU:HD22	0.55	2.16	22	21
1:A:42:ALA:HB1	1:A:65:VAL:CG1	0.55	2.31	8	2
1:A:42:ALA:CB	1:A:65:VAL:HG22	0.55	2.31	8	1
1:A:20:VAL:HG22	1:A:43:ALA:HB1	0.55	1.78	49	1
1:A:53:ILE:HG22	1:A:58:GLU:CB	0.55	2.31	37	1
1:A:52:LYS:O	1:A:77:LEU:HD21	0.55	2.01	51	2
1:A:15:ILE:HD12	1:A:51:HIS:C	0.55	2.23	40	3
1:A:45:VAL:HG11	1:A:65:VAL:HG22	0.55	1.77	20	1
1:A:16:THR:HG22	1:A:51:HIS:CD2	0.55	2.36	5	2
1:A:15:ILE:HD12	1:A:51:HIS:CA	0.55	2.32	4	10
1:A:15:ILE:HG22	1:A:46:ILE:CG2	0.55	2.32	55	7
1:A:15:ILE:HD12	1:A:51:HIS:HB2	0.55	1.78	27	4
1:A:53:ILE:HD12	1:A:58:GLU:HB3	0.55	1.77	43	1
1:A:52:LYS:HG3	1:A:77:LEU:HD13	0.54	1.78	29	1
1:A:53:ILE:HD12	1:A:58:GLU:HB2	0.54	1.79	29	1
1:A:42:ALA:HA	1:A:65:VAL:HG21	0.54	1.78	6	4
1:A:22:LEU:HD22	1:A:29:VAL:HG21	0.54	1.76	43	1
1:A:22:LEU:HD12	1:A:39:TYR:CG	0.54	2.38	48	1
1:A:52:LYS:CD	1:A:77:LEU:HD11	0.54	2.33	7	1
1:A:52:LYS:HA	1:A:77:LEU:HD21	0.54	1.79	35	1
1:A:19:LEU:CG	1:A:43:ALA:HB2	0.54	2.33	53	1
1:A:45:VAL:HG21	1:A:62:LEU:HD22	0.54	1.80	32	3
1:A:19:LEU:HD21	1:A:73:ILE:HD11	0.54	1.79	40	1
1:A:42:ALA:HB2	1:A:69:ILE:HG21	0.54	1.80	20	3
1:A:19:LEU:HD21	1:A:42:ALA:HB3	0.54	1.79	17	3
1:A:49:TYR:CD2	1:A:62:LEU:HD22	0.54	2.38	26	1
1:A:22:LEU:HD13	1:A:39:TYR:CD1	0.53	2.38	37	7
1:A:19:LEU:HD12	1:A:39:TYR:O	0.53	2.03	28	1
1:A:66:GLY:O	1:A:67:THR:HG23	0.53	2.04	28	2
1:A:38:ALA:HB1	1:A:69:ILE:HG12	0.53	1.79	2	2
1:A:19:LEU:HD21	1:A:42:ALA:CB	0.53	2.33	18	1
1:A:15:ILE:O	1:A:19:LEU:HD13	0.53	2.03	26	4
1:A:52:LYS:CG	1:A:77:LEU:HD13	0.53	2.34	29	1
1:A:50:PRO:O	1:A:51:HIS:O	0.53	2.27	17	1
1:A:46:ILE:HD13	1:A:62:LEU:HD12	0.53	1.81	39	1
1:A:46:ILE:CD1	1:A:65:VAL:HG21	0.53	2.34	27	2
1:A:19:LEU:HD23	1:A:43:ALA:CA	0.53	2.34	17	2
1:A:16:THR:HG22	1:A:51:HIS:ND1	0.52	2.18	50	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:ILE:HD11	1:A:53:ILE:HG23	0.52	1.80	45	1
1:A:41:LYS:O	1:A:45:VAL:HG12	0.52	2.05	22	2
1:A:39:TYR:HD1	1:A:69:ILE:HD11	0.52	1.65	24	1
1:A:45:VAL:HG11	1:A:65:VAL:HG23	0.52	1.82	15	1
1:A:66:GLY:O	1:A:70:ALA:HB2	0.52	2.05	23	1
1:A:49:TYR:HE2	1:A:53:ILE:HD13	0.52	1.65	29	1
1:A:65:VAL:HG11	1:A:73:ILE:HD12	0.52	1.81	18	2
1:A:23:ALA:HB1	1:A:36:TYR:HE1	0.52	1.64	27	1
1:A:19:LEU:HD23	1:A:43:ALA:N	0.51	2.19	45	4
1:A:19:LEU:HD13	1:A:43:ALA:N	0.51	2.20	5	1
1:A:77:LEU:N	1:A:77:LEU:CD2	0.51	2.74	7	21
1:A:29:VAL:O	1:A:33:ILE:HD12	0.51	2.06	3	1
1:A:45:VAL:HG13	1:A:62:LEU:HD13	0.51	1.81	25	1
1:A:19:LEU:HD11	1:A:39:TYR:HB3	0.51	1.81	53	1
1:A:22:LEU:CD1	1:A:39:TYR:CE2	0.51	2.94	30	12
1:A:49:TYR:CD2	1:A:50:PRO:HD2	0.51	2.41	24	6
1:A:45:VAL:CG1	1:A:65:VAL:HG22	0.51	2.36	20	1
1:A:50:PRO:O	1:A:51:HIS:CG	0.51	2.64	27	21
1:A:53:ILE:HG21	1:A:58:GLU:CG	0.51	2.36	52	1
1:A:50:PRO:O	1:A:51:HIS:CD2	0.51	2.64	17	10
1:A:19:LEU:HD11	1:A:73:ILE:HG12	0.51	1.82	21	2
1:A:45:VAL:HG22	1:A:45:VAL:O	0.51	2.06	32	12
1:A:53:ILE:HD11	1:A:73:ILE:CG2	0.51	2.35	11	1
1:A:15:ILE:HD11	1:A:52:LYS:N	0.50	2.21	8	2
1:A:65:VAL:HG13	1:A:69:ILE:CG2	0.50	2.37	24	1
1:A:15:ILE:HD12	1:A:51:HIS:CB	0.50	2.36	27	1
1:A:53:ILE:HD12	1:A:58:GLU:CB	0.50	2.37	43	2
1:A:53:ILE:N	1:A:77:LEU:HD13	0.50	2.21	33	1
1:A:49:TYR:CD1	1:A:50:PRO:CD	0.50	2.95	2	20
1:A:25:PHE:HD2	1:A:29:VAL:HG23	0.50	1.65	10	1
1:A:19:LEU:HD13	1:A:73:ILE:HD11	0.50	1.83	52	2
1:A:19:LEU:HD21	1:A:69:ILE:HG21	0.50	1.84	22	1
1:A:45:VAL:HG21	1:A:63:PRO:CD	0.50	2.35	24	2
1:A:29:VAL:HG12	1:A:36:TYR:HD2	0.50	1.67	32	9
1:A:19:LEU:HD13	1:A:42:ALA:HB3	0.50	1.84	29	1
1:A:19:LEU:HD22	1:A:69:ILE:CG2	0.50	2.37	10	1
1:A:19:LEU:CD2	1:A:46:ILE:HD11	0.49	2.37	24	1
1:A:20:VAL:CG2	1:A:43:ALA:HB1	0.49	2.37	49	1
1:A:46:ILE:HD13	1:A:73:ILE:HD13	0.49	1.83	17	1
1:A:19:LEU:HG	1:A:43:ALA:HB2	0.49	1.85	53	1
1:A:53:ILE:HD12	1:A:56:GLY:HA2	0.49	1.83	54	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:ALA:CB	1:A:73:ILE:HG21	0.49	2.38	35	1
1:A:41:LYS:C	1:A:65:VAL:HG21	0.49	2.28	6	1
1:A:22:LEU:CD1	1:A:29:VAL:HG21	0.48	2.37	2	1
1:A:15:ILE:CG2	1:A:46:ILE:HG23	0.48	2.38	35	1
1:A:46:ILE:CD1	1:A:73:ILE:HD12	0.48	2.37	36	2
1:A:19:LEU:HD11	1:A:39:TYR:O	0.48	2.08	42	1
1:A:52:LYS:O	1:A:53:ILE:O	0.48	2.32	51	2
1:A:22:LEU:HD23	1:A:22:LEU:C	0.48	2.28	44	6
1:A:45:VAL:CG1	1:A:65:VAL:HG21	0.48	2.38	24	1
1:A:46:ILE:CD1	1:A:73:ILE:HD11	0.48	2.38	7	1
1:A:62:LEU:CD1	1:A:65:VAL:HG21	0.48	2.38	40	1
1:A:53:ILE:HG21	1:A:58:GLU:HG2	0.48	1.85	52	1
1:A:53:ILE:HD13	1:A:54:LYS:N	0.48	2.24	51	1
1:A:46:ILE:HG22	1:A:49:TYR:HE1	0.48	1.69	24	1
1:A:45:VAL:HG22	1:A:62:LEU:HD13	0.48	1.86	52	1
1:A:45:VAL:CG1	1:A:65:VAL:HG23	0.47	2.39	23	2
1:A:42:ALA:HB1	1:A:65:VAL:HG22	0.47	1.86	9	1
1:A:49:TYR:CZ	1:A:53:ILE:HD13	0.47	2.44	18	1
1:A:62:LEU:HD13	1:A:65:VAL:HG21	0.47	1.85	40	1
1:A:15:ILE:CD1	1:A:51:HIS:CD2	0.47	2.95	17	1
1:A:52:LYS:CG	1:A:77:LEU:HD21	0.47	2.39	17	1
1:A:53:ILE:HD11	1:A:58:GLU:HB2	0.47	1.86	21	1
1:A:16:THR:HG23	1:A:17:ASP:OD1	0.47	2.10	24	1
1:A:29:VAL:CG1	1:A:36:TYR:CD1	0.47	2.98	36	7
1:A:19:LEU:HD23	1:A:43:ALA:CB	0.47	2.39	15	1
1:A:15:ILE:HG22	1:A:19:LEU:HD12	0.47	1.87	29	1
1:A:42:ALA:HB2	1:A:65:VAL:HG13	0.47	1.85	46	5
1:A:52:LYS:O	1:A:53:ILE:CG1	0.46	2.63	7	4
1:A:49:TYR:CZ	1:A:53:ILE:CD1	0.46	2.98	18	1
1:A:39:TYR:CD1	1:A:69:ILE:HD11	0.46	2.45	24	1
1:A:19:LEU:HD12	1:A:46:ILE:CD1	0.46	2.39	5	1
1:A:72:LYS:O	1:A:76:PHE:CZ	0.46	2.68	22	6
1:A:53:ILE:HD13	1:A:58:GLU:CB	0.46	2.40	7	1
1:A:19:LEU:HD13	1:A:43:ALA:CA	0.46	2.39	37	2
1:A:46:ILE:HD12	1:A:65:VAL:HG21	0.46	1.87	37	1
1:A:39:TYR:O	1:A:43:ALA:HB3	0.46	2.10	9	1
1:A:49:TYR:CE2	1:A:62:LEU:CD1	0.46	2.99	26	1
1:A:20:VAL:HG12	1:A:24:ASN:OD1	0.46	2.10	52	1
1:A:18:MET:CB	1:A:76:PHE:CD1	0.46	2.99	55	1
1:A:18:MET:CB	1:A:76:PHE:CZ	0.46	2.99	8	5
1:A:76:PHE:CD1	1:A:76:PHE:N	0.46	2.84	54	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:ALA:HB3	1:A:70:ALA:HB1	0.46	1.88	12	1
1:A:52:LYS:HG3	1:A:77:LEU:HD22	0.46	1.87	29	1
1:A:38:ALA:O	1:A:69:ILE:HD13	0.46	2.11	33	1
1:A:19:LEU:HD11	1:A:42:ALA:HB3	0.46	1.86	22	2
1:A:15:ILE:HG21	1:A:46:ILE:CG1	0.46	2.41	29	1
1:A:53:ILE:H	1:A:77:LEU:HD13	0.46	1.71	33	1
1:A:65:VAL:HG13	1:A:69:ILE:HG21	0.45	1.87	24	1
1:A:46:ILE:HG23	1:A:49:TYR:HE1	0.45	1.71	28	1
1:A:29:VAL:HG11	1:A:39:TYR:CE2	0.45	2.45	35	1
1:A:20:VAL:HG23	1:A:43:ALA:CB	0.45	2.38	46	1
1:A:19:LEU:CD1	1:A:43:ALA:HB2	0.45	2.41	53	1
1:A:18:MET:CB	1:A:76:PHE:CE1	0.45	3.00	48	4
1:A:67:THR:HG22	1:A:67:THR:O	0.45	2.12	12	1
1:A:33:ILE:CG2	1:A:36:TYR:CB	0.45	2.94	31	4
1:A:33:ILE:HG22	1:A:34:HIS:N	0.45	2.26	1	1
1:A:34:HIS:CG	1:A:35:LYS:N	0.45	2.85	8	1
1:A:53:ILE:HD13	1:A:58:GLU:HB3	0.45	1.88	49	1
1:A:53:ILE:HG13	1:A:73:ILE:HG21	0.45	1.86	12	1
1:A:19:LEU:HD11	1:A:39:TYR:HA	0.45	1.87	14	1
1:A:19:LEU:HD13	1:A:42:ALA:CB	0.45	2.42	29	1
1:A:49:TYR:CD2	1:A:53:ILE:HG21	0.45	2.44	53	1
1:A:34:HIS:CD2	1:A:35:LYS:N	0.45	2.85	8	3
1:A:33:ILE:HG23	1:A:36:TYR:HB2	0.45	1.89	11	2
1:A:42:ALA:CA	1:A:65:VAL:HG22	0.45	2.41	8	2
1:A:59:ALA:HB1	1:A:73:ILE:HG13	0.45	1.88	14	1
1:A:15:ILE:CD1	1:A:51:HIS:HB2	0.45	2.41	17	1
1:A:53:ILE:HD11	1:A:59:ALA:N	0.45	2.27	21	1
1:A:59:ALA:HB3	1:A:70:ALA:CB	0.45	2.42	25	1
1:A:39:TYR:CD1	1:A:69:ILE:CD1	0.45	3.00	7	4
1:A:49:TYR:CD2	1:A:62:LEU:CD2	0.45	3.00	26	1
1:A:42:ALA:CA	1:A:65:VAL:HG21	0.44	2.41	6	1
1:A:52:LYS:O	1:A:53:ILE:CG2	0.44	2.65	51	1
1:A:15:ILE:CG2	1:A:46:ILE:CD1	0.44	2.93	50	3
1:A:19:LEU:C	1:A:19:LEU:HD13	0.44	2.33	42	1
1:A:25:PHE:CG	1:A:29:VAL:HG23	0.44	2.47	26	1
1:A:15:ILE:HG21	1:A:46:ILE:CB	0.44	2.43	29	1
1:A:65:VAL:HG12	1:A:69:ILE:CD1	0.44	2.43	29	1
1:A:15:ILE:HG23	1:A:73:ILE:HG12	0.44	1.88	41	1
1:A:53:ILE:HG22	1:A:58:GLU:CD	0.44	2.34	4	1
1:A:15:ILE:CG2	1:A:46:ILE:CG2	0.44	2.95	33	13
1:A:69:ILE:HG22	1:A:69:ILE:O	0.44	2.13	22	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:ILE:HD12	1:A:52:LYS:H	0.44	1.73	24	2
1:A:22:LEU:CD1	1:A:39:TYR:CG	0.43	2.96	53	6
1:A:53:ILE:HG21	1:A:58:GLU:HB3	0.43	1.88	27	1
1:A:46:ILE:HG23	1:A:62:LEU:HD13	0.43	1.90	50	1
1:A:52:LYS:HD3	1:A:77:LEU:HD22	0.43	1.90	3	1
1:A:25:PHE:CB	1:A:29:VAL:HG23	0.43	2.43	21	3
1:A:59:ALA:CB	1:A:70:ALA:HB1	0.43	2.43	21	2
1:A:46:ILE:HG22	1:A:49:TYR:CE1	0.43	2.49	24	1
1:A:51:HIS:CD2	1:A:52:LYS:N	0.43	2.86	24	1
1:A:45:VAL:HG13	1:A:46:ILE:N	0.43	2.28	29	2
1:A:15:ILE:HG21	1:A:46:ILE:HG12	0.43	1.90	37	1
1:A:57:ALA:HB1	1:A:60:LYS:HE3	0.43	1.90	44	1
1:A:19:LEU:CD1	1:A:46:ILE:HD11	0.43	2.43	5	1
1:A:46:ILE:HD13	1:A:73:ILE:CD1	0.43	2.44	17	2
1:A:15:ILE:N	1:A:15:ILE:CD1	0.43	2.81	32	1
1:A:50:PRO:O	1:A:51:HIS:CB	0.43	2.65	29	12
1:A:49:TYR:O	1:A:51:HIS:CD2	0.43	2.71	40	3
1:A:53:ILE:HD11	1:A:73:ILE:HG22	0.43	1.90	11	1
1:A:42:ALA:CB	1:A:65:VAL:CG1	0.43	2.96	35	2
1:A:67:THR:O	1:A:68:LYS:CB	0.43	2.67	32	3
1:A:50:PRO:O	1:A:51:HIS:HB3	0.43	2.14	50	1
1:A:49:TYR:CE2	1:A:62:LEU:CD2	0.43	2.98	4	1
1:A:62:LEU:HD23	1:A:62:LEU:N	0.43	2.27	8	1
1:A:33:ILE:N	1:A:33:ILE:CD1	0.43	2.81	32	2
1:A:14:GLY:O	1:A:76:PHE:CE2	0.43	2.71	2	1
1:A:66:GLY:O	1:A:70:ALA:HB3	0.43	2.14	10	1
1:A:22:LEU:HD11	1:A:39:TYR:CB	0.43	2.44	11	1
1:A:22:LEU:CD1	1:A:39:TYR:CZ	0.43	3.00	1	2
1:A:29:VAL:HG12	1:A:36:TYR:HB2	0.43	1.91	29	1
1:A:35:LYS:O	1:A:39:TYR:CE2	0.43	2.72	50	22
1:A:36:TYR:CD1	1:A:36:TYR:O	0.43	2.72	30	6
1:A:46:ILE:HG22	1:A:47:ALA:N	0.43	2.28	14	2
1:A:46:ILE:HD12	1:A:62:LEU:HD13	0.43	1.91	21	1
1:A:39:TYR:CE1	1:A:69:ILE:CD1	0.43	3.02	47	1
1:A:72:LYS:O	1:A:76:PHE:CE1	0.42	2.72	39	20
1:A:46:ILE:CD1	1:A:73:ILE:HD13	0.42	2.44	17	2
1:A:19:LEU:HD23	1:A:19:LEU:C	0.42	2.34	31	1
1:A:33:ILE:CG1	1:A:36:TYR:HB2	0.42	2.43	35	1
1:A:22:LEU:O	1:A:22:LEU:HD13	0.42	2.14	13	5
1:A:66:GLY:HA3	1:A:69:ILE:HD12	0.42	1.91	29	1
1:A:29:VAL:HG11	1:A:36:TYR:HD1	0.42	1.75	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:LEU:HD13	1:A:73:ILE:CD1	0.42	2.44	52	1
1:A:67:THR:HG23	1:A:68:LYS:N	0.42	2.30	14	1
1:A:25:PHE:O	1:A:26:GLU:CB	0.42	2.67	47	4
1:A:47:ALA:O	1:A:51:HIS:CE1	0.42	2.72	44	3
1:A:22:LEU:O	1:A:25:PHE:CD1	0.42	2.73	31	4
1:A:53:ILE:HG22	1:A:55:SER:O	0.42	2.15	30	1
1:A:53:ILE:HG23	1:A:58:GLU:CB	0.42	2.45	30	1
1:A:50:PRO:C	1:A:51:HIS:CG	0.42	2.92	40	3
1:A:15:ILE:CD1	1:A:46:ILE:HG21	0.42	2.44	21	1
1:A:29:VAL:O	1:A:29:VAL:CG1	0.42	2.68	46	1
1:A:25:PHE:CB	1:A:29:VAL:CG2	0.42	2.98	37	3
1:A:15:ILE:HD12	1:A:52:LYS:N	0.42	2.29	24	3
1:A:46:ILE:CD1	1:A:62:LEU:CD1	0.42	2.98	15	2
1:A:46:ILE:HG23	1:A:51:HIS:HA	0.42	1.92	29	2
1:A:53:ILE:HG22	1:A:54:LYS:N	0.42	2.29	32	1
1:A:46:ILE:O	1:A:51:HIS:CD2	0.42	2.72	26	2
1:A:19:LEU:HD11	1:A:73:ILE:HD13	0.42	1.90	33	1
1:A:16:THR:HB	1:A:47:ALA:HB2	0.42	1.91	40	1
1:A:53:ILE:H	1:A:53:ILE:HD13	0.42	1.74	48	1
1:A:50:PRO:O	1:A:51:HIS:HB2	0.42	2.15	32	1
1:A:51:HIS:O	1:A:52:LYS:CB	0.41	2.66	17	1
1:A:46:ILE:HG23	1:A:49:TYR:CE1	0.41	2.50	28	1
1:A:33:ILE:HD12	1:A:33:ILE:H	0.41	1.74	40	1
1:A:29:VAL:HG13	1:A:36:TYR:HA	0.41	1.92	46	1
1:A:53:ILE:HG23	1:A:58:GLU:HB2	0.41	1.91	30	1
1:A:19:LEU:HD23	1:A:42:ALA:HB3	0.41	1.92	32	1
1:A:22:LEU:CD2	1:A:39:TYR:CE2	0.41	3.00	34	1
1:A:22:LEU:HG	1:A:39:TYR:CD1	0.41	2.50	13	1
1:A:34:HIS:ND1	1:A:34:HIS:N	0.41	2.68	14	3
1:A:33:ILE:HB	1:A:36:TYR:CB	0.41	2.46	43	2
1:A:25:PHE:O	1:A:26:GLU:CG	0.41	2.69	28	1
1:A:19:LEU:CD1	1:A:46:ILE:CD1	0.41	2.99	2	1
1:A:33:ILE:O	1:A:34:HIS:CB	0.41	2.68	8	1
1:A:18:MET:HB2	1:A:76:PHE:CE2	0.41	2.51	14	1
1:A:20:VAL:HG12	1:A:24:ASN:ND2	0.41	2.30	23	1
1:A:14:GLY:O	1:A:76:PHE:CD2	0.41	2.74	54	2
1:A:49:TYR:O	1:A:51:HIS:CE1	0.41	2.74	36	1
1:A:18:MET:HB2	1:A:76:PHE:CZ	0.41	2.51	26	2
1:A:46:ILE:HD11	1:A:73:ILE:CD1	0.41	2.45	7	1
1:A:22:LEU:CD1	1:A:39:TYR:CB	0.41	2.98	11	1
1:A:46:ILE:CG2	1:A:47:ALA:N	0.41	2.84	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ALA:O	1:A:36:TYR:CZ	0.41	2.74	39	2
1:A:20:VAL:O	1:A:20:VAL:HG12	0.41	2.16	19	1
1:A:19:LEU:HD22	1:A:46:ILE:HG13	0.41	1.92	33	1
1:A:19:LEU:HD21	1:A:46:ILE:HD11	0.41	1.93	24	1
1:A:18:MET:CB	1:A:76:PHE:CG	0.41	3.04	37	1
1:A:45:VAL:HG13	1:A:65:VAL:HG23	0.41	1.92	37	1
1:A:39:TYR:CD1	1:A:39:TYR:N	0.41	2.89	36	1
1:A:35:LYS:O	1:A:39:TYR:CZ	0.41	2.73	52	2
1:A:15:ILE:HD11	1:A:53:ILE:HD13	0.41	1.93	2	1
1:A:19:LEU:CD1	1:A:46:ILE:HD12	0.41	2.46	31	2
1:A:29:VAL:O	1:A:33:ILE:HD13	0.41	2.16	2	2
1:A:46:ILE:CD1	1:A:73:ILE:CD1	0.41	2.99	54	3
1:A:52:LYS:HD2	1:A:77:LEU:HD11	0.41	1.92	7	1
1:A:19:LEU:CD2	1:A:69:ILE:CG2	0.41	2.99	10	1
1:A:25:PHE:CD2	1:A:28:ASN:HB2	0.41	2.51	10	1
1:A:22:LEU:O	1:A:25:PHE:CG	0.41	2.74	19	1
1:A:18:MET:HB3	1:A:76:PHE:CE1	0.41	2.51	28	1
1:A:18:MET:HB3	1:A:76:PHE:CZ	0.41	2.51	33	1
1:A:47:ALA:C	1:A:51:HIS:HE2	0.41	2.18	41	1
1:A:15:ILE:CD1	1:A:53:ILE:HG23	0.41	2.46	45	1
1:A:28:ASN:O	1:A:29:VAL:HG23	0.41	2.16	55	1
1:A:19:LEU:CD1	1:A:73:ILE:CD1	0.41	2.99	23	2
1:A:24:ASN:O	1:A:25:PHE:C	0.41	2.60	51	2
1:A:45:VAL:CG1	1:A:65:VAL:CG2	0.41	2.99	27	2
1:A:69:ILE:O	1:A:69:ILE:HG22	0.40	2.16	7	1
1:A:33:ILE:O	1:A:34:HIS:CG	0.40	2.73	8	1
1:A:23:ALA:O	1:A:36:TYR:CE2	0.40	2.74	49	3
1:A:25:PHE:HB3	1:A:29:VAL:HG23	0.40	1.93	26	1
1:A:49:TYR:CD1	1:A:62:LEU:HD21	0.40	2.50	30	1
1:A:23:ALA:O	1:A:36:TYR:CE1	0.40	2.74	38	1
1:A:34:HIS:ND1	1:A:35:LYS:N	0.40	2.70	48	1
1:A:42:ALA:O	1:A:46:ILE:CG1	0.40	2.70	49	1
1:A:69:ILE:H	1:A:69:ILE:HD12	0.40	1.76	52	1
1:A:49:TYR:CE2	1:A:53:ILE:HG22	0.40	2.51	8	1
1:A:49:TYR:O	1:A:51:HIS:N	0.40	2.55	27	1
1:A:72:LYS:O	1:A:76:PHE:CE2	0.40	2.74	33	1
1:A:20:VAL:HG12	1:A:20:VAL:O	0.40	2.15	52	1
1:A:15:ILE:HD13	1:A:46:ILE:HG21	0.40	1.92	20	1
1:A:51:HIS:O	1:A:52:LYS:CG	0.40	2.69	46	1
1:A:22:LEU:HD11	1:A:39:TYR:CE2	0.40	2.51	19	1
1:A:46:ILE:HD11	1:A:65:VAL:CG2	0.40	2.39	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:ILE:O	1:A:49:TYR:CB	0.40	2.69	32	1
1:A:49:TYR:CE2	1:A:53:ILE:CD1	0.40	3.04	32	1
1:A:15:ILE:CG2	1:A:73:ILE:HD12	0.40	2.47	35	1
1:A:15:ILE:HB	1:A:46:ILE:HG21	0.40	1.92	45	1
1:A:46:ILE:CG2	1:A:51:HIS:CB	0.40	2.99	46	1
1:A:19:LEU:HD13	1:A:19:LEU:C	0.40	2.37	53	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	63/87 (72%)	51±2 (81±3%)	9±2 (14±3%)	3±2 (5±3%)	3	23
All	All	3465/4785 (72%)	2805 (81%)	476 (14%)	184 (5%)	3	23

All 20 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	51	HIS	30
1	A	52	LYS	29
1	A	68	LYS	16
1	A	27	LYS	15
1	A	29	VAL	14
1	A	67	THR	12
1	A	53	ILE	12
1	A	66	GLY	9
1	A	25	PHE	9
1	A	34	HIS	7
1	A	50	PRO	7
1	A	13	GLY	5
1	A	55	SER	4
1	A	56	GLY	4
1	A	65	VAL	3
1	A	63	PRO	3

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Mol	Chain	Res	Type	Models (Total)
1	A	15	ILE	2
1	A	14	GLY	1
1	A	33	ILE	1
1	A	35	LYS	1

### 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	49/70 (70%)	39±3 (79±6%)	10±3 (21±6%)	3	31
All	All	2695/3850 (70%)	2123 (79%)	572 (21%)	3	31

All 44 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	49	TYR	38
1	A	40	ARG	38
1	A	25	PHE	37
1	A	39	TYR	33
1	A	22	LEU	31
1	A	46	ILE	30
1	A	65	VAL	27
1	A	76	PHE	26
1	A	19	LEU	22
1	A	27	LYS	21
1	A	18	MET	19
1	A	68	LYS	17
1	A	34	HIS	15
1	A	72	LYS	14
1	A	67	THR	13
1	A	61	LYS	12
1	A	33	ILE	12
1	A	52	LYS	11
1	A	55	SER	11
1	A	75	GLU	11
1	A	28	ASN	10

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Mol	Chain	Res	Type	Models (Total)
1	A	41	LYS	10
1	A	17	ASP	10
1	A	58	GLU	10
1	A	48	LYS	9
1	A	54	LYS	9
1	A	35	LYS	8
1	A	74	ASP	8
1	A	53	ILE	6
1	A	71	GLU	6
1	A	36	TYR	6
1	A	60	LYS	5
1	A	21	GLU	5
1	A	24	ASN	5
1	A	77	LEU	5
1	A	51	HIS	4
1	A	62	LEU	3
1	A	63	PRO	3
1	A	29	VAL	3
1	A	16	THR	3
1	A	69	ILE	2
1	A	44	SER	2
1	A	73	ILE	1
1	A	26	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 monosaccharides 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

No chemical shift data were provided