



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 07:24 AM UTC

PDB ID : 1ZQ3 / pdb\_00001zq3  
Title : NMR Solution Structure of the Bicoid Homeodomain Bound to the Consensus DNA Binding Site TAATCC  
Authors : Baird-Titus, J.M.; Rance, M.; Clark-Baldwin, K.; Ma, J.; Vrushank, D.  
Deposited on : 2005-05-18

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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| wwPDB-RCI                      | : | v_1n_11_5_13_A (Berjanski et al., 2005)                          |
| PANAV                          | : | Wang et al. (2010)                                               |
| wwPDB-ShiftChecker             | : | v1.2                                                             |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

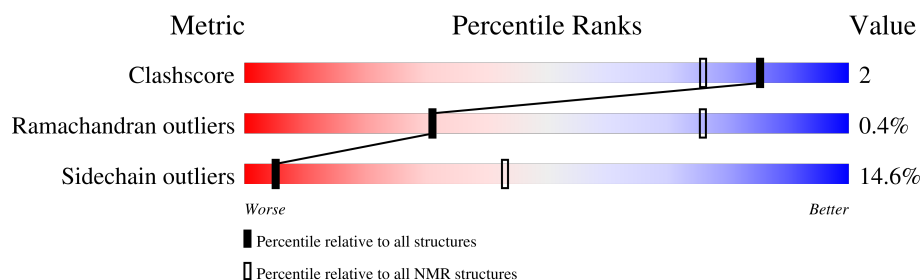
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment 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<br>(#Entries) | NMR archive<br>(#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore            | 229148                      | 14424                     |
| Ramachandran outliers | 224038                      | 12848                     |
| Sidechain outliers    | 223484                      | 12823                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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     | 13     | 77% (yellow) 23% (orange)                    |
| 2   | B     | 13     | 77% (yellow) 23% (orange)                    |
| 3   | P     | 68     | 28% (green) 29% (yellow) . (grey) 38% (cyan) |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 3 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                                    | P:10-P:51 (42)        | 0.45              | 3            |

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 2 clusters. No single-model clusters were found.

| Cluster number | Models                                                        |
|----------------|---------------------------------------------------------------|
| 1              | 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 13, 14, 15, 16, 17, 18, 19, 20 |
| 2              | 11, 12                                                        |

### 3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1960 atoms, of which 871 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called 5'-D(\*GP\*CP\*TP\*CP\*TP\*AP\*AP\*TP\*CP\*CP\*CP\*CP\*G)-3'.

| Mol | Chain | Residues | Atoms |     |     |    |    |    | Trace |
|-----|-------|----------|-------|-----|-----|----|----|----|-------|
| 1   | A     | 13       | Total | C   | H   | N  | O  | P  | 0     |
|     |       |          | 405   | 124 | 148 | 44 | 77 | 12 |       |

- Molecule 2 is a DNA chain called 5'-D(\*CP\*GP\*GP\*GP\*GP\*AP\*TP\*TP\*AP\*GP\*AP\*GP\*C)-3'.

| Mol | Chain | Residues | Atoms |     |     |    |    |    | Trace |
|-----|-------|----------|-------|-----|-----|----|----|----|-------|
| 2   | B     | 13       | Total | C   | H   | N  | O  | P  | 0     |
|     |       |          | 417   | 128 | 147 | 55 | 75 | 12 |       |

- Molecule 3 is a protein called Homeotic bicoid protein.

| Mol | Chain | Residues | Atoms |     |     |     |    | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|-------|
| 3   | P     | 68       | Total | C   | H   | N   | O  | 0     |
|     |       |          | 1138  | 348 | 576 | 115 | 99 |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| P     | 1       | GLY      | -      | cloning artifact | UNP Q9UAM0 |

## 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.

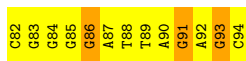
- Molecule 1: 5'-D(\*GP\*CP\*TP\*CP\*TP\*AP\*AP\*TP\*CP\*CP\*CP\*CP\*G)-3'

Chain A: 



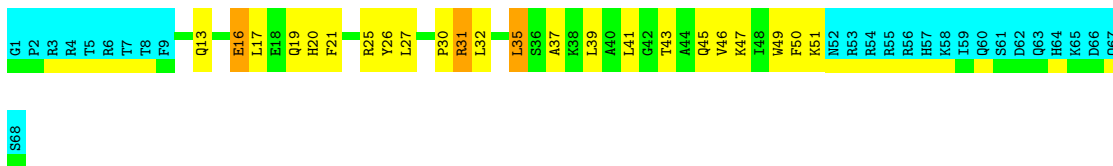
- Molecule 2: 5'-D(\*CP\*GP\*GP\*GP\*GP\*AP\*TP\*TP\*AP\*GP\*AP\*GP\*C)-3'

Chain B: 



- Molecule 3: Homeotic bicoid protein

Chain P: 

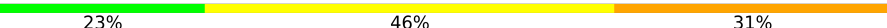


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

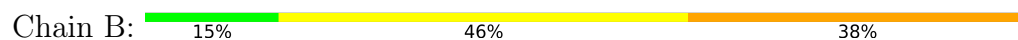
#### 4.2.1 Score per residue for model 1

- Molecule 1: 5'-D(\*GP\*CP\*TP\*CP\*TP\*AP\*AP\*TP\*CP\*CP\*CP\*CP\*G)-3'

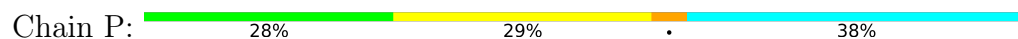
Chain A: 



- Molecule 2: 5'-D(\*CP\*GP\*GP\*GP\*GP\*AP\*TP\*TP\*AP\*GP\*AP\*GP\*C)-3'

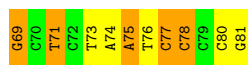
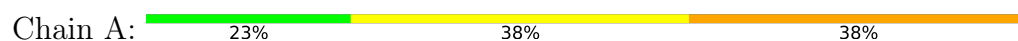


- Molecule 3: Homeotic bicoid protein

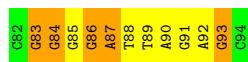
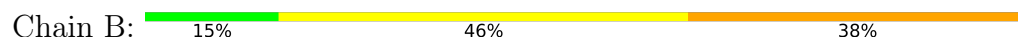


#### 4.2.2 Score per residue for model 2

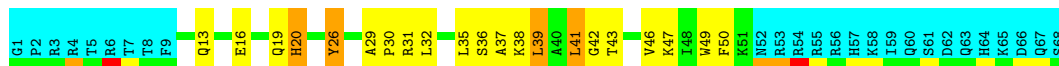
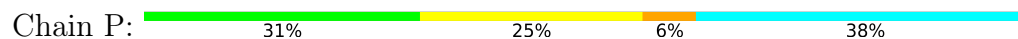
- Molecule 1: 5'-D(\*GP\*CP\*TP\*CP\*TP\*AP\*AP\*TP\*CP\*CP\*CP\*CP\*G)-3'



- Molecule 2: 5'-D(\*CP\*GP\*GP\*GP\*GP\*AP\*TP\*TP\*AP\*GP\*AP\*GP\*C)-3'



- Molecule 3: Homeotic bicoid protein

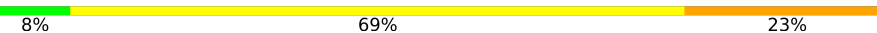


#### 4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: 5'-D(\*GP\*CP\*TP\*CP\*TP\*AP\*AP\*TP\*CP\*CP\*CP\*CP\*G)-3'

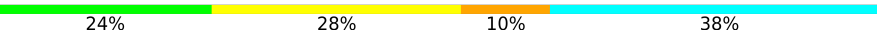


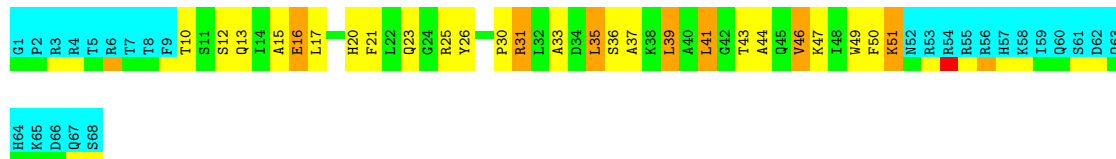
- Molecule 2: 5'-D(\*CP\*GP\*GP\*GP\*GP\*AP\*TP\*TP\*AP\*GP\*AP\*GP\*C)-3'

Chain B:  8% 69% 23%



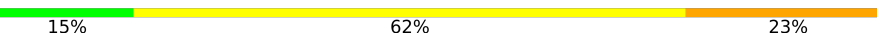
- Molecule 3: Homeotic bicoid protein

Chain P:  24% 28% 10% 38%



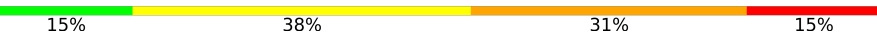
#### 4.2.4 Score per residue for model 4

- Molecule 1: 5'-D(\*GP\*CP\*TP\*CP\*TP\*AP\*AP\*TP\*CP\*CP\*CP\*CP\*G)-3'

Chain A:  15% 62% 23%



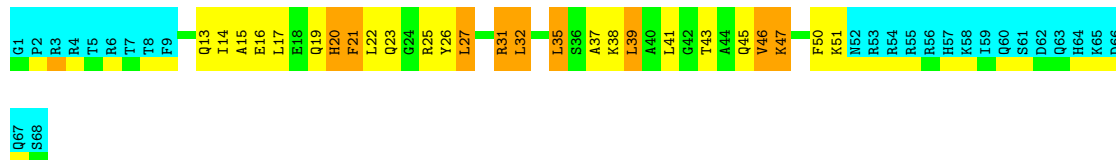
- Molecule 2: 5'-D(\*CP\*GP\*GP\*GP\*GP\*AP\*TP\*TP\*AP\*GP\*AP\*GP\*C)-3'

Chain B:  15% 38% 31% 15%



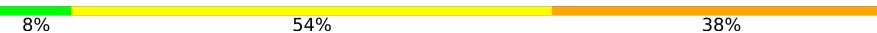
- Molecule 3: Homeotic bicoid protein

Chain P:  24% 25% 13% 38%



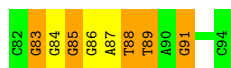
#### 4.2.5 Score per residue for model 5

- Molecule 1: 5'-D(\*GP\*CP\*TP\*CP\*TP\*AP\*AP\*TP\*CP\*CP\*CP\*CP\*G)-3'

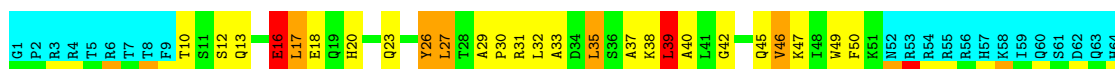
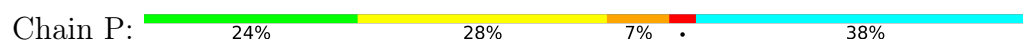
Chain A:  8% 54% 38%



- Molecule 2: 5'-D(\*CP\*GP\*GP\*GP\*GP\*AP\*TP\*TP\*AP\*GP\*AP\*GP\*C)-3'

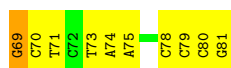


- Molecule 3: Homeotic bicoid protein

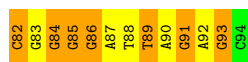


#### 4.2.6 Score per residue for model 6

- Molecule 1: 5'-D(\*GP\*CP\*TP\*CP\*TP\*AP\*AP\*TP\*CP\*CP\*CP\*G)-3'



- Molecule 2: 5'-D(\*CP\*GP\*GP\*GP\*GP\*AP\*TP\*TP\*AP\*GP\*AP\*GP\*C)-3'

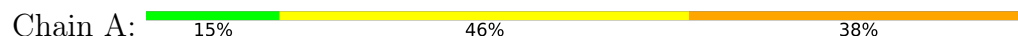


- Molecule 3: Homeotic bicoid protein



#### 4.2.7 Score per residue for model 7

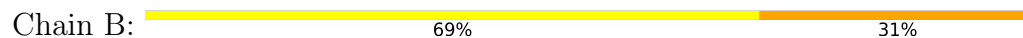
- Molecule 1: 5'-D(\*GP\*CP\*TP\*CP\*TP\*AP\*AP\*TP\*CP\*CP\*CP\*G)-3'



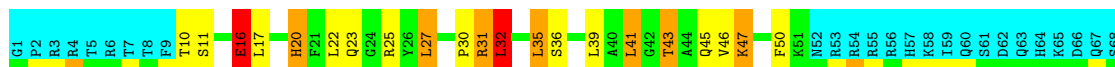
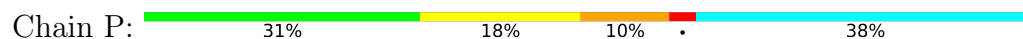




- Molecule 2: 5'-D(\*CP\*GP\*GP\*GP\*GP\*AP\*TP\*TP\*AP\*GP\*AP\*GP\*C)-3'

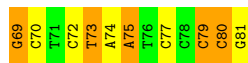
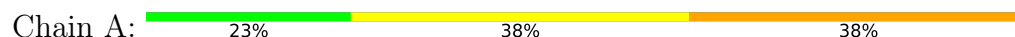


- Molecule 3: Homeotic bicoid protein



#### 4.2.8 Score per residue for model 8

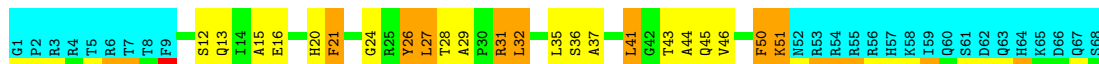
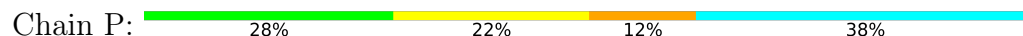
- Molecule 1: 5'-D(\*GP\*CP\*TP\*CP\*TP\*AP\*AP\*TP\*CP\*CP\*CP\*G)-3'



- Molecule 2: 5'-D(\*CP\*GP\*GP\*GP\*GP\*AP\*TP\*TP\*AP\*GP\*AP\*GP\*C)-3'



- Molecule 3: Homeotic bicoid protein

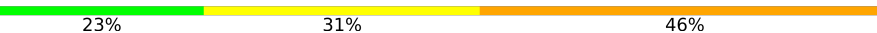


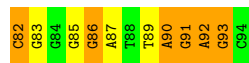
#### 4.2.9 Score per residue for model 9

- Molecule 1: 5'-D(\*GP\*CP\*TP\*CP\*TP\*AP\*AP\*TP\*CP\*CP\*CP\*G)-3'

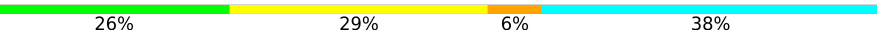


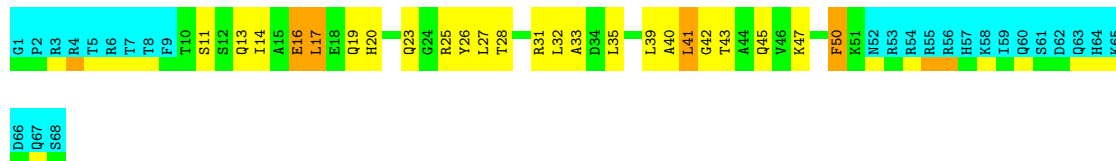
- Molecule 2: 5'-D(\*CP\*GP\*GP\*GP\*GP\*AP\*TP\*TP\*AP\*GP\*AP\*GP\*C)-3'

Chain B: 



- Molecule 3: Homeotic bicoid protein

Chain P: 



#### 4.2.10 Score per residue for model 10

- Molecule 1: 5'-D(\*GP\*CP\*TP\*CP\*TP\*AP\*AP\*TP\*CP\*CP\*CP\*CP\*G)-3'

Chain A: 



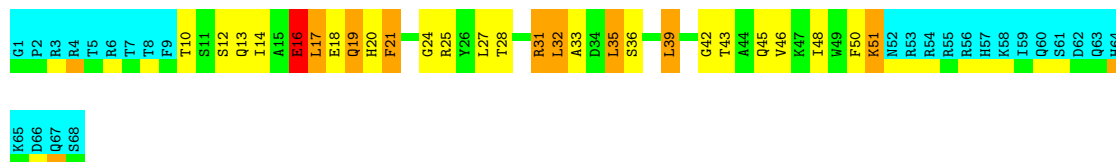
- Molecule 2: 5'-D(\*CP\*GP\*GP\*GP\*GP\*AP\*TP\*TP\*AP\*GP\*AP\*GP\*C)-3'

Chain B: 



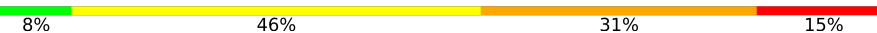
- Molecule 3: Homeotic bicoid protein

Chain P: 



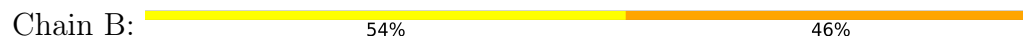
#### 4.2.11 Score per residue for model 11

- Molecule 1: 5'-D(\*GP\*CP\*TP\*CP\*TP\*AP\*AP\*TP\*CP\*CP\*CP\*CP\*G)-3'

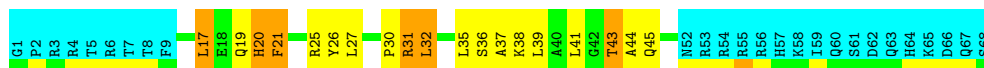
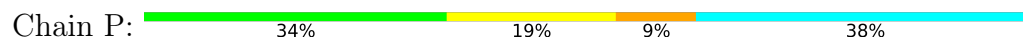
Chain A: 



- Molecule 2: 5'-D(\*CP\*GP\*GP\*GP\*GP\*AP\*TP\*TP\*AP\*GP\*AP\*GP\*C)-3'



- Molecule 3: Homeotic bicoid protein

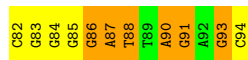


#### 4.2.12 Score per residue for model 12

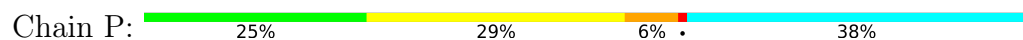
- Molecule 1: 5'-D(\*GP\*CP\*TP\*CP\*TP\*AP\*AP\*TP\*CP\*CP\*CP\*CP\*G)-3'



- Molecule 2: 5'-D(\*CP\*GP\*GP\*GP\*GP\*AP\*TP\*TP\*AP\*GP\*AP\*GP\*C)-3'



- Molecule 3: Homeotic bicoid protein



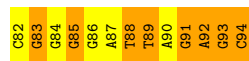
#### 4.2.13 Score per residue for model 13

- Molecule 1: 5'-D(\*GP\*CP\*TP\*CP\*TP\*AP\*AP\*TP\*CP\*CP\*CP\*CP\*G)-3'



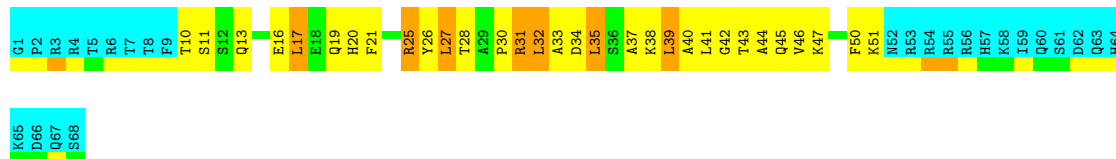
- Molecule 2: 5'-D(\*CP\*GP\*GP\*GP\*GP\*AP\*TP\*TP\*AP\*GP\*AP\*GP\*C)-3'

Chain B: 



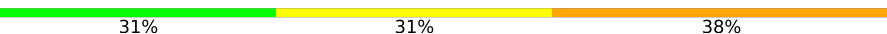
- Molecule 3: Homeotic bicoid protein

Chain P: 



#### 4.2.14 Score per residue for model 14

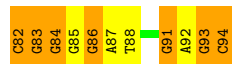
- Molecule 1: 5'-D(\*GP\*CP\*TP\*CP\*TP\*AP\*AP\*TP\*CP\*CP\*CP\*CP\*G)-3'

Chain A: 



- Molecule 2: 5'-D(\*CP\*GP\*GP\*GP\*GP\*AP\*TP\*TP\*AP\*GP\*AP\*GP\*C)-3'

Chain B: 



- Molecule 3: Homeotic bicoid protein

Chain P: 



#### 4.2.15 Score per residue for model 15

- Molecule 1: 5'-D(\*GP\*CP\*TP\*CP\*TP\*AP\*AP\*TP\*CP\*CP\*CP\*CP\*G)-3'

Chain A: 



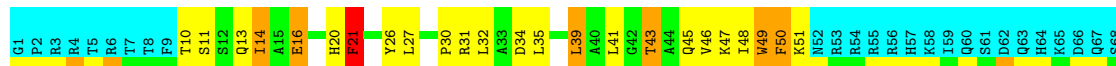
- Molecule 2: 5'-D(\*CP\*GP\*GP\*GP\*GP\*AP\*TP\*TP\*AP\*GP\*AP\*GP\*C)-3'

Chain B: 



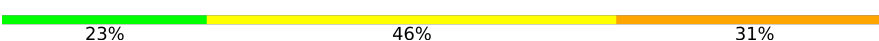
- Molecule 3: Homeotic bicoid protein

Chain P: 



#### 4.2.16 Score per residue for model 16

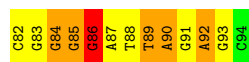
- Molecule 1: 5'-D(\*GP\*CP\*TP\*CP\*TP\*AP\*AP\*TP\*CP\*CP\*CP\*CP\*G)-3'

Chain A: 



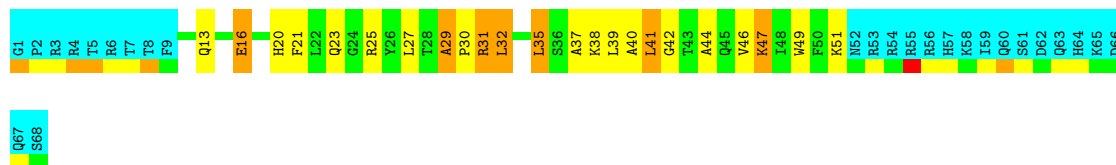
- Molecule 2: 5'-D(\*CP\*GP\*GP\*GP\*GP\*AP\*TP\*TP\*AP\*GP\*AP\*GP\*C)-3'

Chain B: 



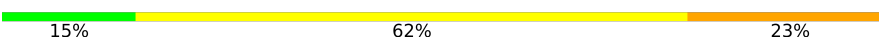
- Molecule 3: Homeotic bicoid protein

Chain P: 



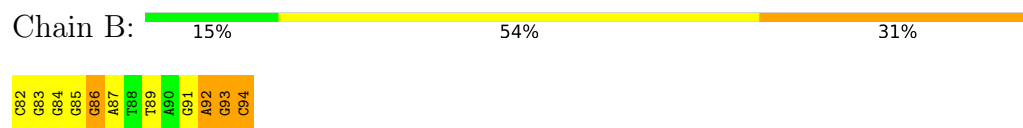
#### 4.2.17 Score per residue for model 17

- Molecule 1: 5'-D(\*GP\*CP\*TP\*CP\*TP\*AP\*AP\*TP\*CP\*CP\*CP\*CP\*G)-3'

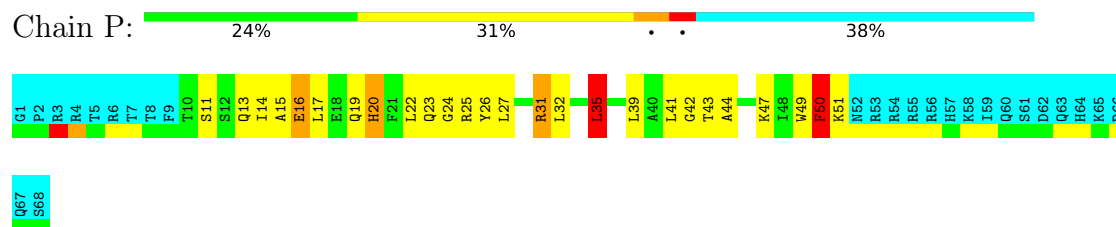
Chain A: 



- Molecule 2: 5'-D(\*CP\*GP\*GP\*GP\*GP\*AP\*TP\*TP\*AP\*GP\*AP\*GP\*C)-3'

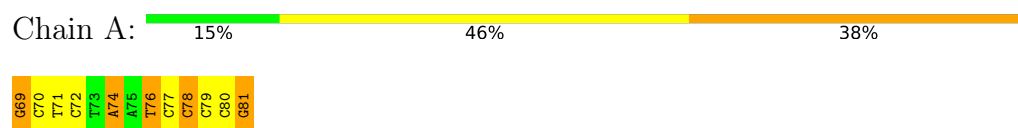


- Molecule 3: Homeotic bicoid protein

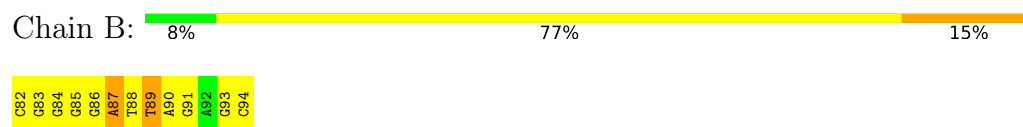


#### 4.2.18 Score per residue for model 18

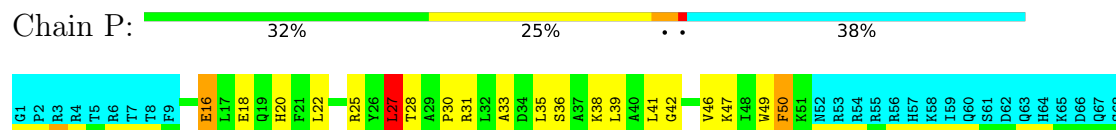
- Molecule 1: 5'-D(\*GP\*CP\*TP\*CP\*TP\*AP\*AP\*TP\*CP\*CP\*CP\*CP\*G)-3'



- Molecule 2: 5'-D(\*CP\*GP\*GP\*GP\*GP\*AP\*TP\*TP\*AP\*GP\*AP\*GP\*C)-3'

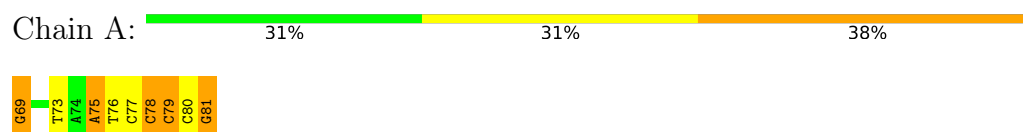


- Molecule 3: Homeotic bicoid protein

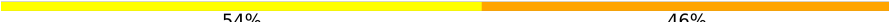


#### 4.2.19 Score per residue for model 19

- Molecule 1: 5'-D(\*GP\*CP\*TP\*CP\*TP\*AP\*AP\*TP\*CP\*CP\*CP\*CP\*G)-3'



- Molecule 2: 5'-D(\*CP\*GP\*GP\*GP\*GP\*AP\*TP\*TP\*AP\*GP\*AP\*GP\*C)-3'

Chain B:  54% 46%



- Molecule 3: Homeotic bicoid protein

Chain P:  34% 19% 9% 38%



#### 4.2.20 Score per residue for model 20

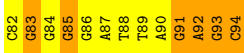
- Molecule 1: 5'-D(\*GP\*CP\*TP\*CP\*TP\*AP\*AP\*TP\*CP\*CP\*CP\*CP\*G)-3'

Chain A:  54% 46%



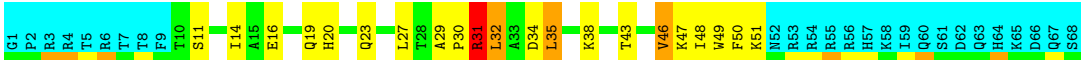
- Molecule 2: 5'-D(\*CP\*GP\*GP\*GP\*GP\*AP\*TP\*TP\*AP\*GP\*AP\*GP\*C)-3'

Chain B:  54% 46%



- Molecule 3: Homeotic bicoid protein

Chain P:  31% 25% 38%



## 5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *protein structure - fast torsion angle dynamics algorithm (CYANA2.0)*, *DNA structure - NUCGEN* and *simulated annealing with NMR-derived energy restraints (AMBER7.0)*, *protein-DNA complex - simulated annealing with NMR-derived energy restraints (AMBER7.0)*, *protein-DNA complex refinement - explicit solvent MD simulations (AMBER7.0)*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| CYANA         | structure solution | 2.0     |
| Amber         | refinement         | 7.0     |

No chemical shift data was provided.



## 6 Model quality

### 6.1 Standard geometry

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     | 1.55±0.08    | 1±1/286 ( 0.3± 0.3%) | 2.26±0.10   | 15±4/438 ( 3.5± 0.9%) |
| 2   | B     | 1.55±0.05    | 1±1/304 ( 0.3± 0.2%) | 2.17±0.07   | 15±4/469 ( 3.1± 0.8%) |
| 3   | P     | 2.02±0.09    | 7±3/339 ( 2.2± 0.8%) | 2.50±0.08   | 23±6/459 ( 4.9± 1.2%) |
| All | All   | 1.74         | 183/18580 ( 1.0%)    | 2.32        | 1053/27320 ( 3.9%)    |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 6.3±1.5   |
| 2   | B     | 0.0±0.0   | 7.5±1.5   |
| 3   | P     | 0.0±0.0   | 1.1±1.1   |
| All | All   | 0         | 298       |

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
|     |       |     |      |         |       |             |          | Worst  | Total |
| 3   | P     | 25  | ARG  | CZ-NH2  | -9.72 | 1.20        | 1.33     | 17     | 3     |
| 3   | P     | 14  | ILE  | C-O     | -9.26 | 1.13        | 1.24     | 9      | 2     |
| 3   | P     | 31  | ARG  | N-CA    | 8.71  | 1.56        | 1.46     | 19     | 5     |
| 3   | P     | 26  | TYR  | CA-C    | 8.55  | 1.62        | 1.52     | 9      | 1     |
| 3   | P     | 20  | HIS  | CD2-NE2 | 8.40  | 1.47        | 1.37     | 6      | 6     |
| 3   | P     | 29  | ALA  | CA-C    | 8.26  | 1.63        | 1.52     | 2      | 2     |
| 3   | P     | 49  | TRP  | N-CA    | 8.13  | 1.56        | 1.46     | 18     | 1     |
| 3   | P     | 32  | LEU  | C-O     | -8.09 | 1.14        | 1.24     | 7      | 1     |
| 3   | P     | 21  | PHE  | N-CA    | 8.06  | 1.56        | 1.46     | 13     | 2     |
| 3   | P     | 24  | GLY  | CA-C    | 7.84  | 1.62        | 1.51     | 19     | 2     |
| 3   | P     | 42  | GLY  | CA-C    | 7.65  | 1.58        | 1.52     | 2      | 2     |
| 3   | P     | 37  | ALA  | CA-C    | 7.51  | 1.62        | 1.52     | 8      | 4     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
|     |       |     |      |         |       |             |          | Worst  | Total |
| 3   | P     | 37  | ALA  | CA-CB   | 7.50  | 1.65        | 1.53     | 1      | 1     |
| 3   | P     | 42  | GLY  | N-CA    | 7.47  | 1.54        | 1.45     | 18     | 1     |
| 3   | P     | 49  | TRP  | NE1-CE2 | 7.38  | 1.45        | 1.37     | 16     | 1     |
| 3   | P     | 40  | ALA  | CA-C    | 7.28  | 1.60        | 1.53     | 13     | 1     |
| 3   | P     | 19  | GLN  | CA-C    | 7.25  | 1.62        | 1.52     | 12     | 1     |
| 2   | B     | 91  | DG   | O3'-P   | -7.21 | 1.50        | 1.61     | 20     | 1     |
| 3   | P     | 41  | LEU  | N-CA    | 7.14  | 1.55        | 1.45     | 9      | 1     |
| 3   | P     | 50  | PHE  | CA-C    | 7.03  | 1.62        | 1.52     | 15     | 3     |
| 3   | P     | 37  | ALA  | N-CA    | -7.02 | 1.38        | 1.46     | 13     | 2     |
| 2   | B     | 84  | DG   | O3'-P   | -6.94 | 1.50        | 1.61     | 3      | 1     |
| 3   | P     | 35  | LEU  | CA-C    | 6.92  | 1.61        | 1.52     | 13     | 2     |
| 3   | P     | 21  | PHE  | CA-C    | 6.86  | 1.62        | 1.52     | 15     | 1     |
| 3   | P     | 15  | ALA  | CA-C    | 6.81  | 1.61        | 1.52     | 3      | 3     |
| 3   | P     | 28  | THR  | CB-OG1  | -6.81 | 1.32        | 1.43     | 18     | 1     |
| 3   | P     | 32  | LEU  | CA-CB   | 6.67  | 1.64        | 1.53     | 14     | 3     |
| 3   | P     | 41  | LEU  | CA-C    | 6.65  | 1.60        | 1.52     | 17     | 3     |
| 3   | P     | 31  | ARG  | NE-CZ   | -6.64 | 1.25        | 1.33     | 7      | 1     |
| 3   | P     | 43  | THR  | C-N     | -6.61 | 1.25        | 1.33     | 10     | 1     |
| 3   | P     | 32  | LEU  | CA-C    | 6.57  | 1.61        | 1.52     | 19     | 2     |
| 3   | P     | 40  | ALA  | CA-CB   | 6.57  | 1.62        | 1.53     | 16     | 1     |
| 3   | P     | 36  | SER  | N-CA    | -6.51 | 1.38        | 1.46     | 10     | 1     |
| 3   | P     | 29  | ALA  | N-CA    | 6.50  | 1.53        | 1.46     | 20     | 3     |
| 3   | P     | 33  | ALA  | CA-CB   | 6.46  | 1.63        | 1.53     | 13     | 1     |
| 1   | A     | 71  | DT   | O3'-P   | -6.43 | 1.51        | 1.61     | 17     | 2     |
| 1   | A     | 80  | DC   | C5'-C4' | 6.41  | 1.65        | 1.52     | 17     | 1     |
| 3   | P     | 13  | GLN  | N-CA    | 6.40  | 1.54        | 1.46     | 3      | 1     |
| 3   | P     | 47  | LYS  | N-CA    | 6.37  | 1.53        | 1.46     | 17     | 1     |
| 3   | P     | 43  | THR  | CB-OG1  | -6.35 | 1.33        | 1.43     | 3      | 2     |
| 3   | P     | 17  | LEU  | CA-C    | -6.34 | 1.44        | 1.52     | 7      | 1     |
| 3   | P     | 41  | LEU  | C-O     | -6.18 | 1.16        | 1.24     | 19     | 1     |
| 1   | A     | 76  | DT   | C5-C7   | 6.16  | 1.62        | 1.50     | 3      | 1     |
| 3   | P     | 44  | ALA  | CA-C    | 6.16  | 1.60        | 1.52     | 3      | 2     |
| 3   | P     | 13  | GLN  | CA-C    | 6.16  | 1.60        | 1.52     | 4      | 2     |
| 3   | P     | 26  | TYR  | C-N     | 6.14  | 1.41        | 1.33     | 15     | 1     |
| 3   | P     | 15  | ALA  | CA-CB   | -6.11 | 1.43        | 1.53     | 4      | 1     |
| 3   | P     | 25  | ARG  | CD-NE   | 6.10  | 1.54        | 1.46     | 12     | 2     |
| 3   | P     | 20  | HIS  | CB-CG   | 6.09  | 1.58        | 1.50     | 8      | 2     |
| 2   | B     | 86  | DG   | O3'-P   | -6.07 | 1.52        | 1.61     | 19     | 1     |
| 3   | P     | 20  | HIS  | ND1-CE1 | 6.07  | 1.38        | 1.32     | 15     | 1     |
| 3   | P     | 20  | HIS  | N-CA    | -6.05 | 1.39        | 1.46     | 18     | 1     |
| 3   | P     | 38  | LYS  | CA-C    | 6.04  | 1.60        | 1.52     | 18     | 1     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
|     |       |     |      |         |       |             |          | Worst  | Total |
| 3   | P     | 50  | PHE  | N-CA    | -6.04 | 1.39        | 1.46     | 5      | 2     |
| 1   | A     | 79  | DC   | O3'-P   | -6.03 | 1.52        | 1.61     | 12     | 1     |
| 3   | P     | 29  | ALA  | C-N     | 6.01  | 1.41        | 1.34     | 14     | 1     |
| 1   | A     | 73  | DT   | O3'-P   | -5.91 | 1.52        | 1.61     | 2      | 2     |
| 3   | P     | 12  | SER  | CA-C    | 5.91  | 1.60        | 1.52     | 12     | 2     |
| 3   | P     | 32  | LEU  | N-CA    | -5.91 | 1.39        | 1.46     | 5      | 1     |
| 3   | P     | 33  | ALA  | CA-C    | 5.91  | 1.60        | 1.52     | 10     | 1     |
| 3   | P     | 38  | LYS  | N-CA    | 5.88  | 1.53        | 1.46     | 19     | 2     |
| 3   | P     | 47  | LYS  | C-N     | 5.88  | 1.41        | 1.34     | 13     | 1     |
| 1   | A     | 70  | DC   | O3'-P   | -5.83 | 1.52        | 1.61     | 13     | 1     |
| 3   | P     | 43  | THR  | CA-C    | 5.80  | 1.60        | 1.52     | 11     | 1     |
| 3   | P     | 30  | PRO  | N-CA    | -5.79 | 1.40        | 1.47     | 7      | 1     |
| 3   | P     | 43  | THR  | CA-CB   | 5.79  | 1.62        | 1.53     | 19     | 2     |
| 3   | P     | 20  | HIS  | CG-CD2  | 5.79  | 1.42        | 1.35     | 16     | 2     |
| 2   | B     | 84  | DG   | C4'-O4' | -5.76 | 1.33        | 1.45     | 16     | 1     |
| 3   | P     | 13  | GLN  | C-O     | -5.72 | 1.17        | 1.24     | 19     | 2     |
| 1   | A     | 74  | DA   | O3'-P   | 5.72  | 1.69        | 1.61     | 13     | 1     |
| 3   | P     | 22  | LEU  | N-CA    | 5.69  | 1.53        | 1.46     | 7      | 2     |
| 3   | P     | 51  | LYS  | C-O     | -5.69 | 1.17        | 1.24     | 19     | 1     |
| 3   | P     | 24  | GLY  | N-CA    | 5.67  | 1.53        | 1.45     | 8      | 1     |
| 3   | P     | 16  | GLU  | C-N     | -5.64 | 1.26        | 1.33     | 13     | 1     |
| 3   | P     | 14  | ILE  | N-CA    | 5.61  | 1.53        | 1.46     | 4      | 2     |
| 2   | B     | 91  | DG   | C4'-O4' | -5.58 | 1.34        | 1.45     | 11     | 1     |
| 3   | P     | 20  | HIS  | CE1-NE2 | 5.57  | 1.38        | 1.32     | 1      | 2     |
| 3   | P     | 30  | PRO  | CA-C    | 5.54  | 1.60        | 1.52     | 18     | 1     |
| 3   | P     | 23  | GLN  | CA-C    | 5.53  | 1.60        | 1.52     | 16     | 2     |
| 3   | P     | 20  | HIS  | CA-C    | 5.50  | 1.60        | 1.52     | 6      | 1     |
| 3   | P     | 17  | LEU  | N-CA    | -5.49 | 1.39        | 1.46     | 7      | 1     |
| 2   | B     | 94  | DC   | C5'-C4' | 5.45  | 1.63        | 1.52     | 11     | 1     |
| 2   | B     | 87  | DA   | C1'-N9  | 5.44  | 1.57        | 1.46     | 1      | 1     |
| 3   | P     | 21  | PHE  | CA-CB   | 5.44  | 1.61        | 1.53     | 16     | 1     |
| 3   | P     | 12  | SER  | N-CA    | 5.42  | 1.53        | 1.46     | 3      | 2     |
| 2   | B     | 89  | DT   | O3'-P   | -5.40 | 1.53        | 1.61     | 17     | 1     |
| 3   | P     | 45  | GLN  | N-CA    | -5.40 | 1.39        | 1.46     | 4      | 1     |
| 1   | A     | 76  | DT   | O3'-P   | -5.38 | 1.53        | 1.61     | 1      | 1     |
| 1   | A     | 80  | DC   | O3'-P   | -5.38 | 1.53        | 1.61     | 4      | 1     |
| 2   | B     | 93  | DG   | C4'-O4' | -5.37 | 1.34        | 1.45     | 15     | 2     |
| 2   | B     | 86  | DG   | C5-C6   | 5.37  | 1.52        | 1.42     | 14     | 1     |
| 1   | A     | 72  | DC   | O3'-P   | -5.36 | 1.53        | 1.61     | 18     | 1     |
| 3   | P     | 49  | TRP  | C-O     | 5.35  | 1.30        | 1.24     | 20     | 1     |
| 2   | B     | 92  | DA   | O3'-P   | -5.34 | 1.53        | 1.61     | 2      | 1     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
|     |       |     |      |         |       |             |          | Worst  | Total |
| 3   | P     | 14  | ILE  | CA-C    | -5.32 | 1.46        | 1.52     | 17     | 2     |
| 3   | P     | 46  | VAL  | CA-C    | 5.32  | 1.59        | 1.52     | 5      | 2     |
| 1   | A     | 76  | DT   | C4'-O4' | -5.32 | 1.34        | 1.45     | 11     | 1     |
| 3   | P     | 39  | LEU  | CA-CB   | -5.28 | 1.44        | 1.53     | 10     | 2     |
| 2   | B     | 92  | DA   | C6-N6   | -5.24 | 1.23        | 1.34     | 7      | 1     |
| 2   | B     | 94  | DC   | C4-N4   | -5.24 | 1.23        | 1.34     | 8      | 1     |
| 1   | A     | 72  | DC   | C3'-C2' | 5.23  | 1.63        | 1.52     | 5      | 2     |
| 3   | P     | 45  | GLN  | CA-CB   | -5.23 | 1.45        | 1.53     | 7      | 1     |
| 3   | P     | 46  | VAL  | N-CA    | 5.23  | 1.52        | 1.46     | 16     | 1     |
| 3   | P     | 20  | HIS  | CA-CB   | -5.23 | 1.44        | 1.53     | 6      | 1     |
| 1   | A     | 73  | DT   | P-O5'   | -5.23 | 1.50        | 1.60     | 16     | 1     |
| 3   | P     | 16  | GLU  | CA-C    | -5.22 | 1.46        | 1.52     | 1      | 1     |
| 3   | P     | 33  | ALA  | N-CA    | 5.21  | 1.52        | 1.46     | 3      | 2     |
| 3   | P     | 29  | ALA  | CA-CB   | 5.21  | 1.60        | 1.53     | 8      | 1     |
| 1   | A     | 79  | DC   | O4'-C1' | 5.21  | 1.52        | 1.41     | 11     | 1     |
| 3   | P     | 10  | THR  | CB-OG1  | -5.21 | 1.35        | 1.43     | 5      | 1     |
| 3   | P     | 22  | LEU  | CA-CB   | 5.20  | 1.61        | 1.53     | 1      | 1     |
| 3   | P     | 38  | LYS  | C-N     | -5.17 | 1.26        | 1.33     | 2      | 1     |
| 3   | P     | 46  | VAL  | C-N     | -5.17 | 1.27        | 1.33     | 20     | 1     |
| 3   | P     | 22  | LEU  | CA-C    | 5.16  | 1.59        | 1.52     | 4      | 1     |
| 3   | P     | 35  | LEU  | N-CA    | -5.14 | 1.40        | 1.46     | 5      | 1     |
| 3   | P     | 27  | LEU  | CA-CB   | 5.11  | 1.61        | 1.53     | 15     | 1     |
| 3   | P     | 47  | LYS  | CA-CB   | 5.11  | 1.61        | 1.53     | 4      | 1     |
| 3   | P     | 31  | ARG  | CZ-NH1  | -5.10 | 1.25        | 1.32     | 13     | 1     |
| 3   | P     | 20  | HIS  | CG-ND1  | 5.09  | 1.43        | 1.38     | 19     | 1     |
| 3   | P     | 43  | THR  | N-CA    | 5.07  | 1.52        | 1.46     | 2      | 1     |
| 3   | P     | 45  | GLN  | C-O     | -5.05 | 1.18        | 1.24     | 7      | 1     |
| 1   | A     | 78  | DC   | O3'-P   | -5.05 | 1.53        | 1.61     | 9      | 1     |
| 2   | B     | 82  | DC   | O3'-P   | -5.04 | 1.53        | 1.61     | 9      | 1     |
| 3   | P     | 31  | ARG  | CA-C    | 5.03  | 1.59        | 1.52     | 7      | 1     |
| 1   | A     | 74  | DA   | C1'-N9  | 5.03  | 1.56        | 1.46     | 9      | 1     |
| 3   | P     | 51  | LYS  | N-CA    | 5.01  | 1.52        | 1.46     | 1      | 1     |
| 2   | B     | 93  | DG   | O3'-P   | -5.01 | 1.53        | 1.61     | 4      | 1     |

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|------------|--------|-------------|----------|--------|-------|
|     |       |     |      |            |        |             |          | Worst  | Total |
| 1   | A     | 73  | DT   | O4'-C1'-N1 | 11.38  | 125.48      | 108.40   | 9      | 5     |
| 3   | P     | 19  | GLN  | OE1-CD-NE2 | -11.33 | 111.27      | 122.60   | 19     | 6     |
| 3   | P     | 45  | GLN  | OE1-CD-NE2 | -10.71 | 111.89      | 122.60   | 8      | 8     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 3   | P     | 31  | ARG  | NE-CZ-NH2   | 10.54 | 128.69      | 119.20   | 20     | 3     |
| 1   | A     | 72  | DC   | C4'-C3'-O3' | 10.34 | 125.51      | 110.00   | 9      | 4     |
| 3   | P     | 49  | TRP  | CA-C-O      | -9.85 | 110.66      | 121.00   | 15     | 1     |
| 3   | P     | 37  | ALA  | CA-C-N      | 9.83  | 133.63      | 120.65   | 6      | 4     |
| 3   | P     | 37  | ALA  | C-N-CA      | 9.83  | 133.63      | 120.65   | 6      | 4     |
| 3   | P     | 23  | GLN  | OE1-CD-NE2  | -9.64 | 112.96      | 122.60   | 7      | 4     |
| 2   | B     | 87  | DA   | O3'-P-O5'   | -9.41 | 89.89       | 104.00   | 6      | 4     |
| 3   | P     | 38  | LYS  | CA-C-N      | 9.21  | 132.62      | 120.28   | 13     | 3     |
| 3   | P     | 38  | LYS  | C-N-CA      | 9.21  | 132.62      | 120.28   | 13     | 3     |
| 1   | A     | 81  | DG   | O4'-C1'-N9  | 9.19  | 122.18      | 108.40   | 17     | 8     |
| 2   | B     | 91  | DG   | O3'-P-O5'   | -9.02 | 90.47       | 104.00   | 20     | 1     |
| 2   | B     | 94  | DC   | O5'-C5'-C4' | 8.94  | 124.21      | 110.80   | 17     | 2     |
| 3   | P     | 16  | GLU  | CA-C-O      | -8.92 | 110.97      | 120.42   | 5      | 3     |
| 3   | P     | 29  | ALA  | O-C-N       | 8.82  | 128.93      | 120.55   | 6      | 1     |
| 3   | P     | 16  | GLU  | CA-CB-CG    | 8.72  | 131.55      | 114.10   | 18     | 15    |
| 2   | B     | 90  | DA   | O4'-C1'-N9  | 8.56  | 121.24      | 108.40   | 18     | 4     |
| 3   | P     | 31  | ARG  | CA-C-N      | 8.55  | 131.56      | 120.44   | 19     | 10    |
| 3   | P     | 31  | ARG  | C-N-CA      | 8.55  | 131.56      | 120.44   | 19     | 10    |
| 2   | B     | 93  | DG   | C4'-C3'-O3' | 8.47  | 122.71      | 110.00   | 13     | 1     |
| 3   | P     | 47  | LYS  | O-C-N       | 8.41  | 131.08      | 122.08   | 2      | 2     |
| 2   | B     | 83  | DG   | O3'-P-O5'   | -8.39 | 91.41       | 104.00   | 13     | 6     |
| 2   | B     | 92  | DA   | C4'-C3'-O3' | -8.36 | 97.47       | 110.00   | 15     | 5     |
| 2   | B     | 88  | DT   | P-O5'-C5'   | 8.35  | 132.53      | 120.00   | 8      | 1     |
| 3   | P     | 29  | ALA  | CA-C-N      | 8.34  | 127.64      | 118.97   | 12     | 1     |
| 3   | P     | 29  | ALA  | C-N-CA      | 8.34  | 127.64      | 118.97   | 12     | 1     |
| 3   | P     | 25  | ARG  | N-CA-C      | 8.33  | 121.29      | 111.71   | 11     | 2     |
| 1   | A     | 78  | DC   | C5'-C4'-O4' | 8.31  | 121.86      | 109.40   | 5      | 2     |
| 1   | A     | 75  | DA   | N1-C6-N6    | -8.28 | 106.58      | 119.00   | 19     | 5     |
| 3   | P     | 25  | ARG  | NH1-CZ-NH2  | -8.28 | 108.54      | 119.30   | 13     | 2     |
| 3   | P     | 17  | LEU  | CA-C-N      | 8.23  | 131.65      | 120.54   | 5      | 2     |
| 3   | P     | 17  | LEU  | C-N-CA      | 8.23  | 131.65      | 120.54   | 5      | 2     |
| 2   | B     | 84  | DG   | O5'-C5'-C4' | 8.21  | 123.12      | 110.80   | 10     | 3     |
| 1   | A     | 75  | DA   | O5'-C5'-C4' | 8.19  | 123.08      | 110.80   | 19     | 3     |
| 3   | P     | 15  | ALA  | CA-C-O      | -8.12 | 112.29      | 120.82   | 8      | 1     |
| 2   | B     | 91  | DG   | N3-C2-N2    | -8.05 | 107.62      | 119.70   | 7      | 1     |
| 2   | B     | 93  | DG   | C2'-C3'-O3' | -8.05 | 99.43       | 111.50   | 13     | 3     |
| 2   | B     | 82  | DC   | C3'-C2'-C1' | 8.01  | 113.62      | 101.60   | 7      | 1     |
| 3   | P     | 27  | LEU  | N-CA-C      | 7.97  | 121.01      | 109.14   | 5      | 3     |
| 1   | A     | 80  | DC   | O3'-P-O5'   | -7.95 | 92.08       | 104.00   | 2      | 3     |
| 2   | B     | 88  | DT   | O5'-C5'-C4' | 7.93  | 122.69      | 110.80   | 13     | 2     |
| 1   | A     | 77  | DC   | O5'-C5'-C4' | 7.92  | 122.68      | 110.80   | 4      | 3     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 1   | A     | 74  | DA   | O5'-C5'-C4' | 7.90  | 122.65      | 110.80   | 2      | 3     |
| 3   | P     | 34  | ASP  | O-C-N       | -7.86 | 113.86      | 122.03   | 20     | 1     |
| 3   | P     | 20  | HIS  | CA-CB-CG    | -7.83 | 105.97      | 113.80   | 7      | 5     |
| 2   | B     | 85  | DG   | P-O5'-C5'   | 7.81  | 131.71      | 120.00   | 3      | 1     |
| 2   | B     | 93  | DG   | C3'-C2'-C1' | 7.73  | 113.19      | 101.60   | 1      | 1     |
| 2   | B     | 85  | DG   | O4'-C1'-N9  | 7.68  | 119.93      | 108.40   | 20     | 3     |
| 3   | P     | 51  | LYS  | CA-C-O      | -7.67 | 112.77      | 120.82   | 17     | 2     |
| 3   | P     | 30  | PRO  | N-CA-CB     | 7.64  | 111.40      | 103.23   | 12     | 8     |
| 1   | A     | 75  | DA   | P-O3'-C3'   | 7.63  | 131.64      | 120.20   | 20     | 2     |
| 1   | A     | 70  | DC   | N1-C2-O2    | 7.61  | 130.62      | 119.20   | 12     | 2     |
| 3   | P     | 37  | ALA  | CA-C-O      | -7.60 | 113.07      | 120.90   | 2      | 1     |
| 3   | P     | 50  | PHE  | CA-C-N      | 7.60  | 131.08      | 120.29   | 9      | 5     |
| 3   | P     | 50  | PHE  | C-N-CA      | 7.60  | 131.08      | 120.29   | 9      | 5     |
| 1   | A     | 76  | DT   | C1'-O4'-C4' | -7.59 | 98.31       | 109.70   | 18     | 1     |
| 3   | P     | 21  | PHE  | CA-CB-CG    | 7.58  | 121.38      | 113.80   | 12     | 2     |
| 3   | P     | 25  | ARG  | NE-CZ-NH1   | 7.56  | 129.06      | 121.50   | 13     | 2     |
| 1   | A     | 80  | DC   | C4'-C3'-C2' | -7.53 | 91.10       | 102.40   | 12     | 1     |
| 1   | A     | 78  | DC   | O4'-C1'-N1  | -7.53 | 97.11       | 108.40   | 18     | 4     |
| 1   | A     | 70  | DC   | O5'-C5'-C4' | 7.49  | 122.04      | 110.80   | 8      | 4     |
| 2   | B     | 89  | DT   | O4'-C1'-N1  | -7.49 | 97.16       | 108.40   | 6      | 1     |
| 2   | B     | 90  | DA   | C2'-C3'-O3' | 7.49  | 122.74      | 111.50   | 15     | 2     |
| 3   | P     | 42  | GLY  | O-C-N       | -7.49 | 113.25      | 122.76   | 16     | 1     |
| 3   | P     | 31  | ARG  | CA-C-O      | -7.48 | 112.90      | 120.90   | 11     | 1     |
| 2   | B     | 84  | DG   | C2'-C3'-O3' | -7.47 | 100.29      | 111.50   | 11     | 3     |
| 1   | A     | 71  | DT   | C6-C5-C7    | -7.46 | 112.82      | 124.00   | 9      | 3     |
| 1   | A     | 79  | DC   | N3-C4-N4    | -7.43 | 106.76      | 117.90   | 19     | 1     |
| 1   | A     | 81  | DG   | O4'-C1'-C2' | -7.41 | 95.28       | 106.40   | 18     | 2     |
| 1   | A     | 75  | DA   | C5'-C4'-O4' | 7.39  | 120.49      | 109.40   | 8      | 2     |
| 2   | B     | 89  | DT   | C6-C5-C7    | -7.39 | 112.92      | 124.00   | 16     | 6     |
| 3   | P     | 43  | THR  | N-CA-C      | 7.38  | 120.27      | 111.33   | 7      | 4     |
| 3   | P     | 17  | LEU  | CA-C-O      | -7.37 | 113.08      | 120.82   | 4      | 6     |
| 1   | A     | 73  | DT   | C6-C5-C7    | -7.36 | 112.95      | 124.00   | 19     | 5     |
| 3   | P     | 10  | THR  | CA-CB-CG2   | 7.36  | 123.02      | 110.50   | 3      | 5     |
| 3   | P     | 42  | GLY  | CA-C-O      | -7.35 | 114.94      | 121.41   | 13     | 2     |
| 3   | P     | 50  | PHE  | CA-CB-CG    | 7.33  | 121.13      | 113.80   | 3      | 7     |
| 2   | B     | 85  | DG   | O3'-P-O5'   | -7.31 | 93.04       | 104.00   | 4      | 1     |
| 3   | P     | 17  | LEU  | O-C-N       | 7.29  | 129.85      | 122.12   | 9      | 1     |
| 2   | B     | 88  | DT   | C5'-C4'-O4' | 7.26  | 120.29      | 109.40   | 14     | 2     |
| 2   | B     | 94  | DC   | C5'-C4'-C3' | -7.25 | 104.03      | 114.90   | 20     | 2     |
| 3   | P     | 11  | SER  | CA-C-N      | 7.22  | 129.83      | 120.44   | 9      | 4     |
| 3   | P     | 11  | SER  | C-N-CA      | 7.22  | 129.83      | 120.44   | 9      | 4     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 3   | P     | 31  | ARG  | NH1-CZ-NH2  | -7.21 | 109.92      | 119.30   | 20     | 3     |
| 1   | A     | 70  | DC   | C4'-C3'-O3' | -7.20 | 99.19       | 110.00   | 15     | 4     |
| 3   | P     | 31  | ARG  | CD-NE-CZ    | 7.20  | 134.48      | 124.40   | 17     | 2     |
| 2   | B     | 82  | DC   | N3-C2-O2    | -7.17 | 111.14      | 121.90   | 9      | 7     |
| 1   | A     | 74  | DA   | N1-C6-N6    | -7.17 | 108.24      | 119.00   | 3      | 6     |
| 1   | A     | 78  | DC   | C3'-C2'-C1' | 7.16  | 112.34      | 101.60   | 12     | 2     |
| 1   | A     | 79  | DC   | C5'-C4'-O4' | 7.16  | 120.14      | 109.40   | 9      | 2     |
| 2   | B     | 91  | DG   | O5'-C5'-C4' | 7.16  | 121.53      | 110.80   | 5      | 4     |
| 1   | A     | 78  | DC   | C2'-C3'-O3' | 7.12  | 122.18      | 111.50   | 2      | 2     |
| 2   | B     | 88  | DT   | N3-C4-O4    | -7.09 | 111.97      | 122.60   | 2      | 3     |
| 3   | P     | 32  | LEU  | CA-C-O      | -7.07 | 113.40      | 120.82   | 10     | 2     |
| 2   | B     | 93  | DG   | O4'-C1'-C2' | -7.06 | 95.81       | 106.40   | 1      | 2     |
| 2   | B     | 93  | DG   | N1-C6-O6    | -7.06 | 109.41      | 120.00   | 10     | 1     |
| 1   | A     | 70  | DC   | N3-C4-N4    | -7.06 | 107.31      | 117.90   | 7      | 3     |
| 1   | A     | 71  | DT   | O4'-C1'-N1  | 7.04  | 118.96      | 108.40   | 20     | 3     |
| 1   | A     | 78  | DC   | C5'-C4'-C3' | 7.03  | 125.45      | 114.90   | 12     | 3     |
| 1   | A     | 78  | DC   | N3-C4-N4    | -7.03 | 107.36      | 117.90   | 15     | 3     |
| 3   | P     | 51  | LYS  | CA-C-N      | 7.01  | 129.55      | 120.44   | 16     | 2     |
| 3   | P     | 51  | LYS  | C-N-CA      | 7.01  | 129.55      | 120.44   | 16     | 2     |
| 2   | B     | 82  | DC   | N3-C4-N4    | -7.00 | 107.40      | 117.90   | 9      | 2     |
| 3   | P     | 27  | LEU  | CA-C-N      | 7.00  | 133.85      | 121.75   | 4      | 6     |
| 3   | P     | 27  | LEU  | C-N-CA      | 7.00  | 133.85      | 121.75   | 4      | 6     |
| 3   | P     | 25  | ARG  | NE-CZ-NH2   | 7.00  | 125.50      | 119.20   | 3      | 5     |
| 2   | B     | 88  | DT   | N1-C1'-C2'  | 6.99  | 123.99      | 113.50   | 8      | 3     |
| 1   | A     | 80  | DC   | N3-C2-O2    | -6.99 | 111.42      | 121.90   | 20     | 4     |
| 3   | P     | 31  | ARG  | NE-CZ-NH1   | 6.99  | 128.49      | 121.50   | 2      | 3     |
| 2   | B     | 91  | DG   | N9-C1'-C2'  | 6.99  | 123.98      | 113.50   | 6      | 1     |
| 3   | P     | 49  | TRP  | CB-CG-CD2   | 6.98  | 136.58      | 126.80   | 5      | 3     |
| 1   | A     | 79  | DC   | N3-C2-O2    | -6.97 | 111.45      | 121.90   | 11     | 4     |
| 2   | B     | 82  | DC   | P-O3'-C3'   | 6.96  | 130.64      | 120.20   | 1      | 2     |
| 1   | A     | 70  | DC   | N3-C2-O2    | -6.96 | 111.46      | 121.90   | 12     | 5     |
| 2   | B     | 90  | DA   | C8-N9-C1'   | 6.96  | 137.49      | 127.05   | 16     | 1     |
| 3   | P     | 41  | LEU  | CA-C-N      | 6.94  | 126.58      | 119.92   | 13     | 5     |
| 3   | P     | 41  | LEU  | C-N-CA      | 6.94  | 126.58      | 119.92   | 13     | 5     |
| 3   | P     | 46  | VAL  | N-CA-C      | -6.94 | 104.01      | 110.53   | 5      | 1     |
| 2   | B     | 92  | DA   | O5'-C5'-C4' | 6.94  | 121.21      | 110.80   | 11     | 2     |
| 2   | B     | 89  | DT   | C2'-C3'-O3' | 6.94  | 121.91      | 111.50   | 13     | 3     |
| 1   | A     | 70  | DC   | O4'-C4'-C3' | 6.93  | 115.80      | 105.40   | 20     | 1     |
| 2   | B     | 86  | DG   | N9-C1'-C2'  | 6.93  | 123.90      | 113.50   | 9      | 3     |
| 2   | B     | 93  | DG   | O4'-C1'-N9  | 6.92  | 118.78      | 108.40   | 13     | 2     |
| 3   | P     | 45  | GLN  | CA-C-O      | -6.92 | 113.22      | 120.55   | 11     | 3     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 2   | B     | 90  | DA   | C1'-O4'-C4' | -6.90 | 99.35       | 109.70   | 9      | 2     |
| 3   | P     | 51  | LYS  | N-CA-C      | 6.90  | 118.49      | 110.97   | 19     | 2     |
| 3   | P     | 47  | LYS  | CA-C-O      | -6.88 | 113.51      | 121.07   | 2      | 3     |
| 1   | A     | 69  | DG   | O4'-C1'-N9  | 6.87  | 118.71      | 108.40   | 20     | 2     |
| 2   | B     | 87  | DA   | N1-C6-N6    | -6.87 | 108.69      | 119.00   | 18     | 4     |
| 3   | P     | 44  | ALA  | O-C-N       | -6.87 | 114.84      | 122.12   | 13     | 3     |
| 2   | B     | 93  | DG   | C5'-C4'-O4' | 6.86  | 119.69      | 109.40   | 18     | 2     |
| 1   | A     | 72  | DC   | P-O3'-C3'   | 6.86  | 130.49      | 120.20   | 9      | 2     |
| 2   | B     | 89  | DT   | O5'-C5'-C4' | 6.83  | 121.04      | 110.80   | 7      | 2     |
| 2   | B     | 87  | DA   | C2'-C3'-O3' | 6.82  | 121.73      | 111.50   | 1      | 2     |
| 2   | B     | 89  | DT   | N3-C4-O4    | -6.81 | 112.39      | 122.60   | 15     | 3     |
| 1   | A     | 80  | DC   | C2'-C3'-O3' | 6.81  | 121.72      | 111.50   | 19     | 2     |
| 2   | B     | 91  | DG   | N1-C6-O6    | -6.79 | 109.81      | 120.00   | 18     | 1     |
| 3   | P     | 44  | ALA  | CA-C-O      | -6.77 | 113.71      | 120.82   | 8      | 3     |
| 3   | P     | 10  | THR  | OG1-CB-CG2  | -6.74 | 95.81       | 109.30   | 5      | 1     |
| 1   | A     | 69  | DG   | P-O3'-C3'   | 6.74  | 130.31      | 120.20   | 3      | 5     |
| 3   | P     | 15  | ALA  | CA-C-N      | 6.74  | 129.20      | 120.44   | 17     | 3     |
| 3   | P     | 15  | ALA  | C-N-CA      | 6.74  | 129.20      | 120.44   | 17     | 3     |
| 1   | A     | 77  | DC   | O3'-P-O5'   | -6.73 | 93.90       | 104.00   | 10     | 1     |
| 3   | P     | 20  | HIS  | CB-CG-CD2   | -6.73 | 122.45      | 131.20   | 17     | 5     |
| 1   | A     | 79  | DC   | O3'-P-O5'   | -6.72 | 93.92       | 104.00   | 16     | 2     |
| 3   | P     | 12  | SER  | CA-C-N      | 6.72  | 129.58      | 120.44   | 5      | 1     |
| 3   | P     | 12  | SER  | C-N-CA      | 6.72  | 129.58      | 120.44   | 5      | 1     |
| 3   | P     | 20  | HIS  | CE1-NE2-CD2 | -6.72 | 102.28      | 109.00   | 5      | 1     |
| 3   | P     | 44  | ALA  | N-CA-C      | 6.72  | 119.46      | 111.33   | 11     | 1     |
| 3   | P     | 50  | PHE  | O-C-N       | -6.71 | 115.05      | 122.03   | 10     | 2     |
| 2   | B     | 86  | DG   | O4'-C1'-N9  | 6.71  | 118.47      | 108.40   | 10     | 3     |
| 3   | P     | 40  | ALA  | N-CA-CB     | -6.71 | 101.92      | 112.46   | 9      | 1     |
| 2   | B     | 82  | DC   | N1-C1'-C2'  | 6.71  | 123.56      | 113.50   | 6      | 2     |
| 1   | A     | 71  | DT   | O4'-C1'-C2' | -6.71 | 96.34       | 106.40   | 10     | 1     |
| 2   | B     | 87  | DA   | C5-C6-N1    | 6.70  | 127.65      | 117.60   | 18     | 1     |
| 1   | A     | 77  | DC   | O4'-C1'-N1  | 6.69  | 118.43      | 108.40   | 8      | 1     |
| 2   | B     | 91  | DG   | C2'-C3'-O3' | 6.68  | 121.52      | 111.50   | 5      | 5     |
| 3   | P     | 33  | ALA  | N-CA-C      | 6.67  | 118.34      | 111.14   | 18     | 2     |
| 2   | B     | 94  | DC   | N3-C2-O2    | -6.65 | 111.92      | 121.90   | 13     | 3     |
| 2   | B     | 93  | DG   | O5'-C5'-C4' | 6.65  | 120.78      | 110.80   | 14     | 3     |
| 3   | P     | 35  | LEU  | N-CA-C      | 6.65  | 118.53      | 111.28   | 10     | 2     |
| 1   | A     | 79  | DC   | N1-C1'-C2'  | 6.62  | 123.43      | 113.50   | 11     | 1     |
| 1   | A     | 70  | DC   | C2'-C3'-O3' | 6.61  | 121.41      | 111.50   | 11     | 3     |
| 2   | B     | 83  | DG   | O5'-C5'-C4' | 6.61  | 120.71      | 110.80   | 19     | 1     |
| 1   | A     | 76  | DT   | N1-C1'-C2'  | 6.60  | 123.41      | 113.50   | 14     | 1     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 1   | A     | 70  | DC   | O4'-C1'-N1  | -6.59 | 98.52       | 108.40   | 10     | 2     |
| 3   | P     | 50  | PHE  | CA-C-O      | 6.58  | 127.53      | 119.97   | 3      | 2     |
| 1   | A     | 71  | DT   | C5-C4-O4    | 6.58  | 132.46      | 122.60   | 12     | 1     |
| 2   | B     | 92  | DA   | N1-C6-N6    | -6.57 | 109.15      | 119.00   | 19     | 6     |
| 1   | A     | 81  | DG   | C2'-C3'-O3' | -6.56 | 101.66      | 111.50   | 9      | 2     |
| 3   | P     | 32  | LEU  | N-CA-CB     | -6.56 | 100.50      | 110.01   | 20     | 3     |
| 2   | B     | 86  | DG   | N3-C2-N2    | -6.56 | 109.86      | 119.70   | 12     | 2     |
| 2   | B     | 88  | DT   | C4'-C3'-O3' | -6.54 | 100.20      | 110.00   | 13     | 1     |
| 2   | B     | 90  | DA   | C5'-C4'-O4' | 6.53  | 119.19      | 109.40   | 10     | 1     |
| 1   | A     | 76  | DT   | O4'-C4'-C3' | 6.52  | 115.18      | 105.40   | 18     | 1     |
| 1   | A     | 69  | DG   | C4'-C3'-C2' | -6.52 | 92.63       | 102.40   | 2      | 1     |
| 1   | A     | 76  | DT   | O5'-C5'-C4' | 6.50  | 120.56      | 110.80   | 9      | 4     |
| 1   | A     | 79  | DC   | C4'-C3'-O3' | -6.49 | 100.27      | 110.00   | 19     | 5     |
| 1   | A     | 74  | DA   | C4'-C3'-O3' | -6.48 | 100.28      | 110.00   | 6      | 1     |
| 1   | A     | 80  | DC   | N1-C2-O2    | 6.48  | 128.92      | 119.20   | 20     | 2     |
| 1   | A     | 80  | DC   | C5'-C4'-O4' | -6.48 | 99.69       | 109.40   | 11     | 2     |
| 2   | B     | 86  | DG   | P-O3'-C3'   | 6.47  | 129.91      | 120.20   | 14     | 1     |
| 1   | A     | 81  | DG   | N1-C6-O6    | -6.47 | 110.29      | 120.00   | 19     | 1     |
| 1   | A     | 71  | DT   | C3'-C2'-C1' | 6.47  | 111.30      | 101.60   | 20     | 3     |
| 2   | B     | 86  | DG   | C3'-C2'-C1' | -6.47 | 91.90       | 101.60   | 1      | 1     |
| 2   | B     | 88  | DT   | C6-C5-C7    | -6.45 | 114.33      | 124.00   | 13     | 6     |
| 3   | P     | 24  | GLY  | CA-C-N      | 6.45  | 133.94      | 121.18   | 10     | 2     |
| 3   | P     | 24  | GLY  | C-N-CA      | 6.45  | 133.94      | 121.18   | 10     | 2     |
| 1   | A     | 72  | DC   | O3'-P-O5'   | 6.45  | 113.67      | 104.00   | 14     | 1     |
| 2   | B     | 92  | DA   | P-O3'-C3'   | 6.42  | 129.83      | 120.20   | 7      | 4     |
| 1   | A     | 70  | DC   | O3'-P-O5'   | 6.42  | 113.63      | 104.00   | 5      | 1     |
| 1   | A     | 73  | DT   | C2'-C3'-O3' | 6.41  | 121.12      | 111.50   | 5      | 1     |
| 1   | A     | 80  | DC   | C1'-O4'-C4' | -6.40 | 100.09      | 109.70   | 16     | 1     |
| 2   | B     | 84  | DG   | C4'-C3'-O3' | -6.40 | 100.40      | 110.00   | 3      | 3     |
| 2   | B     | 89  | DT   | C5-C4-O4    | 6.39  | 132.19      | 122.60   | 16     | 3     |
| 1   | A     | 75  | DA   | O3'-P-O5'   | -6.39 | 94.41       | 104.00   | 9      | 2     |
| 2   | B     | 87  | DA   | O5'-C5'-C4' | 6.39  | 120.39      | 110.80   | 10     | 3     |
| 1   | A     | 73  | DT   | O4'-C1'-C2' | -6.37 | 96.84       | 106.40   | 9      | 3     |
| 1   | A     | 69  | DG   | C5'-C4'-O4' | 6.36  | 118.94      | 109.40   | 7      | 1     |
| 3   | P     | 35  | LEU  | CA-C-O      | -6.35 | 112.66      | 119.97   | 16     | 1     |
| 2   | B     | 87  | DA   | N9-C1'-C2'  | 6.35  | 123.02      | 113.50   | 11     | 1     |
| 3   | P     | 45  | GLN  | CG-CD-OE1   | 6.35  | 133.50      | 120.80   | 7      | 1     |
| 3   | P     | 36  | SER  | N-CA-C      | 6.34  | 118.72      | 111.11   | 18     | 1     |
| 3   | P     | 21  | PHE  | O-C-N       | -6.34 | 115.40      | 122.12   | 4      | 1     |
| 1   | A     | 71  | DT   | C5'-C4'-C3' | -6.33 | 105.40      | 114.90   | 2      | 1     |
| 2   | B     | 82  | DC   | O4'-C1'-C2' | 6.33  | 115.89      | 106.40   | 10     | 1     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 1   | A     | 71  | DT   | N3-C4-O4    | -6.32 | 113.11      | 122.60   | 15     | 2     |
| 3   | P     | 27  | LEU  | O-C-N       | -6.32 | 115.59      | 122.79   | 18     | 2     |
| 3   | P     | 30  | PRO  | N-CD-CG     | 6.32  | 112.67      | 103.20   | 6      | 1     |
| 3   | P     | 20  | HIS  | CB-CG-ND1   | 6.31  | 132.17      | 122.70   | 5      | 2     |
| 3   | P     | 46  | VAL  | CA-C-N      | 6.31  | 128.64      | 120.44   | 19     | 4     |
| 3   | P     | 46  | VAL  | C-N-CA      | 6.31  | 128.64      | 120.44   | 19     | 4     |
| 3   | P     | 20  | HIS  | CB-CA-C     | 6.30  | 123.17      | 109.99   | 13     | 2     |
| 2   | B     | 94  | DC   | N3-C4-N4    | -6.30 | 108.45      | 117.90   | 7      | 1     |
| 3   | P     | 16  | GLU  | CB-CA-C     | -6.30 | 100.95      | 110.90   | 2      | 1     |
| 2   | B     | 91  | DG   | C5'-C4'-O4' | 6.28  | 118.82      | 109.40   | 15     | 1     |
| 1   | A     | 71  | DT   | C4-C5-C7    | -6.28 | 112.98      | 122.40   | 10     | 1     |
| 3   | P     | 39  | LEU  | CA-C-O      | -6.27 | 113.17      | 120.20   | 19     | 2     |
| 1   | A     | 75  | DA   | C5-C6-N6    | 6.27  | 132.81      | 123.40   | 19     | 1     |
| 3   | P     | 47  | LYS  | CA-C-N      | 6.27  | 128.58      | 120.56   | 16     | 2     |
| 3   | P     | 47  | LYS  | C-N-CA      | 6.27  | 128.58      | 120.56   | 16     | 2     |
| 3   | P     | 22  | LEU  | CA-C-O      | 6.26  | 127.06      | 119.49   | 12     | 2     |
| 1   | A     | 76  | DT   | P-O3'-C3'   | 6.25  | 129.58      | 120.20   | 12     | 1     |
| 1   | A     | 75  | DA   | C2'-C3'-O3' | 6.25  | 120.88      | 111.50   | 19     | 1     |
| 2   | B     | 85  | DG   | C2'-C3'-O3' | -6.25 | 102.12      | 111.50   | 8      | 3     |
| 2   | B     | 89  | DT   | O3'-P-O5'   | -6.25 | 94.63       | 104.00   | 5      | 1     |
| 3   | P     | 36  | SER  | CA-C-N      | 6.25  | 128.56      | 120.44   | 8      | 4     |
| 3   | P     | 36  | SER  | C-N-CA      | 6.25  | 128.56      | 120.44   | 8      | 4     |
| 1   | A     | 71  | DT   | N3-C2-O2    | -6.24 | 112.65      | 122.00   | 3      | 1     |
| 2   | B     | 86  | DG   | C4'-C3'-C2' | 6.23  | 111.75      | 102.40   | 1      | 1     |
| 2   | B     | 85  | DG   | O5'-C5'-C4' | 6.23  | 120.14      | 110.80   | 19     | 2     |
| 3   | P     | 29  | ALA  | CA-C-O      | -6.22 | 112.60      | 118.33   | 5      | 2     |
| 3   | P     | 23  | GLN  | CA-C-O      | 6.21  | 127.12      | 119.79   | 4      | 1     |
| 2   | B     | 85  | DG   | N1-C6-O6    | -6.20 | 110.70      | 120.00   | 5      | 1     |
| 3   | P     | 31  | ARG  | O-C-N       | 6.20  | 128.79      | 122.09   | 20     | 1     |
| 3   | P     | 51  | LYS  | O-C-N       | 6.19  | 128.45      | 122.07   | 8      | 2     |
| 3   | P     | 20  | HIS  | N-CA-C      | 6.19  | 119.00      | 111.82   | 9      | 1     |
| 3   | P     | 27  | LEU  | CA-C-O      | 6.19  | 128.78      | 121.36   | 1      | 4     |
| 3   | P     | 39  | LEU  | CD1-CG-CD2  | 6.18  | 124.40      | 110.80   | 15     | 1     |
| 3   | P     | 49  | TRP  | CB-CA-C     | -6.18 | 101.13      | 110.90   | 18     | 1     |
| 3   | P     | 26  | TYR  | CA-C-N      | 6.18  | 133.34      | 121.54   | 12     | 3     |
| 3   | P     | 26  | TYR  | C-N-CA      | 6.18  | 133.34      | 121.54   | 12     | 3     |
| 3   | P     | 38  | LYS  | CA-C-O      | -6.18 | 113.94      | 120.55   | 2      | 1     |
| 3   | P     | 23  | GLN  | O-C-N       | -6.18 | 113.41      | 122.43   | 5      | 1     |
| 3   | P     | 13  | GLN  | CA-CB-CG    | -6.17 | 101.75      | 114.10   | 16     | 3     |
| 3   | P     | 48  | ILE  | CA-C-O      | -6.17 | 114.63      | 121.17   | 6      | 3     |
| 2   | B     | 86  | DG   | O5'-C5'-C4' | 6.15  | 120.03      | 110.80   | 16     | 6     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 1   | A     | 70  | DC   | C4-C5-C6    | -6.15 | 108.38      | 117.60   | 8      | 1     |
| 3   | P     | 32  | LEU  | CA-C-N      | 6.14  | 128.42      | 120.44   | 5      | 5     |
| 3   | P     | 32  | LEU  | C-N-CA      | 6.14  | 128.42      | 120.44   | 5      | 5     |
| 3   | P     | 49  | TRP  | O-C-N       | 6.14  | 128.41      | 122.03   | 15     | 1     |
| 3   | P     | 34  | ASP  | CA-C-O      | -6.13 | 114.38      | 120.70   | 13     | 1     |
| 2   | B     | 94  | DC   | C1'-O4'-C4' | -6.12 | 100.51      | 109.70   | 10     | 3     |
| 2   | B     | 83  | DG   | C5'-C4'-O4' | 6.12  | 118.57      | 109.40   | 15     | 2     |
| 3   | P     | 10  | THR  | CA-C-N      | 6.11  | 129.31      | 120.38   | 10     | 2     |
| 3   | P     | 10  | THR  | C-N-CA      | 6.11  | 129.31      | 120.38   | 10     | 2     |
| 1   | A     | 76  | DT   | N3-C4-O4    | -6.11 | 113.43      | 122.60   | 10     | 2     |
| 2   | B     | 93  | DG   | O3'-P-O5'   | -6.10 | 94.85       | 104.00   | 2      | 3     |
| 2   | B     | 89  | DT   | N1-C1'-C2'  | 6.10  | 122.65      | 113.50   | 11     | 3     |
| 3   | P     | 43  | THR  | CA-CB-OG1   | 6.10  | 118.74      | 109.60   | 4      | 1     |
| 2   | B     | 91  | DG   | O4'-C1'-N9  | 6.10  | 117.54      | 108.40   | 12     | 1     |
| 2   | B     | 88  | DT   | C5-C4-O4    | 6.09  | 131.73      | 122.60   | 7      | 3     |
| 1   | A     | 71  | DT   | O3'-P-O5'   | 6.08  | 113.12      | 104.00   | 2      | 2     |
| 1   | A     | 74  | DA   | C5'-C4'-O4' | 6.07  | 118.51      | 109.40   | 12     | 1     |
| 2   | B     | 85  | DG   | N3-C4-N9    | 6.06  | 135.09      | 126.00   | 2      | 1     |
| 3   | P     | 41  | LEU  | O-C-N       | -6.06 | 116.34      | 123.25   | 2      | 2     |
| 1   | A     | 78  | DC   | O4'-C1'-C2' | 6.06  | 115.49      | 106.40   | 16     | 1     |
| 3   | P     | 47  | LYS  | CB-CG-CD    | 6.05  | 125.22      | 111.30   | 4      | 2     |
| 2   | B     | 87  | DA   | P-O3'-C3'   | 6.04  | 129.26      | 120.20   | 2      | 1     |
| 3   | P     | 41  | LEU  | N-CA-C      | 6.04  | 118.25      | 109.07   | 2      | 1     |
| 2   | B     | 91  | DG   | C4-N9-C1'   | -6.04 | 117.94      | 127.00   | 15     | 1     |
| 1   | A     | 70  | DC   | P-O3'-C3'   | 6.04  | 129.25      | 120.20   | 10     | 1     |
| 1   | A     | 79  | DC   | P-O3'-C3'   | 6.03  | 129.25      | 120.20   | 18     | 2     |
| 2   | B     | 88  | DT   | C5'-C4'-C3' | -6.03 | 105.85      | 114.90   | 20     | 2     |
| 2   | B     | 82  | DC   | C4'-C3'-O3' | -6.03 | 100.95      | 110.00   | 11     | 1     |
| 1   | A     | 73  | DT   | N3-C4-O4    | -6.02 | 113.57      | 122.60   | 20     | 1     |
| 1   | A     | 72  | DC   | N1-C1'-C2'  | 6.02  | 122.53      | 113.50   | 15     | 1     |
| 3   | P     | 31  | ARG  | CB-CA-C     | -6.02 | 101.43      | 110.88   | 7      | 1     |
| 1   | A     | 76  | DT   | C4-C5-C7    | -6.02 | 113.38      | 122.40   | 20     | 2     |
| 3   | P     | 19  | GLN  | N-CA-C      | 6.01  | 117.83      | 111.28   | 4      | 2     |
| 2   | B     | 84  | DG   | N1-C6-O6    | -6.01 | 110.99      | 120.00   | 6      | 1     |
| 1   | A     | 77  | DC   | N3-C2-O2    | -6.00 | 112.90      | 121.90   | 19     | 7     |
| 1   | A     | 79  | DC   | C2'-C3'-O3' | 6.00  | 120.50      | 111.50   | 1      | 2     |
| 2   | B     | 83  | DG   | C4'-C3'-O3' | -6.00 | 101.00      | 110.00   | 7      | 2     |
| 2   | B     | 84  | DG   | O3'-P-O5'   | -5.99 | 95.02       | 104.00   | 19     | 1     |
| 1   | A     | 74  | DA   | P-O3'-C3'   | 5.99  | 129.18      | 120.20   | 3      | 2     |
| 1   | A     | 78  | DC   | O5'-C5'-C4' | 5.99  | 119.78      | 110.80   | 6      | 4     |
| 2   | B     | 82  | DC   | C5'-C4'-C3' | 5.98  | 123.87      | 114.90   | 1      | 1     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 3   | P     | 45  | GLN  | CB-CG-CD    | 5.98  | 122.76      | 112.60   | 8      | 1     |
| 3   | P     | 26  | TYR  | CA-CB-CG    | 5.97  | 124.64      | 113.90   | 5      | 1     |
| 2   | B     | 89  | DT   | P-O3'-C3'   | 5.97  | 129.15      | 120.20   | 9      | 1     |
| 1   | A     | 77  | DC   | O4'-C1'-C2' | -5.97 | 97.45       | 106.40   | 13     | 1     |
| 3   | P     | 32  | LEU  | N-CA-C      | 5.96  | 118.26      | 111.11   | 8      | 2     |
| 3   | P     | 13  | GLN  | CA-C-O      | -5.96 | 114.56      | 120.82   | 6      | 2     |
| 3   | P     | 23  | GLN  | N-CA-C      | 5.94  | 120.26      | 112.89   | 20     | 1     |
| 2   | B     | 82  | DC   | C1'-O4'-C4' | -5.94 | 100.79      | 109.70   | 10     | 1     |
| 2   | B     | 88  | DT   | C4-C5-C7    | -5.92 | 113.52      | 122.40   | 19     | 1     |
| 3   | P     | 30  | PRO  | CA-C-N      | 5.91  | 128.52      | 120.54   | 13     | 3     |
| 3   | P     | 30  | PRO  | C-N-CA      | 5.91  | 128.52      | 120.54   | 13     | 3     |
| 3   | P     | 18  | GLU  | N-CA-C      | 5.91  | 117.39      | 111.07   | 10     | 1     |
| 3   | P     | 46  | VAL  | O-C-N       | -5.91 | 115.74      | 121.83   | 18     | 1     |
| 3   | P     | 36  | SER  | O-C-N       | 5.91  | 128.38      | 122.12   | 2      | 1     |
| 3   | P     | 49  | TRP  | CB-CG-CD1   | -5.90 | 118.05      | 126.90   | 5      | 2     |
| 3   | P     | 43  | THR  | CA-C-N      | 5.90  | 128.67      | 120.29   | 19     | 2     |
| 3   | P     | 43  | THR  | C-N-CA      | 5.90  | 128.67      | 120.29   | 19     | 2     |
| 1   | A     | 72  | DC   | C2'-C3'-O3' | 5.88  | 120.32      | 111.50   | 15     | 2     |
| 1   | A     | 70  | DC   | N3-C4-C5    | 5.87  | 130.60      | 121.80   | 8      | 1     |
| 3   | P     | 19  | GLN  | CG-CD-NE2   | 5.87  | 125.20      | 116.40   | 19     | 1     |
| 1   | A     | 79  | DC   | O5'-C5'-C4' | 5.87  | 119.60      | 110.80   | 11     | 1     |
| 2   | B     | 82  | DC   | C5'-C4'-O4' | 5.86  | 118.19      | 109.40   | 15     | 1     |
| 1   | A     | 73  | DT   | N1-C1'-C2'  | 5.85  | 122.27      | 113.50   | 4      | 2     |
| 2   | B     | 90  | DA   | N1-C6-N6    | -5.84 | 110.23      | 119.00   | 7      | 5     |
| 2   | B     | 85  | DG   | N3-C2-N2    | -5.83 | 110.96      | 119.70   | 5      | 1     |
| 3   | P     | 49  | TRP  | N-CA-CB     | 5.83  | 118.67      | 109.82   | 16     | 1     |
| 2   | B     | 88  | DT   | C2'-C3'-O3' | 5.82  | 120.23      | 111.50   | 19     | 2     |
| 2   | B     | 88  | DT   | O3'-P-O5'   | -5.82 | 95.28       | 104.00   | 15     | 2     |
| 3   | P     | 38  | LYS  | N-CA-C      | 5.82  | 118.84      | 111.69   | 12     | 1     |
| 3   | P     | 14  | ILE  | O-C-N       | -5.81 | 116.03      | 121.90   | 15     | 1     |
| 1   | A     | 75  | DA   | C3'-C2'-C1' | 5.81  | 110.32      | 101.60   | 10     | 1     |
| 1   | A     | 74  | DA   | C5'-C4'-C3' | 5.81  | 123.62      | 114.90   | 7      | 2     |
| 3   | P     | 13  | GLN  | O-C-N       | 5.81  | 128.06      | 122.07   | 17     | 2     |
| 2   | B     | 88  | DT   | N3-C2-O2    | -5.80 | 113.29      | 122.00   | 14     | 1     |
| 3   | P     | 42  | GLY  | CA-C-N      | 5.80  | 129.52      | 120.82   | 5      | 3     |
| 3   | P     | 42  | GLY  | C-N-CA      | 5.80  | 129.52      | 120.82   | 5      | 3     |
| 1   | A     | 72  | DC   | O4'-C4'-C3' | 5.80  | 114.10      | 105.40   | 12     | 1     |
| 2   | B     | 94  | DC   | N1-C2-O2    | 5.79  | 127.89      | 119.20   | 4      | 2     |
| 3   | P     | 12  | SER  | N-CA-C      | 5.79  | 117.67      | 111.36   | 8      | 1     |
| 1   | A     | 74  | DA   | C5-C6-N6    | 5.78  | 132.06      | 123.40   | 20     | 1     |
| 2   | B     | 86  | DG   | C2'-C3'-O3' | 5.77  | 120.15      | 111.50   | 7      | 1     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 1   | A     | 73  | DT   | N3-C2-O2    | -5.76 | 113.36      | 122.00   | 10     | 1     |
| 2   | B     | 83  | DG   | C1'-O4'-C4' | -5.76 | 101.06      | 109.70   | 8      | 1     |
| 2   | B     | 89  | DT   | C3'-C2'-C1' | -5.75 | 92.97       | 101.60   | 7      | 1     |
| 1   | A     | 76  | DT   | C3'-C2'-C1' | 5.75  | 110.23      | 101.60   | 9      | 1     |
| 3   | P     | 20  | HIS  | O-C-N       | 5.75  | 129.34      | 122.27   | 9      | 1     |
| 2   | B     | 87  | DA   | C8-N9-C1'   | 5.74  | 135.66      | 127.05   | 6      | 2     |
| 1   | A     | 76  | DT   | C2'-C3'-O3' | 5.74  | 120.10      | 111.50   | 18     | 1     |
| 2   | B     | 82  | DC   | N1-C2-O2    | 5.73  | 127.80      | 119.20   | 9      | 1     |
| 1   | A     | 69  | DG   | O5'-C5'-C4' | 5.72  | 119.38      | 110.80   | 11     | 3     |
| 1   | A     | 72  | DC   | N1-C2-O2    | 5.71  | 127.77      | 119.20   | 18     | 1     |
| 3   | P     | 37  | ALA  | O-C-N       | 5.70  | 128.19      | 122.03   | 2      | 1     |
| 3   | P     | 25  | ARG  | CA-C-N      | 5.70  | 131.52      | 122.62   | 17     | 1     |
| 3   | P     | 25  | ARG  | C-N-CA      | 5.70  | 131.52      | 122.62   | 17     | 1     |
| 3   | P     | 10  | THR  | O-C-N       | 5.70  | 129.88      | 123.27   | 7      | 1     |
| 2   | B     | 88  | DT   | C4'-C3'-C2' | -5.69 | 93.86       | 102.40   | 19     | 1     |
| 1   | A     | 78  | DC   | O4'-C4'-C3' | 5.69  | 113.93      | 105.40   | 9      | 1     |
| 3   | P     | 26  | TYR  | CB-CG-CD2   | -5.68 | 112.29      | 120.80   | 8      | 2     |
| 3   | P     | 21  | PHE  | CA-C-O      | -5.67 | 114.51      | 120.63   | 3      | 2     |
| 2   | B     | 87  | DA   | C1'-O4'-C4' | -5.67 | 101.20      | 109.70   | 6      | 1     |
| 3   | P     | 28  | THR  | CA-C-N      | 5.67  | 127.17      | 120.09   | 10     | 1     |
| 3   | P     | 28  | THR  | C-N-CA      | 5.67  | 127.17      | 120.09   | 10     | 1     |
| 1   | A     | 76  | DT   | C6-N1-C1'   | 5.67  | 127.85      | 119.35   | 12     | 1     |
| 1   | A     | 76  | DT   | O4'-C1'-N1  | 5.66  | 116.89      | 108.40   | 15     | 2     |
| 3   | P     | 49  | TRP  | CG-CD2-CE3  | -5.66 | 128.24      | 133.90   | 15     | 2     |
| 1   | A     | 73  | DT   | O3'-P-O5'   | -5.66 | 95.52       | 104.00   | 15     | 3     |
| 3   | P     | 18  | GLU  | O-C-N       | -5.66 | 116.24      | 122.07   | 10     | 1     |
| 1   | A     | 81  | DG   | C4-C5-C6    | -5.65 | 110.62      | 119.10   | 11     | 1     |
| 1   | A     | 80  | DC   | O4'-C1'-C2' | -5.65 | 97.93       | 106.40   | 3      | 1     |
| 3   | P     | 16  | GLU  | CB-CG-CD    | 5.65  | 122.20      | 112.60   | 10     | 2     |
| 1   | A     | 79  | DC   | N1-C2-O2    | 5.64  | 127.66      | 119.20   | 8      | 1     |
| 3   | P     | 20  | HIS  | ND1-CE1-NE2 | 5.63  | 114.03      | 108.40   | 5      | 2     |
| 2   | B     | 87  | DA   | C5'-C4'-O4' | 5.63  | 117.85      | 109.40   | 7      | 1     |
| 1   | A     | 70  | DC   | O4'-C1'-C2' | -5.63 | 97.95       | 106.40   | 13     | 2     |
| 2   | B     | 87  | DA   | C3'-C2'-C1' | -5.62 | 93.17       | 101.60   | 6      | 1     |
| 3   | P     | 39  | LEU  | CA-C-N      | 5.62  | 132.26      | 121.54   | 4      | 2     |
| 3   | P     | 39  | LEU  | C-N-CA      | 5.62  | 132.26      | 121.54   | 4      | 2     |
| 2   | B     | 93  | DG   | N3-C2-N2    | -5.61 | 111.28      | 119.70   | 19     | 1     |
| 2   | B     | 91  | DG   | C5'-C4'-C3' | -5.61 | 106.48      | 114.90   | 1      | 2     |
| 2   | B     | 94  | DC   | O4'-C4'-C3' | 5.61  | 113.81      | 105.40   | 10     | 2     |
| 3   | P     | 41  | LEU  | CA-C-O      | -5.61 | 114.88      | 121.44   | 8      | 1     |
| 2   | B     | 84  | DG   | P-O3'-C3'   | 5.60  | 128.61      | 120.20   | 13     | 1     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 2   | B     | 94  | DC   | C5'-C4'-O4' | -5.60 | 101.00      | 109.40   | 10     | 2     |
| 3   | P     | 18  | GLU  | CA-C-O      | -5.59 | 114.94      | 120.70   | 18     | 1     |
| 1   | A     | 78  | DC   | P-O3'-C3'   | 5.59  | 128.59      | 120.20   | 20     | 1     |
| 1   | A     | 69  | DG   | N1-C6-O6    | -5.59 | 111.61      | 120.00   | 19     | 2     |
| 1   | A     | 77  | DC   | C5-C4-N4    | 5.58  | 128.67      | 120.30   | 4      | 1     |
| 1   | A     | 75  | DA   | O4'-C1'-C2' | -5.58 | 98.03       | 106.40   | 10     | 2     |
| 1   | A     | 80  | DC   | O4'-C4'-C3' | 5.57  | 113.75      | 105.40   | 16     | 2     |
| 1   | A     | 76  | DT   | N3-C2-O2    | -5.57 | 113.65      | 122.00   | 7      | 1     |
| 2   | B     | 85  | DG   | C3'-C2'-C1' | -5.56 | 93.27       | 101.60   | 1      | 1     |
| 2   | B     | 86  | DG   | P-O5'-C5'   | 5.56  | 128.34      | 120.00   | 6      | 1     |
| 3   | P     | 16  | GLU  | N-CA-C      | -5.55 | 105.13      | 111.07   | 10     | 3     |
| 1   | A     | 74  | DA   | O3'-P-O5'   | -5.55 | 95.67       | 104.00   | 13     | 2     |
| 2   | B     | 83  | DG   | C2'-C3'-O3' | 5.55  | 119.82      | 111.50   | 2      | 3     |
| 2   | B     | 87  | DA   | O4'-C1'-C2' | -5.55 | 98.08       | 106.40   | 3      | 1     |
| 2   | B     | 90  | DA   | C5'-C4'-C3' | -5.55 | 106.58      | 114.90   | 9      | 1     |
| 3   | P     | 18  | GLU  | CA-C-N      | 5.54  | 127.70      | 120.28   | 10     | 1     |
| 3   | P     | 18  | GLU  | C-N-CA      | 5.54  | 127.70      | 120.28   | 10     | 1     |
| 3   | P     | 48  | ILE  | N-CA-CB     | 5.53  | 117.39      | 110.47   | 15     | 1     |
| 1   | A     | 73  | DT   | C4'-C3'-C2' | -5.53 | 94.11       | 102.40   | 11     | 1     |
| 1   | A     | 76  | DT   | C6-C5-C7    | -5.53 | 115.71      | 124.00   | 18     | 1     |
| 2   | B     | 85  | DG   | O4'-C1'-C2' | -5.53 | 98.11       | 106.40   | 2      | 1     |
| 2   | B     | 93  | DG   | C5'-C4'-C3' | -5.53 | 106.61      | 114.90   | 20     | 1     |
| 2   | B     | 83  | DG   | N9-C1'-C2'  | 5.50  | 121.75      | 113.50   | 20     | 1     |
| 3   | P     | 49  | TRP  | CD2-CE3-CZ3 | 5.50  | 125.75      | 118.60   | 3      | 1     |
| 3   | P     | 22  | LEU  | O-C-N       | -5.50 | 116.29      | 122.12   | 17     | 1     |
| 3   | P     | 36  | SER  | CA-C-O      | 5.49  | 126.37      | 120.55   | 7      | 2     |
| 1   | A     | 80  | DC   | O5'-C5'-C4' | 5.49  | 119.04      | 110.80   | 19     | 1     |
| 1   | A     | 70  | DC   | C2-N1-C1'   | -5.49 | 111.46      | 119.70   | 4      | 1     |
| 3   | P     | 19  | GLN  | CA-C-O      | -5.49 | 114.73      | 120.55   | 20     | 2     |
| 3   | P     | 46  | VAL  | CA-CB-CG1   | 5.49  | 119.73      | 110.40   | 15     | 1     |
| 1   | A     | 72  | DC   | C5'-C4'-C3' | 5.48  | 123.12      | 114.90   | 9      | 1     |
| 1   | A     | 78  | DC   | N3-C2-O2    | -5.48 | 113.69      | 121.90   | 12     | 2     |
| 1   | A     | 78  | DC   | N1-C1'-C2'  | 5.48  | 121.72      | 113.50   | 18     | 1     |
| 1   | A     | 81  | DG   | C5-N7-C8    | -5.48 | 95.99       | 104.20   | 10     | 1     |
| 1   | A     | 77  | DC   | O4'-C4'-C3' | 5.48  | 113.61      | 105.40   | 19     | 1     |
| 2   | B     | 94  | DC   | N1-C1'-C2'  | 5.47  | 121.71      | 113.50   | 3      | 1     |
| 1   | A     | 75  | DA   | C5'-C4'-C3' | 5.47  | 123.11      | 114.90   | 13     | 1     |
| 1   | A     | 80  | DC   | N1-C1'-C2'  | 5.46  | 121.70      | 113.50   | 17     | 3     |
| 3   | P     | 49  | TRP  | NE1-CE2-CD2 | -5.46 | 100.31      | 107.40   | 3      | 1     |
| 1   | A     | 81  | DG   | C6-C5-N7    | 5.46  | 138.29      | 130.10   | 11     | 1     |
| 3   | P     | 26  | TYR  | O-C-N       | -5.46 | 116.89      | 123.27   | 9      | 1     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 1   | A     | 73  | DT   | O4'-C4'-C3' | 5.45  | 113.58      | 105.40   | 13     | 1     |
| 1   | A     | 75  | DA   | C5-C6-N1    | 5.44  | 125.76      | 117.60   | 7      | 3     |
| 1   | A     | 81  | DG   | C1'-O4'-C4' | -5.43 | 101.55      | 109.70   | 1      | 2     |
| 1   | A     | 77  | DC   | P-O3'-C3'   | 5.43  | 128.35      | 120.20   | 7      | 2     |
| 1   | A     | 69  | DG   | C4'-C3'-O3' | -5.43 | 101.85      | 110.00   | 6      | 1     |
| 1   | A     | 81  | DG   | O5'-C5'-C4' | 5.42  | 118.92      | 110.80   | 7      | 2     |
| 1   | A     | 72  | DC   | O4'-C1'-N1  | 5.42  | 116.52      | 108.40   | 3      | 2     |
| 1   | A     | 75  | DA   | C4'-C3'-O3' | -5.41 | 101.89      | 110.00   | 2      | 3     |
| 3   | P     | 35  | LEU  | N-CA-CB     | 5.39  | 118.04      | 110.12   | 17     | 1     |
| 1   | A     | 72  | DC   | N3-C2-O2    | -5.38 | 113.83      | 121.90   | 14     | 1     |
| 3   | P     | 43  | THR  | CA-C-O      | 5.38  | 126.44      | 120.63   | 10     | 1     |
| 2   | B     | 87  | DA   | C4'-C3'-O3' | -5.38 | 101.94      | 110.00   | 19     | 1     |
| 3   | P     | 17  | LEU  | CD1-CG-CD2  | -5.37 | 98.99       | 110.80   | 13     | 3     |
| 1   | A     | 74  | DA   | O4'-C1'-N9  | -5.37 | 100.35      | 108.40   | 5      | 1     |
| 1   | A     | 79  | DC   | C5'-C4'-C3' | -5.37 | 106.85      | 114.90   | 6      | 1     |
| 3   | P     | 34  | ASP  | CA-CB-CG    | 5.35  | 117.95      | 112.60   | 15     | 1     |
| 1   | A     | 73  | DT   | C5'-C4'-O4' | 5.35  | 117.43      | 109.40   | 5      | 1     |
| 2   | B     | 90  | DA   | C3'-C2'-C1' | -5.34 | 93.59       | 101.60   | 11     | 1     |
| 1   | A     | 76  | DT   | O4'-C1'-C2' | 5.34  | 114.41      | 106.40   | 18     | 1     |
| 3   | P     | 43  | THR  | OG1-CB-CG2  | -5.34 | 98.63       | 109.30   | 4      | 1     |
| 3   | P     | 51  | LYS  | CG-CD-CE    | 5.34  | 123.57      | 111.30   | 12     | 1     |
| 2   | B     | 86  | DG   | C5'-C4'-C3' | 5.33  | 122.90      | 114.90   | 7      | 1     |
| 2   | B     | 85  | DG   | C5'-C4'-C3' | -5.31 | 106.93      | 114.90   | 14     | 3     |
| 2   | B     | 92  | DA   | C2'-C3'-O3' | -5.31 | 103.54      | 111.50   | 10     | 3     |
| 2   | B     | 90  | DA   | P-O3'-C3'   | 5.31  | 128.16      | 120.20   | 12     | 2     |
| 1   | A     | 78  | DC   | C2-N3-C4    | -5.30 | 112.04      | 120.00   | 6      | 1     |
| 3   | P     | 47  | LYS  | N-CA-C      | 5.30  | 117.06      | 111.28   | 7      | 1     |
| 2   | B     | 86  | DG   | N1-C6-O6    | -5.30 | 112.05      | 120.00   | 5      | 2     |
| 2   | B     | 91  | DG   | C3'-C2'-C1' | 5.30  | 109.55      | 101.60   | 8      | 2     |
| 1   | A     | 77  | DC   | N3-C4-N4    | -5.30 | 109.95      | 117.90   | 4      | 1     |
| 2   | B     | 86  | DG   | C8-N9-C1'   | -5.30 | 119.05      | 127.00   | 2      | 1     |
| 3   | P     | 11  | SER  | N-CA-C      | 5.29  | 117.73      | 111.33   | 20     | 1     |
| 2   | B     | 88  | DT   | C1'-O4'-C4' | -5.28 | 101.78      | 109.70   | 3      | 2     |
| 3   | P     | 28  | THR  | CA-CB-OG1   | 5.28  | 117.51      | 109.60   | 9      | 1     |
| 2   | B     | 89  | DT   | O4'-C1'-C2' | 5.27  | 114.31      | 106.40   | 2      | 2     |
| 3   | P     | 40  | ALA  | O-C-N       | 5.26  | 129.75      | 123.33   | 13     | 1     |
| 3   | P     | 35  | LEU  | O-C-N       | -5.26 | 116.16      | 122.15   | 6      | 1     |
| 3   | P     | 31  | ARG  | N-CA-C      | 5.26  | 117.42      | 111.11   | 13     | 1     |
| 3   | P     | 20  | HIS  | CA-C-N      | 5.26  | 127.28      | 120.44   | 14     | 1     |
| 3   | P     | 20  | HIS  | C-N-CA      | 5.26  | 127.28      | 120.44   | 14     | 1     |
| 1   | A     | 72  | DC   | C1'-O4'-C4' | -5.26 | 101.81      | 109.70   | 18     | 1     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 3   | P     | 50  | PHE  | N-CA-CB     | 5.25  | 117.58      | 109.91   | 6      | 2     |
| 1   | A     | 81  | DG   | C4'-C3'-O3' | 5.25  | 117.88      | 110.00   | 14     | 1     |
| 1   | A     | 80  | DC   | C4'-C3'-O3' | -5.25 | 102.12      | 110.00   | 4      | 1     |
| 3   | P     | 13  | GLN  | OE1-CD-NE2  | -5.24 | 117.36      | 122.60   | 9      | 2     |
| 2   | B     | 94  | DC   | C2'-C3'-O3' | -5.24 | 103.63      | 111.50   | 18     | 1     |
| 3   | P     | 32  | LEU  | CB-CA-C     | 5.24  | 119.20      | 110.81   | 11     | 1     |
| 1   | A     | 75  | DA   | C6-C5-N7    | 5.24  | 140.16      | 132.30   | 15     | 1     |
| 2   | B     | 90  | DA   | C4-C5-C6    | -5.23 | 109.05      | 116.90   | 10     | 1     |
| 3   | P     | 49  | TRP  | NE1-CE2-CZ2 | 5.23  | 137.94      | 130.10   | 3      | 1     |
| 2   | B     | 93  | DG   | N1-C2-N2    | -5.23 | 108.45      | 116.30   | 12     | 1     |
| 3   | P     | 34  | ASP  | N-CA-C      | 5.23  | 116.66      | 111.07   | 1      | 1     |
| 2   | B     | 88  | DT   | P-O3'-C3'   | 5.23  | 128.04      | 120.20   | 19     | 1     |
| 2   | B     | 92  | DA   | C4-C5-C6    | -5.22 | 109.07      | 116.90   | 1      | 1     |
| 1   | A     | 71  | DT   | P-O3'-C3'   | 5.22  | 128.03      | 120.20   | 12     | 2     |
| 3   | P     | 39  | LEU  | N-CA-C      | 5.22  | 116.97      | 111.28   | 13     | 1     |
| 1   | A     | 70  | DC   | C5'-C4'-C3' | 5.22  | 122.72      | 114.90   | 17     | 1     |
| 2   | B     | 86  | DG   | N1-C2-N2    | 5.22  | 124.12      | 116.30   | 18     | 1     |
| 1   | A     | 78  | DC   | C4'-C3'-O3' | -5.21 | 102.18      | 110.00   | 18     | 1     |
| 1   | A     | 77  | DC   | C5'-C4'-O4' | 5.21  | 117.21      | 109.40   | 18     | 1     |
| 3   | P     | 31  | ARG  | CA-CB-CG    | 5.21  | 124.51      | 114.10   | 11     | 1     |
| 1   | A     | 71  | DT   | C2-N1-C1'   | -5.21 | 111.54      | 119.35   | 2      | 1     |
| 3   | P     | 16  | GLU  | CA-C-N      | 5.20  | 127.20      | 120.44   | 8      | 1     |
| 3   | P     | 16  | GLU  | C-N-CA      | 5.20  | 127.20      | 120.44   | 8      | 1     |
| 1   | A     | 77  | DC   | N1-C1'-C2'  | 5.18  | 121.27      | 113.50   | 16     | 1     |
| 1   | A     | 73  | DT   | P-O3'-C3'   | 5.18  | 127.97      | 120.20   | 4      | 1     |
| 3   | P     | 51  | LYS  | CB-CG-CD    | 5.18  | 123.21      | 111.30   | 13     | 1     |
| 2   | B     | 84  | DG   | C5-C6-N1    | 5.17  | 119.46      | 111.70   | 19     | 1     |
| 1   | A     | 81  | DG   | N7-C8-N9    | 5.17  | 121.25      | 113.50   | 10     | 1     |
| 1   | A     | 69  | DG   | C2'-C3'-O3' | 5.17  | 119.25      | 111.50   | 15     | 1     |
| 1   | A     | 76  | DT   | C5-C4-O4    | 5.15  | 130.32      | 122.60   | 10     | 2     |
| 3   | P     | 26  | TYR  | CB-CG-CD1   | 5.14  | 128.52      | 120.80   | 8      | 1     |
| 3   | P     | 21  | PHE  | CA-C-N      | 5.14  | 127.68      | 120.28   | 8      | 1     |
| 3   | P     | 21  | PHE  | C-N-CA      | 5.14  | 127.68      | 120.28   | 8      | 1     |
| 1   | A     | 77  | DC   | C5'-C4'-C3' | -5.13 | 107.20      | 114.90   | 20     | 1     |
| 3   | P     | 28  | THR  | N-CA-C      | -5.13 | 101.50      | 109.14   | 13     | 1     |
| 1   | A     | 76  | DT   | P-O5'-C5'   | 5.12  | 127.69      | 120.00   | 5      | 1     |
| 2   | B     | 85  | DG   | C4'-C3'-O3' | 5.11  | 117.67      | 110.00   | 13     | 1     |
| 3   | P     | 46  | VAL  | CG1-CB-CG2  | -5.11 | 99.56       | 110.80   | 4      | 1     |
| 1   | A     | 69  | DG   | C4-N9-C1'   | -5.11 | 119.34      | 127.00   | 3      | 1     |
| 2   | B     | 87  | DA   | C4-C5-C6    | -5.11 | 109.24      | 116.90   | 9      | 1     |
| 2   | B     | 91  | DG   | C4'-C3'-O3' | -5.10 | 102.34      | 110.00   | 14     | 1     |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|-------|-------------|----------|--------|-------|
|     |       |     |      |             |       |             |          | Worst  | Total |
| 2   | B     | 91  | DG   | P-O3'-C3'   | 5.10  | 127.85      | 120.20   | 16     | 2     |
| 2   | B     | 90  | DA   | O3'-P-O5'   | 5.10  | 111.65      | 104.00   | 1      | 1     |
| 2   | B     | 92  | DA   | O4'-C1'-N9  | 5.10  | 116.05      | 108.40   | 1      | 1     |
| 1   | A     | 81  | DG   | C5'-C4'-O4' | -5.10 | 101.75      | 109.40   | 19     | 1     |
| 3   | P     | 51  | LYS  | CB-CA-C     | -5.10 | 103.11      | 110.96   | 15     | 1     |
| 1   | A     | 70  | DC   | C1'-O4'-C4' | 5.09  | 117.34      | 109.70   | 5      | 1     |
| 3   | P     | 46  | VAL  | CA-C-O      | -5.09 | 115.77      | 121.17   | 1      | 1     |
| 2   | B     | 89  | DT   | C4'-C3'-O3' | -5.08 | 102.37      | 110.00   | 4      | 1     |
| 3   | P     | 13  | GLN  | N-CA-C      | -5.08 | 105.66      | 111.14   | 2      | 1     |
| 2   | B     | 85  | DG   | C5-C6-O6    | 5.07  | 135.91      | 128.30   | 3      | 1     |
| 3   | P     | 11  | SER  | CA-CB-OG    | 5.07  | 121.23      | 111.10   | 15     | 1     |
| 2   | B     | 90  | DA   | C4-N9-C1'   | -5.06 | 119.46      | 127.05   | 16     | 1     |
| 1   | A     | 71  | DT   | C2'-C3'-O3' | 5.06  | 119.09      | 111.50   | 18     | 1     |
| 2   | B     | 91  | DG   | N1-C2-N3    | 5.05  | 131.58      | 124.00   | 11     | 1     |
| 1   | A     | 71  | DT   | C5'-C4'-O4' | 5.05  | 116.97      | 109.40   | 7      | 1     |
| 2   | B     | 93  | DG   | N9-C1'-C2'  | 5.05  | 121.07      | 113.50   | 19     | 1     |
| 1   | A     | 80  | DC   | C5'-C4'-C3' | -5.04 | 107.34      | 114.90   | 2      | 1     |
| 3   | P     | 49  | TRP  | CA-C-N      | 5.04  | 127.34      | 120.54   | 5      | 1     |
| 3   | P     | 49  | TRP  | C-N-CA      | 5.04  | 127.34      | 120.54   | 5      | 1     |
| 3   | P     | 33  | ALA  | CA-C-N      | 5.04  | 126.99      | 120.44   | 9      | 1     |
| 3   | P     | 33  | ALA  | C-N-CA      | 5.04  | 126.99      | 120.44   | 9      | 1     |
| 1   | A     | 76  | DT   | C4'-C3'-O3' | 5.04  | 117.55      | 110.00   | 3      | 1     |
| 3   | P     | 51  | LYS  | N-CA-CB     | 5.03  | 117.25      | 109.91   | 15     | 1     |
| 1   | A     | 75  | DA   | O4'-C1'-N9  | -5.02 | 100.86      | 108.40   | 16     | 2     |
| 2   | B     | 84  | DG   | N3-C4-C5    | -5.02 | 120.87      | 128.40   | 8      | 1     |
| 1   | A     | 74  | DA   | C6-C5-N7    | 5.02  | 139.83      | 132.30   | 4      | 1     |
| 3   | P     | 16  | GLU  | O-C-N       | 5.02  | 127.24      | 122.07   | 12     | 1     |
| 2   | B     | 84  | DG   | C3'-C2'-C1' | 5.01  | 109.12      | 101.60   | 14     | 1     |
| 1   | A     | 77  | DC   | P-O5'-C5'   | 5.01  | 127.52      | 120.00   | 4      | 1     |
| 2   | B     | 85  | DG   | C4-N9-C1'   | -5.00 | 119.50      | 127.00   | 2      | 1     |
| 1   | A     | 79  | DC   | O4'-C1'-N1  | 5.00  | 115.91      | 108.40   | 5      | 1     |
| 2   | B     | 87  | DA   | C5'-C4'-C3' | -5.00 | 107.40      | 114.90   | 9      | 1     |
| 2   | B     | 82  | DC   | C2-N3-C4    | -5.00 | 112.49      | 120.00   | 16     | 1     |
| 2   | B     | 90  | DA   | P-O5'-C5'   | 5.00  | 127.50      | 120.00   | 15     | 1     |

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 69  | DG   | Sidechain | 18             |

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| Mol | Chain | Res | Type | Group               | Models (Total) |
|-----|-------|-----|------|---------------------|----------------|
| 1   | A     | 81  | DG   | Sidechain           | 18             |
| 2   | B     | 91  | DG   | Sidechain           | 17             |
| 2   | B     | 85  | DG   | Sidechain           | 15             |
| 2   | B     | 93  | DG   | Sidechain           | 15             |
| 2   | B     | 84  | DG   | Sidechain           | 14             |
| 1   | A     | 75  | DA   | Sidechain           | 13             |
| 2   | B     | 82  | DC   | Sidechain           | 13             |
| 2   | B     | 83  | DG   | Sidechain           | 13             |
| 1   | A     | 76  | DT   | Sidechain           | 12             |
| 2   | B     | 86  | DG   | Sidechain           | 12             |
| 1   | A     | 73  | DT   | Sidechain           | 12             |
| 2   | B     | 92  | DA   | Sidechain           | 11             |
| 2   | B     | 88  | DT   | Sidechain           | 10             |
| 1   | A     | 74  | DA   | Sidechain           | 9              |
| 2   | B     | 89  | DT   | Sidechain           | 9              |
| 2   | B     | 87  | DA   | Sidechain           | 9              |
| 1   | A     | 70  | DC   | Sidechain           | 9              |
| 1   | A     | 78  | DC   | Sidechain           | 7              |
| 1   | A     | 72  | DC   | Sidechain           | 7              |
| 2   | B     | 90  | DA   | Sidechain           | 7              |
| 1   | A     | 71  | DT   | Sidechain           | 6              |
| 2   | B     | 94  | DC   | Sidechain           | 6              |
| 1   | A     | 79  | DC   | Sidechain           | 6              |
| 1   | A     | 80  | DC   | Sidechain           | 5              |
| 1   | A     | 77  | DC   | Sidechain           | 4              |
| 3   | P     | 20  | HIS  | Sidechain,Mainchain | 4              |
| 3   | P     | 26  | TYR  | Sidechain           | 3              |
| 3   | P     | 50  | PHE  | Sidechain           | 3              |
| 3   | P     | 31  | ARG  | Sidechain           | 3              |
| 3   | P     | 25  | ARG  | Sidechain           | 2              |
| 3   | P     | 42  | GLY  | Mainchain           | 1              |
| 3   | P     | 46  | VAL  | Mainchain           | 1              |
| 3   | P     | 21  | PHE  | Sidechain           | 1              |
| 3   | P     | 11  | SER  | Mainchain           | 1              |
| 3   | P     | 14  | ILE  | Mainchain           | 1              |
| 3   | P     | 38  | LYS  | Mainchain           | 1              |

## 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     | 257   | 148      | 140      | 0±0     |
| 2   | B     | 270   | 147      | 141      | 0±0     |
| 3   | P     | 332   | 344      | 344      | 3±2     |
| All | All   | 17180 | 12780    | 12492    | 65      |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 3:P:16:GLU:HB2  | 3:P:39:LEU:HD11 | 0.62     | 1.71        | 17     | 4     |
| 3:P:48:ILE:HD13 | 3:P:51:LYS:HE2  | 0.58     | 1.74        | 10     | 1     |
| 3:P:17:LEU:HD13 | 3:P:49:TRP:CG   | 0.56     | 2.35        | 14     | 1     |
| 3:P:13:GLN:HE22 | 3:P:41:LEU:HD21 | 0.55     | 1.58        | 15     | 2     |
| 3:P:17:LEU:CD2  | 3:P:39:LEU:HD11 | 0.53     | 2.33        | 9      | 5     |
| 3:P:39:LEU:HD13 | 3:P:41:LEU:HD12 | 0.52     | 1.82        | 16     | 1     |
| 3:P:27:LEU:HD11 | 3:P:46:VAL:HG12 | 0.52     | 1.81        | 13     | 3     |
| 3:P:27:LEU:HD12 | 3:P:47:LYS:HA   | 0.52     | 1.82        | 7      | 2     |
| 3:P:20:HIS:CD2  | 3:P:35:LEU:HD11 | 0.51     | 2.40        | 4      | 4     |
| 3:P:17:LEU:CD2  | 3:P:39:LEU:HD21 | 0.51     | 2.35        | 3      | 2     |
| 3:P:16:GLU:HB3  | 3:P:39:LEU:HD12 | 0.51     | 1.82        | 5      | 1     |
| 3:P:32:LEU:C    | 3:P:32:LEU:HD23 | 0.50     | 2.32        | 6      | 1     |
| 3:P:27:LEU:CD1  | 3:P:47:LYS:HA   | 0.49     | 2.37        | 18     | 1     |
| 3:P:29:ALA:N    | 3:P:30:PRO:HD2  | 0.48     | 2.23        | 16     | 1     |
| 3:P:27:LEU:HD13 | 3:P:32:LEU:CD1  | 0.47     | 2.40        | 4      | 1     |
| 2:B:85:DG:N7    | 3:P:51:LYS:HE3  | 0.47     | 2.25        | 3      | 1     |
| 3:P:35:LEU:HD12 | 3:P:39:LEU:CD2  | 0.47     | 2.39        | 19     | 1     |
| 2:B:93:DG:C5    | 2:B:94:DC:C4    | 0.47     | 3.03        | 17     | 1     |
| 3:P:21:PHE:CD1  | 3:P:21:PHE:C    | 0.47     | 2.93        | 15     | 2     |
| 3:P:17:LEU:HB3  | 3:P:49:TRP:CZ3  | 0.47     | 2.44        | 17     | 1     |
| 3:P:17:LEU:HD21 | 3:P:39:LEU:HD11 | 0.46     | 1.86        | 13     | 3     |
| 3:P:16:GLU:HB2  | 3:P:39:LEU:CD2  | 0.46     | 2.41        | 10     | 1     |
| 3:P:16:GLU:HB3  | 3:P:39:LEU:CD1  | 0.45     | 2.42        | 5      | 1     |
| 3:P:17:LEU:HG   | 3:P:39:LEU:HD21 | 0.45     | 1.89        | 6      | 2     |
| 2:B:82:DC:H2''  | 2:B:83:DG:C8    | 0.44     | 2.48        | 10     | 1     |
| 2:B:88:DT:H2'   | 2:B:89:DT:H72   | 0.43     | 1.90        | 4      | 1     |
| 3:P:16:GLU:HB3  | 3:P:39:LEU:HD21 | 0.43     | 1.89        | 7      | 1     |
| 2:B:93:DG:C2    | 2:B:94:DC:C2    | 0.43     | 3.07        | 14     | 1     |
| 3:P:27:LEU:HD11 | 3:P:50:PHE:CE2  | 0.43     | 2.49        | 17     | 1     |
| 3:P:32:LEU:C    | 3:P:32:LEU:CD2  | 0.43     | 2.92        | 6      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 3:P:20:HIS:HB2  | 3:P:35:LEU:HD11 | 0.43     | 1.91        | 17     | 1     |
| 3:P:32:LEU:HD21 | 3:P:43:THR:CA   | 0.42     | 2.44        | 7      | 1     |
| 3:P:21:PHE:CD2  | 3:P:25:ARG:HA   | 0.42     | 2.49        | 4      | 1     |
| 3:P:28:THR:H    | 3:P:31:ARG:HB2  | 0.42     | 1.75        | 8      | 1     |
| 1:A:75:DA:C2    | 1:A:76:DT:C2    | 0.42     | 3.08        | 10     | 1     |
| 3:P:27:LEU:HD21 | 3:P:50:PHE:CD2  | 0.42     | 2.50        | 17     | 1     |
| 3:P:17:LEU:HB3  | 3:P:49:TRP:CE3  | 0.41     | 2.50        | 17     | 1     |
| 3:P:49:TRP:CE3  | 3:P:50:PHE:CD2  | 0.41     | 3.07        | 15     | 1     |
| 1:A:76:DT:C4    | 1:A:77:DC:N4    | 0.41     | 2.89        | 11     | 1     |
| 3:P:32:LEU:HD21 | 3:P:43:THR:O    | 0.41     | 2.16        | 15     | 1     |
| 3:P:49:TRP:CE3  | 3:P:50:PHE:CE2  | 0.41     | 3.08        | 15     | 1     |
| 3:P:35:LEU:HG   | 3:P:39:LEU:HD11 | 0.41     | 1.91        | 3      | 1     |
| 3:P:17:LEU:HD21 | 3:P:46:VAL:HG13 | 0.40     | 1.93        | 5      | 1     |
| 3:P:17:LEU:HD21 | 3:P:39:LEU:HD21 | 0.40     | 1.93        | 5      | 1     |
| 3:P:32:LEU:CD2  | 3:P:43:THR:HB   | 0.40     | 2.47        | 1      | 1     |
| 3:P:13:GLN:HA   | 3:P:39:LEU:CD1  | 0.40     | 2.46        | 15     | 1     |

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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 |    |
|-----|-------|----------------|--------------|------------|------------|-------------|----|
| 3   | P     | 42/68 (62%)    | 40±1 (95±3%) | 2±1 (5±3%) | 0±0 (0±1%) | 31          | 76 |
| All | All   | 840/1360 (62%) | 799 (95%)    | 38 (5%)    | 3 (0%)     | 31          | 76 |

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 3   | P     | 40  | ALA  | 1              |
| 3   | P     | 27  | LEU  | 1              |
| 3   | P     | 24  | GLY  | 1              |

### 6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

| Mol | Chain | Analysed       | Rotameric    | Outliers    | Percentiles |
|-----|-------|----------------|--------------|-------------|-------------|
| 3   | P     | 34/59 (58%)    | 29±1 (85±4%) | 5±1 (15±4%) | 5 43        |
| All | All   | 680/1180 (58%) | 581 (85%)    | 99 (15%)    | 5 43        |

All 17 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) |
|-----|-------|-----|------|----------------|
| 3   | P     | 35  | LEU  | 20             |
| 3   | P     | 31  | ARG  | 11             |
| 3   | P     | 32  | LEU  | 10             |
| 3   | P     | 16  | GLU  | 9              |
| 3   | P     | 47  | LYS  | 7              |
| 3   | P     | 27  | LEU  | 6              |
| 3   | P     | 41  | LEU  | 5              |
| 3   | P     | 39  | LEU  | 4              |
| 3   | P     | 51  | LYS  | 4              |
| 3   | P     | 21  | PHE  | 4              |
| 3   | P     | 19  | GLN  | 4              |
| 3   | P     | 43  | THR  | 4              |
| 3   | P     | 26  | TYR  | 3              |
| 3   | P     | 45  | GLN  | 3              |
| 3   | P     | 46  | VAL  | 2              |
| 3   | P     | 38  | LYS  | 2              |
| 3   | P     | 12  | SER  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided