# Full wwPDB NMR Structure Validation Report (i)

Feb 13, 2022 – 11:07 PM EST

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|---|---|---|
| PDB ID | : | 1HRZ |
| Title | : | THE 3D STRUCTURE OF THE HUMAN SRY-DNA COMPLEX SOLVED BY MULTI-DIMENSIONAL HETERONUCLEAR-EDITED AND-FILTERED NMR |
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| Deposited on | : | 1995-05-09 |

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

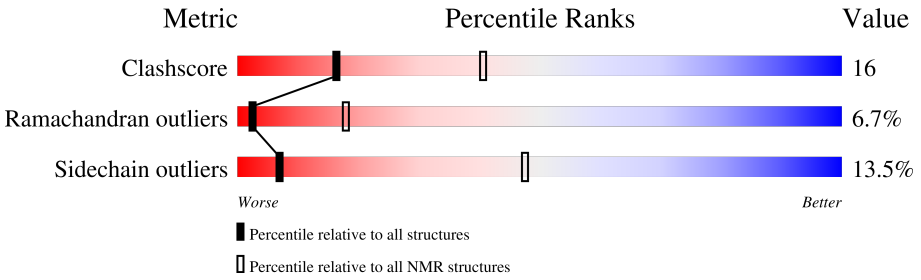
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| ShiftChecker | : | 2.26 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.26 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




| Metric | Whole archive (#Entries) | NMR archive (#Entries) |
|---|---|---|
| Clashscore | 158937 | 12864 |
| Ramachandran outliers | 154571 | 11451 |
| Sidechain outliers | 154315 | 11428 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | B | 8 | 38% 62% |
| 2 | C | 8 | 12% 50% 38% |
| 3 | A | 76 | 50% 38% 5% • • |

# 2 Ensemble composition and analysis (i)

This entry contains 35 models. Model 27 is the overall representative, medoid model (most similar to other models).

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

| Well-defined (core) protein residues | | | |
|---|---|---|---|
| **Well-defined core** | **Residue range (total)** | **Backbone RMSD (Å)** | **Medoid model** |
| 1 | A:5-A:75 (71) | 0.42 | 27 |

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

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

The models can be grouped into 9 clusters and 3 single-model clusters were found.

| Cluster number | Models |
|---|---|
| 1 | 18, 22, 23, 27, 28, 29 |
| 2 | 8, 16, 17, 25, 26, 33 |
| 3 | 3, 11, 13, 15, 34 |
| 4 | 6, 14, 30, 35 |
| 5 | 1, 5, 31 |
| 6 | 9, 20 |
| 7 | 12, 24 |
| 8 | 7, 32 |
| 9 | 2, 10 |
| Single-model clusters | 4; 19; 21 |

# 3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1794 atoms, of which 828 are hydrogens and 0 are deuteriums.

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

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | P | |
| 1 | B | 8 | 250 | 77 | 90 | 34 | 42 | 7 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | P | |
| 2 | C | 8 | 256 | 79 | 94 | 26 | 50 | 7 | 0 |

- Molecule 3 is a protein called HUMAN SRY.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | |
| 3 | A | 73 | 1288 | 409 | 644 | 123 | 107 | 5 | 0 |

# 4 Residue-property plots (i)

## 4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

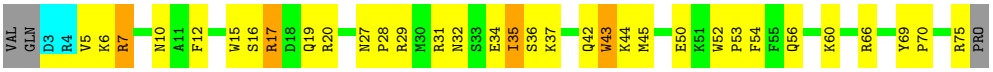
Chain B: 38% 62%

• Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 50% 38%

• Molecule 3: HUMAN SRY

Chain A: 50% 38% 5%




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

Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

• Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 38% 50% 12%

• Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 38% 50%

G9 T10 T11 T12 G13 T14 G15 C16

• Molecule 3: HUMAN SRY

Chain A: 49% 36% 9%

VAL GLN D3 R4 V5 K6 R7 N10 A11 F12 W15 S16 R17 D18 Q19 R20 N27 P28 R29 N32 S33 E34 I35 S36 Y41 Q42 W43 K44 M45 E50 K51 W52 P53 F54 E57 A58 Q59 K60 L61 Q62 R66 P70 R75 PRO

### 4.2.2 Score per residue for model 2

• Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 38% 62%

G1 C2 A3 C4 A5 A6 A7 C8

• Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 50% 38%

G9 T10 T11 T12 G13 T14 G15 C16

• Molecule 3: HUMAN SRY

Chain A: 51% 36% 5%

VAL GLN D3 R4 V5 K6 R7 N10 A11 F12 W15 S16 R17 D18 Q19 R29 M30 R31 N32 S33 E34 I35 S36 K37 Y41 Q42 W43 K44 M45 L46 T47 E50 K51 W52 P53 F54 F55 Q56 A63 E67 P70 N71 Y72 R75 PRO

### 4.2.3 Score per residue for model 3

• Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 12% 75% 12%

G1 C2 A3 C4 A5 A6 A7 C8

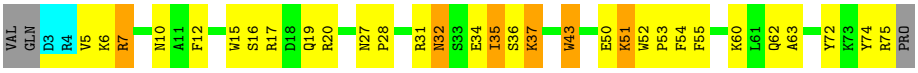
• Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 62% 25%

G9 T10 T11 T12 G13 T14 G15 C16

• Molecule 3: HUMAN SRY

Chain A: 53% 33% 8%



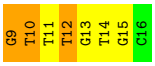

### 4.2.4 Score per residue for model 4

• Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 12% 88%

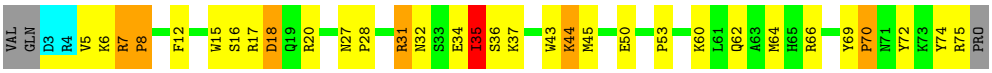
• Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 50% 38%




• Molecule 3: HUMAN SRY

Chain A: 51% 33% 8%




### 4.2.5 Score per residue for model 5

• Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

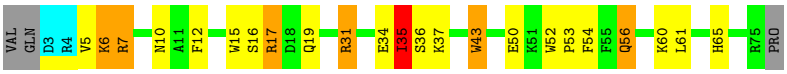
Chain B: 38% 50% 12%

• Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 38% 50%

• Molecule 3: HUMAN SRY

Chain A: 63% 21% 8%



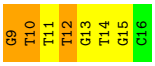

### 4.2.6 Score per residue for model 6

- Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 38% 50% 12%

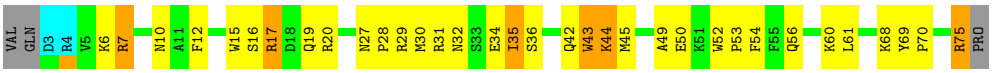
- Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 50% 38%




- Molecule 3: HUMAN SRY

Chain A: 49% 37% 8%



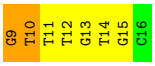

### 4.2.7 Score per residue for model 7

- Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 25% 62% 12%

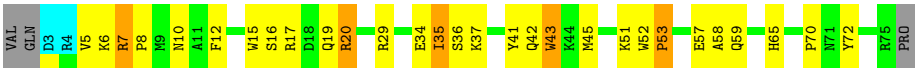
- Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 62% 25%




- Molecule 3: HUMAN SRY

Chain A: 55% 32% 7%



### 4.2.8 Score per residue for model 8

- Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 25% 62% 12%

G1 C2 A3 C4 A5 A6 A7 C8

- Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 50% 38%

G9 T10 T11 T12 G13 T14 G15 C16

- Molecule 3: HUMAN SRY

Chain A: 53% 29% 11%

VAL GLN D3 R4 R7 N10 V14 W15 S16 R17 D18 Q19 R20 R29 M30 R31 N32 S33 E34 I35 S36 K37 Q42 W43 K44 M45 E50 K51 W52 P53 F54 E57 A58 Q59 Q62 R66 Y69 P70 N71 Y72 R75 PRO

### 4.2.9 Score per residue for model 9

- Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 38% 62%

G1 C2 A3 C4 A5 A6 A7 C8

- Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 50% 38%

G9 T10 T11 T12 G13 T14 G15 C16

- Molecule 3: HUMAN SRY

Chain A: 53% 33% 7%

VAL GLN D3 R4 V5 K6 R7 N10 A11 F12 I13 V14 W15 S16 R17 D18 Q19 R20 R29 M30 R31 N32 S33 E34 I35 S36 Y41 Q42 W43 K44 M45 E50 P53 F54 K60 L61 H65 R66 Y72 R75 PRO

### 4.2.10 Score per residue for model 10

- Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 38% 62%

G1 C2 A3 C4 A5 A6 A7 C8

• Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 50% 38%

G9 T10 T11 T12 G13 T14 G15 C16

• Molecule 3: HUMAN SRY

Chain A: 49% 34% 9%

VAL GLN D3 R4 V5 K6 R7 W15 S16 R17 D18 Q19 R20 R21 R29 M30 R31 N32 S33 E34 I35 S36 K37 Q38 L39 Q42 W43 K44 M45 E50 K51 W52 P53 F54 F55 Q56 E57 A58 Q59 H65 R66 P70 R75 PRO

### 4.2.11 Score per residue for model 11

• Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 38% 62%

G1 C2 A3 C4 A5 A6 A7 C8

• Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 62% 25%

G9 T10 T11 T12 G13 T14 G15 C16

• Molecule 3: HUMAN SRY

Chain A: 57% 28% 7%

VAL GLN D3 R4 V5 K6 R7 W15 S16 R17 D18 Q19 R20 R31 E34 I35 S36 L39 G40 Y41 Q42 W43 K44 M45 E50 K51 W52 P53 F54 A63 E67 K68 Y69 P70 R75 PRO

### 4.2.12 Score per residue for model 12

• Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 25% 75%

G1 C2 A3 C4 A5 A6 A7 C8

• Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 38% 50%

G9 T10 T11 T12 G13 T14 G15 C16

• Molecule 3: HUMAN SRY

Chain A: 43% 42% 5%

VAL GLN D3 R4 V5 K6 R7 N10 A11 F12 W15 S16 R17 D18 Q19 R20 R21 K22 L25 E26 N27 P28 R29 M30 R31 N32 S33 E34 I35 S36 Y41 Q42 W43 K44 M45 E50 K51 W52 P53 F54 F55 Q56 E57 A58 Q59 K60 L61 M64 P70 N71 Y72 R75

PRO

### 4.2.13 Score per residue for model 13

• Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 38% 62%

G1 C2 A3 C4 A5 A6 A7 C8

• Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 50% 38%

G9 T10 T11 T12 G13 T14 G15 C16

• Molecule 3: HUMAN SRY

Chain A: 50% 36% 7%

VAL GLN D3 R4 V5 K6 R7 P8 M9 N10 A11 F12 I13 V14 W15 S16 Q19 R20 N27 P28 R31 E34 I35 S36 K37 W43 K44 M45 E50 P53 F54 E57 A58 Q59 A63 R66 E67 P70 K73 Y74 R75 PRO

### 4.2.14 Score per residue for model 14

• Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 25% 62% 12%

G1 C2 A3 C4 A5 A6 A7 C8

• Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 50% 38%

G9 T10 T11 T12 G13 T14 G15 C16

• Molecule 3: HUMAN SRY

Chain A: 57% 21% 14%

VAL GLN D3 R4 V5 K6 R7 W15 S16 R17 D18 Q19 R20 R29 M30 R31 N32 S33 E34 I35 S36 K37 Q42 W43 K44 M45 E50 K51 W52 P53 F54 F55 Q56 K60 L61 R66 Y69 P70 R75 PRO

### 4.2.15 Score per residue for model 15

• Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 12% 88%

G1 C2 A3 C4 A5 A6 A7 C8

• Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 50% 38%

G9 T10 T11 T12 G13 T14 G15 C16

• Molecule 3: HUMAN SRY

Chain A: 39% 41% 12%

VAL GLN D3 R4 V5 K6 R7 P8 M9 F12 W15 S16 R17 R20 R21 K22 N27 P28 R31 N32 S33 E34 I35 S36 K37 Q42 W43 K44 M45 E50 K51 W52 P53 F54 F55 Q56 E57 A58 Q59 K60 A63 M64 H65 R66 E67 K68 Y69 P70 N71 Y72 R75

PRO

### 4.2.16 Score per residue for model 16

• Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 38% 62%

G1 C2 A3 C4 A5 A6 A7 C8

• Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 38% 50%

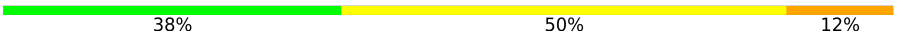
• Molecule 3: HUMAN SRY

Chain A:

### 4.2.17 Score per residue for model 17

• Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B:

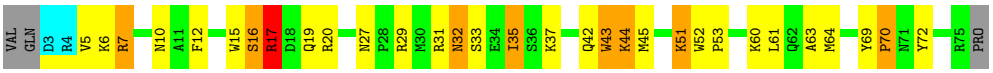


• Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C:

• Molecule 3: HUMAN SRY

Chain A:



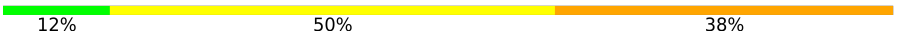

### 4.2.18 Score per residue for model 18

• Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B:

• Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C:



• Molecule 3: HUMAN SRY

Chain A: 57% 29% 8%

VAL GLN D3 R4 V5 K6 R7 N10 A11 F12 W15 S16 R17 D18 Q19 R20 R31 N32 S33 E34 I35 S36 K37 W43 E50 K51 W52 P53 F54 K60 L61 R66 P70 N71 R75 PRO

### 4.2.19 Score per residue for model 19

- Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 38% 62%

G1 C2 A3 C4 A5 A6 A7 C8

- Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 50% 38%

G9 T10 T11 T12 G13 T14 G15 C16

- Molecule 3: HUMAN SRY

Chain A: 51% 30% 11%

VAL GLN D3 R4 V5 K6 R7 P8 K9 N10 A11 F12 W15 S16 R17 D18 Q19 R20 R21 N27 P28 R29 M30 R31 N32 S33 E34 I35 S36 K37 W43 K44 M45 E50 K51 F54 E57 A58 Q59 K60 Y69 P70 Y74 R75 PRO

### 4.2.20 Score per residue for model 20

- Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 25% 75%

G1 C2 A3 C4 A5 A6 A7 C8

- Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 62% 25%

G9 T10 T11 T12 G13 T14 G15 C16

- Molecule 3: HUMAN SRY

Chain A: 54% 28% 12%

VAL GLN D3 R4 V5 K6 R7 N10 A11 F12 W15 S16 R17 D18 Q19 R20 R21 L25 E26 N27 P28 R31 N32 I35 S36 K37 Q42 W43 K44 M45 E50 K51 W52 P53 F54 F55 Q56 K60 L61 P70 R75 PRO

### 4.2.21 Score per residue for model 21

- Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 25% 75%

G1 C2 A3 C4 A5 A6 A7 C8

- Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 50% 38%

G9 T10 T11 T12 G13 T14 G15 C16

- Molecule 3: HUMAN SRY

Chain A: 57% 30% 7%

VAL GLN D3 R4 V5 K6 R7 N10 W15 S16 R17 D18 Q19 R20 P28 N32 S33 E34 I35 S36 K37 Q38 L39 Q42 W43 K44 M45 E50 K51 W52 P53 F54 F55 Q56 Q62 R66 R75 PRO

### 4.2.22 Score per residue for model 22

- Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 38% 38% 25%

G1 C2 A3 C4 A5 A6 A7 C8

- Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 25% 62%

G9 T10 T11 T12 G13 T14 G15 C16

- Molecule 3: HUMAN SRY

Chain A: 45% 38% 9%

VAL GLN D3 R4 V5 K6 R7 P8 M9 N10 A11 F12 W15 S16 R17 D18 Q19 R20 N27 P28 R29 M30 R31 N32 S33 E34 I35 S36 K37 Q42 W43 K44 M45 A49 E50 K51 W52 P53 F54 F55 Q56 Q62 A63 M64 H65 R66 E67 P70 Y74 R75 PRO

### 4.2.23 Score per residue for model 23

- Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 25% 75%

G1 C2 A3 C4 A5 A6 A7 C8

• Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 50% 38%

G9 T10 T11 T12 G13 T14 G15 C16

• Molecule 3: HUMAN SRY

Chain A: 51% 34% 8% • •

VAL GLN D3 R4 V5 K6 R7 F12 W15 S16 R17 D18 Q19 N27 P28 R31 E34 I35 S36 K37 Y41 Q42 W43 K44 M45 K51 W52 P53 Q56 E57 A58 Q59 K60 L61 Q62 P70 Y74 R75 PRO

### 4.2.24 Score per residue for model 24

• Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 38% 62%

G1 C2 A3 C4 A5 A6 A7 C8

• Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 50% 38%

G9 T10 T11 T12 G13 T14 G15 C16

• Molecule 3: HUMAN SRY

Chain A: 50% 37% 7% • •

VAL GLN D3 R4 V5 K6 R7 P8 M9 N10 A11 F12 W15 S16 R17 D18 Q19 P28 R31 N32 S33 E34 I35 S36 K37 Q42 W43 K44 M45 E50 K51 W52 P53 F54 F55 Q56 K60 L61 Q62 A63 M64 H65 R75 PRO

### 4.2.25 Score per residue for model 25

• Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 12% 62% 25%

G1 C2 A3 C4 A5 A6 A7 C8

• Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 50% 38%

G9 T10 T11 T12 G13 T14 G15 C16

• Molecule 3: HUMAN SRY

Chain A: 57% 26% 9%

VAL GLN D3 R4 V5 K6 R7 N10 A11 F12 W15 S16 R17 D18 Q19 R20 N27 P28 R29 N32 S33 E34 T35 S36 Q42 W43 K44 M45 W52 P53 Q56 K60 M64 Y69 P70 R75 PRO

### 4.2.26 Score per residue for model 26

• Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 25% 75%

G1 C2 A3 C4 A5 A6 A7 C8

• Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 62% 25%

G9 T10 T11 T12 G13 T14 G15 C16

• Molecule 3: HUMAN SRY

Chain A: 57% 29% 7%

VAL GLN D3 R4 V5 K6 R7 N10 A11 F12 W15 S16 R17 D18 Q19 R20 R21 R31 E34 T35 S36 K37 Y41 Q42 W43 W52 P53 F54 F55 Q56 A63 E67 K68 Y69 P70 N71 Y72 K73 Y74 R75 PRO

### 4.2.27 Score per residue for model 27 (medoid)

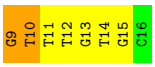
• Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 38% 62%

G1 C2 A3 C4 A5 A6 A7 C8

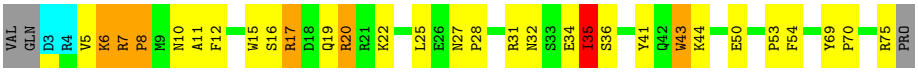
• Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 62% 25%




• Molecule 3: HUMAN SRY

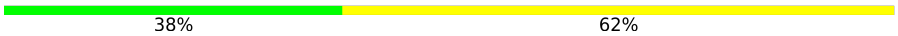
Chain A:




### 4.2.28 Score per residue for model 28

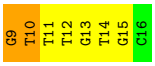
• Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B:



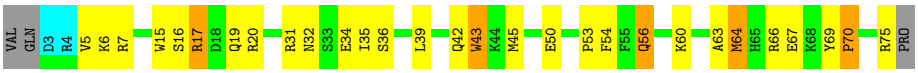
• Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C:




• Molecule 3: HUMAN SRY

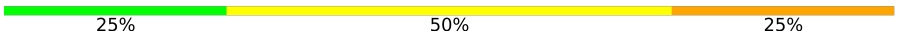
Chain A:




### 4.2.29 Score per residue for model 29

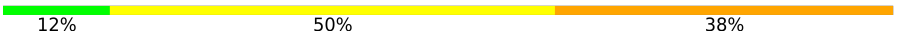
• Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B:



• Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C:



• Molecule 3: HUMAN SRY

Chain A: 42% 36% 14%

VAL GLN D3 R4 V5 K6 R7 P8 F12 W15 S16 R17 D18 Q19 R20 R21 K22 M23 N27 P28 R29 M30 R31 N32 S33 E34 I35 S36 Q42 W43 K44 M45 W52 P53 Q56 E57 A58 Q59 K60 L61 M64 H65 R66 Y69 P70 N71 Y72 K73 Y74 R75 PRO

### 4.2.30 Score per residue for model 30

- Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 25% 75%

G1 C2 A3 C4 A5 A6 A7 C8

- Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 50% 38%

G9 T10 T11 T12 G13 T14 G15 C16

- Molecule 3: HUMAN SRY

Chain A: 46% 39% 8%

VAL GLN D3 R4 V5 K6 R7 P8 F12 W15 S16 R17 D18 Q19 R20 N27 P28 R29 M30 R31 N32 S33 E34 I35 S36 Y41 Q42 W43 K44 M45 W52 P53 F54 F55 Q56 E57 A58 Q59 Q62 A63 R66 E67 K68 Y69 P70 R75 PRO

### 4.2.31 Score per residue for model 31

- Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 38% 50% 12%

G1 C2 A3 C4 A5 A6 A7 C8

- Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 50% 38%

G9 T10 T11 T12 G13 T14 G15 C16

- Molecule 3: HUMAN SRY

Chain A: 61% 25% 7%

VAL GLN D3 R4 V5 K6 R7 F12 W15 S16 R17 D18 Q19 R20 R31 E34 I35 S36 Q42 W43 K44 M45 E50 P53 F54 K60 L61 Q62 Y69 P70 R75 PRO

### 4.2.32 Score per residue for model 32

- Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 12% 75% 12%

G1 C2 A3 C4 A5 A6 A7 C8

- Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 38% 50%

G9 T10 T11 T12 G13 T14 G15 C16

- Molecule 3: HUMAN SRY

Chain A: 55% 26% 12%

VAL GLN D3 R4 V5 K6 R7 P8 W15 S16 R17 D18 Q19 R20 N32 S33 E34 I35 S36 K37 Q42 W43 K44 M45 L46 T47 E48 A49 E50 P53 E57 A58 Q59 Q62 A63 M64 H65 R66 E67 R75 PRO

### 4.2.33 Score per residue for model 33

- Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 38% 62%

G1 C2 A3 C4 A5 A6 A7 C8

- Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 38% 50%

G9 T10 T11 T12 G13 T14 G15 C16

- Molecule 3: HUMAN SRY

Chain A: 53% 32% 9%

VAL GLN D3 R4 V5 K6 R7 P8 M9 N10 A11 F12 W15 S16 R17 D18 Q19 R20 R21 R29 M30 R31 N32 S33 E34 I35 S36 Q42 W43 K44 M45 P53 E57 A58 Q59 H65 Y69 P70 N71 R75 PRO

### 4.2.34 Score per residue for model 34

- Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 38% 62%

G1 C2 A3 C4 A5 A6 A7 C8

• Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 62% 25%

G9 T10 T11 T12 G13 T14 G15 C16

• Molecule 3: HUMAN SRY

Chain A: 43% 36% 12%

VAL GLN D3 R4 V5 K6 R7 N10 A11 W15 S16 R17 D18 Q19 R20 R21 N27 P28 R31 N32 S33 E34 I35 S36 Q42 W43 K44 M45 E50 K51 W52 P53 F54 F55 Q56 E57 A58 Q59 K60 L61 R66 Y69 P70 N71 R75 PRO

### 4.2.35 Score per residue for model 35

• Molecule 1: DNA (5'-D(*GP*CP*AP*CP*AP*AP*AP*C)-3')

Chain B: 38% 62%

G1 C2 A3 C4 A5 A6 A7 C8

• Molecule 2: DNA (5'-D(*GP*TP*TP*TP*GP*TP*GP*C)-3')

Chain C: 12% 62% 25%

G9 T10 T11 T12 G13 T14 G15 C16

• Molecule 3: HUMAN SRY

Chain A: 53% 28% 12%

VAL GLN D3 R4 V5 K6 R7 P8 W15 S16 R17 D18 Q19 R29 M30 R31 N32 S33 E34 I35 S36 K37 Q38 L39 G40 Y41 Q42 W43 K44 M45 P53 F54 K60 L61 R66 E67 K68 Y69 Y72 R75 PRO

# 5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *?*.

Of the ? calculated structures, 35 were deposited, based on the following criterion: *?*.

The authors did not provide any information on software used for structure solution, optimization or refinement.

No chemical shift data was provided.

# 6 Model quality (i)

## 6.1 Standard geometry (i)

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #Z>5 | RMSZ | #Z>5 |
| 1 | B | 1.39±0.02 | 0±0/180 ( 0.0± 0.1%) | 2.88±0.01 | 16±1/275 ( 6.0± 0.2%) |
| 2 | C | 1.55±0.02 | 3±1/180 ( 1.8± 0.5%) | 2.67±0.01 | 15±1/277 ( 5.5± 0.5%) |
| 3 | A | 1.11±0.01 | 0±0/642 ( 0.0± 0.0%) | 0.96±0.01 | 0±0/858 ( 0.0± 0.0%) |
| All | All | 1.25 | 118/35070 ( 0.3%) | 1.89 | 1109/49350 ( 2.2%) |

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 | B | 1.0±0.0 | 0.0±0.0 |
| 2 | C | 1.0±0.0 | 0.0±0.0 |
| 3 | A | 0.0±0.0 | 0.0±0.2 |
| All | All | 70 | 1 |

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 |
| 2 | C | 14 | DT | C5-C7 | 6.52 | 1.53 | 1.50 | 11 | 35 |
| 2 | C | 11 | DT | C5-C7 | 6.46 | 1.53 | 1.50 | 27 | 32 |
| 2 | C | 10 | DT | C5-C7 | 6.07 | 1.53 | 1.50 | 8 | 26 |
| 2 | C | 12 | DT | C5-C7 | 6.00 | 1.53 | 1.50 | 18 | 23 |
| 1 | B | 1 | DG | N9-C8 | -5.21 | 1.34 | 1.37 | 8 | 2 |

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($^o$) | Ideal($^o$) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | B | 1 | DG | N7-C8-N9 | 14.37 | 120.28 | 113.10 | 25 | 35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 2 | C | 13 | DG | N7-C8-N9 | 14.29 | 120.24 | 113.10 | 3 | 35 |
| 2 | C | 15 | DG | N7-C8-N9 | 14.17 | 120.18 | 113.10 | 33 | 35 |
| 2 | C | 9 | DG | N7-C8-N9 | 14.14 | 120.17 | 113.10 | 9 | 35 |
| 1 | B | 6 | DA | N7-C8-N9 | 12.82 | 120.21 | 113.80 | 7 | 35 |
| 1 | B | 3 | DA | N7-C8-N9 | 12.73 | 120.17 | 113.80 | 11 | 35 |
| 1 | B | 7 | DA | N7-C8-N9 | 12.67 | 120.14 | 113.80 | 29 | 35 |
| 1 | B | 5 | DA | N7-C8-N9 | 12.62 | 120.11 | 113.80 | 25 | 35 |
| 2 | C | 13 | DG | C8-N9-C4 | -9.61 | 102.56 | 106.40 | 32 | 35 |
| 2 | C | 9 | DG | C8-N9-C4 | -9.49 | 102.61 | 106.40 | 22 | 35 |
| 1 | B | 1 | DG | C8-N9-C4 | -9.47 | 102.61 | 106.40 | 21 | 35 |
| 2 | C | 15 | DG | C8-N9-C4 | -9.46 | 102.62 | 106.40 | 14 | 35 |
| 1 | B | 6 | DA | C8-N9-C4 | -8.90 | 102.24 | 105.80 | 7 | 35 |
| 1 | B | 7 | DA | C8-N9-C4 | -8.88 | 102.25 | 105.80 | 14 | 35 |
| 1 | B | 5 | DA | C8-N9-C4 | -8.69 | 102.32 | 105.80 | 9 | 35 |
| 1 | B | 3 | DA | C8-N9-C4 | -8.47 | 102.41 | 105.80 | 27 | 35 |
| 2 | C | 9 | DG | C5-N7-C8 | -8.37 | 100.12 | 104.30 | 7 | 35 |
| 2 | C | 13 | DG | C5-N7-C8 | -8.27 | 100.16 | 104.30 | 1 | 35 |
| 1 | B | 1 | DG | C5-N7-C8 | -8.27 | 100.17 | 104.30 | 4 | 35 |
| 2 | C | 15 | DG | C5-N7-C8 | -8.20 | 100.20 | 104.30 | 16 | 35 |
| 1 | B | 3 | DA | C5-N7-C8 | -8.04 | 99.88 | 103.90 | 15 | 35 |
| 1 | B | 7 | DA | C5-N7-C8 | -7.80 | 100.00 | 103.90 | 8 | 35 |
| 1 | B | 5 | DA | C5-N7-C8 | -7.72 | 100.04 | 103.90 | 4 | 35 |
| 1 | B | 6 | DA | C5-N7-C8 | -7.67 | 100.07 | 103.90 | 9 | 35 |
| 1 | B | 5 | DA | O4'-C1'-N9 | 6.53 | 112.57 | 108.00 | 31 | 34 |
| 2 | C | 14 | DT | O4'-C1'-N1 | 6.50 | 112.55 | 108.00 | 7 | 12 |
| 2 | C | 10 | DT | C6-C5-C7 | -6.38 | 119.07 | 122.90 | 12 | 34 |
| 2 | C | 12 | DT | C6-C5-C7 | -6.34 | 119.10 | 122.90 | 5 | 34 |
| 1 | B | 7 | DA | O4'-C1'-N9 | 6.28 | 112.39 | 108.00 | 17 | 12 |
| 2 | C | 11 | DT | C6-C5-C7 | -6.21 | 119.17 | 122.90 | 6 | 18 |
| 2 | C | 15 | DG | O4'-C1'-N9 | 5.84 | 112.09 | 108.00 | 8 | 4 |
| 1 | B | 2 | DC | O4'-C1'-N1 | 5.80 | 112.06 | 108.00 | 15 | 2 |
| 2 | C | 14 | DT | C6-C5-C7 | -5.72 | 119.47 | 122.90 | 7 | 4 |
| 3 | A | 7 | ARG | NE-CZ-NH1 | 5.65 | 123.12 | 120.30 | 8 | 1 |
| 2 | C | 10 | DT | C4-C5-C6 | 5.57 | 121.34 | 118.00 | 11 | 35 |
| 2 | C | 13 | DG | O4'-C1'-N9 | 5.50 | 111.85 | 108.00 | 34 | 4 |
| 2 | C | 12 | DT | C4-C5-C6 | 5.43 | 121.26 | 118.00 | 4 | 33 |
| 2 | C | 12 | DT | O4'-C1'-N1 | 5.39 | 111.77 | 108.00 | 22 | 5 |
| 2 | C | 9 | DG | O4'-C1'-N9 | 5.36 | 111.75 | 108.00 | 14 | 12 |
| 1 | B | 3 | DA | O4'-C1'-N9 | 5.33 | 111.73 | 108.00 | 12 | 1 |
| 2 | C | 11 | DT | C4-C5-C6 | 5.30 | 121.18 | 118.00 | 5 | 19 |
| 2 | C | 14 | DT | C4-C5-C6 | 5.10 | 121.06 | 118.00 | 33 | 4 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | B | 1 | DG | O4'-C1'-N9 | 5.08 | 111.56 | 108.00 | 9 | 1 |

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

| Mol | Chain | Res | Type | Atoms | Models (Total) |
|---|---|---|---|---|---|
| 1 | B | 5 | DA | C3' | 35 |
| 2 | C | 9 | DG | C3' | 35 |

All unique planar outliers are listed below.

| Mol | Chain | Res | Type | Group | Models (Total) |
|---|---|---|---|---|---|
| 3 | A | 7 | ARG | Sidechain | 1 |

## 6.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|---|---|---|---|---|---|
| 1 | B | 160 | 90 | 90 | 1±1 |
| 2 | C | 162 | 94 | 94 | 2±1 |
| 3 | A | 625 | 627 | 627 | 26±5 |
| All | All | 33145 | 28385 | 28385 | 975 |

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 16.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 3:A:19:GLN:NE2 | 3:A:39:LEU:HD21 | 0.74 | 1.97 | 28 | 2 |
| 3:A:7:ARG:NE | 3:A:7:ARG:H | 0.70 | 1.84 | 14 | 8 |
| 3:A:5:VAL:HG12 | 3:A:6:LYS:H | 0.68 | 1.46 | 7 | 7 |
| 3:A:56:GLN:NE2 | 3:A:56:GLN:N | 0.67 | 2.43 | 16 | 9 |
| 3:A:56:GLN:H | 3:A:56:GLN:NE2 | 0.66 | 1.89 | 28 | 3 |
| 3:A:35:ILE:C | 3:A:35:ILE:HD13 | 0.65 | 2.12 | 20 | 31 |
| 3:A:56:GLN:NE2 | 3:A:56:GLN:H | 0.64 | 1.90 | 16 | 5 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 3:A:7:ARG:NE | 3:A:7:ARG:N | 0.64 | 2.46 | 3 | 5 |
| 3:A:7:ARG:CG | 3:A:7:ARG:HH11 | 0.63 | 2.06 | 8 | 3 |
| 3:A:31:ARG:NE | 3:A:31:ARG:H | 0.62 | 1.93 | 14 | 1 |
| 3:A:15:TRP:CE3 | 3:A:43:TRP:CH2 | 0.62 | 2.87 | 12 | 30 |
| 3:A:32:ASN:N | 3:A:32:ASN:ND2 | 0.62 | 2.47 | 32 | 2 |
| 3:A:7:ARG:HH11 | 3:A:7:ARG:H | 0.61 | 1.36 | 15 | 3 |
| 3:A:7:ARG:CD | 3:A:7:ARG:N | 0.60 | 2.64 | 1 | 11 |
| 3:A:64:MET:SD | 3:A:64:MET:N | 0.60 | 2.74 | 29 | 3 |
| 3:A:7:ARG:CG | 3:A:7:ARG:NH1 | 0.60 | 2.65 | 8 | 1 |
| 3:A:22:LYS:NZ | 3:A:23:MET:N | 0.59 | 2.50 | 29 | 1 |
| 3:A:5:VAL:HG12 | 3:A:6:LYS:N | 0.59 | 2.12 | 5 | 23 |
| 3:A:41:TYR:CE1 | 3:A:45:MET:SD | 0.59 | 2.95 | 35 | 1 |
| 3:A:20:ARG:HH11 | 3:A:20:ARG:CB | 0.58 | 2.12 | 7 | 3 |
| 3:A:15:TRP:O | 3:A:19:GLN:N | 0.58 | 2.37 | 33 | 32 |
| 3:A:27:ASN:N | 3:A:28:PRO:CD | 0.58 | 2.66 | 23 | 16 |
| 3:A:52:TRP:CD1 | 3:A:56:GLN:NE2 | 0.57 | 2.72 | 14 | 3 |
| 3:A:31:ARG:NE | 3:A:31:ARG:N | 0.57 | 2.51 | 14 | 1 |
| 3:A:19:GLN:NE2 | 3:A:22:LYS:NZ | 0.57 | 2.52 | 12 | 1 |
| 3:A:7:ARG:N | 3:A:7:ARG:CD | 0.57 | 2.67 | 3 | 4 |
| 3:A:22:LYS:HZ2 | 3:A:23:MET:N | 0.57 | 1.97 | 29 | 1 |
| 3:A:50:GLU:O | 3:A:54:PHE:CE2 | 0.57 | 2.58 | 19 | 21 |
| 3:A:69:TYR:N | 3:A:70:PRO:CD | 0.57 | 2.68 | 14 | 16 |
| 3:A:9:MET:SD | 3:A:9:MET:N | 0.57 | 2.77 | 15 | 2 |
| 3:A:5:VAL:O | 3:A:7:ARG:NH1 | 0.56 | 2.38 | 13 | 7 |
| 3:A:20:ARG:HH11 | 3:A:20:ARG:CG | 0.56 | 2.13 | 7 | 3 |
| 3:A:34:GLU:OE1 | 3:A:34:GLU:N | 0.56 | 2.38 | 22 | 3 |
| 3:A:31:ARG:O | 3:A:32:ASN:ND2 | 0.56 | 2.39 | 14 | 1 |
| 2:C:12:DT:O2 | 3:A:12:PHE:CD2 | 0.56 | 2.59 | 15 | 19 |
| 3:A:50:GLU:O | 3:A:54:PHE:CE1 | 0.56 | 2.59 | 18 | 2 |
| 3:A:52:TRP:O | 3:A:56:GLN:NE2 | 0.55 | 2.38 | 2 | 12 |
| 3:A:60:LYS:O | 3:A:64:MET:SD | 0.55 | 2.65 | 24 | 6 |
| 3:A:31:ARG:CG | 3:A:31:ARG:HH11 | 0.55 | 2.14 | 26 | 6 |
| 3:A:71:ASN:N | 3:A:71:ASN:HD22 | 0.55 | 2.00 | 18 | 4 |
| 3:A:5:VAL:O | 3:A:7:ARG:CZ | 0.55 | 2.55 | 11 | 3 |
| 3:A:29:ARG:CG | 3:A:29:ARG:HH11 | 0.54 | 2.16 | 8 | 7 |
| 3:A:32:ASN:N | 3:A:32:ASN:OD1 | 0.54 | 2.41 | 28 | 5 |
| 3:A:32:ASN:N | 3:A:32:ASN:HD22 | 0.54 | 2.00 | 32 | 2 |
| 3:A:14:VAL:HG11 | 3:A:54:PHE:CD1 | 0.54 | 2.37 | 9 | 3 |
| 3:A:16:SER:OG | 3:A:20:ARG:NH2 | 0.54 | 2.41 | 6 | 2 |
| 3:A:17:ARG:CA | 3:A:17:ARG:HH11 | 0.54 | 2.16 | 6 | 1 |
| 3:A:50:GLU:O | 3:A:54:PHE:CD2 | 0.54 | 2.61 | 19 | 11 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 3:A:34:GLU:O | 3:A:36:SER:N | 0.54 | 2.40 | 13 | 28 |
| 1:B:7:DA:C4 | 1:B:8:DC:C5 | 0.54 | 2.96 | 14 | 2 |
| 3:A:50:GLU:O | 3:A:54:PHE:CZ | 0.54 | 2.61 | 1 | 2 |
| 3:A:50:GLU:N | 3:A:50:GLU:OE1 | 0.54 | 2.40 | 3 | 2 |
| 3:A:29:ARG:CG | 3:A:29:ARG:NH1 | 0.54 | 2.71 | 8 | 2 |
| 3:A:75:ARG:CG | 3:A:75:ARG:NH1 | 0.53 | 2.71 | 1 | 6 |
| 3:A:70:PRO:O | 3:A:72:TYR:N | 0.53 | 2.42 | 12 | 3 |
| 3:A:15:TRP:CD2 | 3:A:43:TRP:CH2 | 0.53 | 2.97 | 27 | 9 |
| 1:B:1:DG:C5 | 1:B:2:DC:N4 | 0.53 | 2.76 | 29 | 4 |
| 3:A:7:ARG:HH11 | 3:A:7:ARG:N | 0.53 | 2.02 | 34 | 3 |
| 1:B:8:DC:O4' | 3:A:20:ARG:NH2 | 0.53 | 2.42 | 4 | 2 |
| 3:A:20:ARG:CG | 3:A:20:ARG:NH1 | 0.53 | 2.71 | 13 | 10 |
| 2:C:13:DG:H21 | 3:A:10:ASN:ND2 | 0.53 | 2.02 | 1 | 5 |
| 3:A:66:ARG:NH1 | 3:A:66:ARG:CG | 0.53 | 2.70 | 21 | 4 |
| 3:A:31:ARG:CG | 3:A:31:ARG:NH1 | 0.53 | 2.71 | 26 | 2 |
| 3:A:6:LYS:HZ1 | 3:A:65:HIS:CD2 | 0.52 | 2.22 | 10 | 1 |
| 3:A:10:ASN:N | 3:A:10:ASN:ND2 | 0.52 | 2.55 | 13 | 2 |
| 3:A:17:ARG:CG | 3:A:17:ARG:HH11 | 0.52 | 2.18 | 17 | 1 |
| 3:A:52:TRP:CD1 | 3:A:56:GLN:OE1 | 0.52 | 2.61 | 30 | 1 |
| 3:A:31:ARG:NH1 | 3:A:31:ARG:CG | 0.52 | 2.70 | 9 | 5 |
| 1:B:8:DC:O3' | 3:A:28:PRO:O | 0.52 | 2.27 | 21 | 1 |
| 3:A:56:GLN:N | 3:A:56:GLN:HE21 | 0.52 | 2.03 | 20 | 3 |
| 3:A:8:PRO:CG | 3:A:65:HIS:CE1 | 0.52 | 2.93 | 7 | 1 |
| 3:A:29:ARG:NH1 | 3:A:29:ARG:CG | 0.52 | 2.71 | 33 | 6 |
| 3:A:75:ARG:CG | 3:A:75:ARG:HH11 | 0.52 | 2.17 | 1 | 4 |
| 3:A:66:ARG:CG | 3:A:66:ARG:HH11 | 0.52 | 2.17 | 21 | 4 |
| 3:A:17:ARG:CG | 3:A:17:ARG:NH1 | 0.51 | 2.73 | 17 | 1 |
| 3:A:58:ALA:O | 3:A:62:GLN:NE2 | 0.51 | 2.42 | 23 | 1 |
| 3:A:66:ARG:CG | 3:A:66:ARG:NH1 | 0.51 | 2.72 | 34 | 1 |
| 3:A:5:VAL:O | 3:A:7:ARG:NE | 0.51 | 2.44 | 12 | 1 |
| 3:A:20:ARG:CG | 3:A:20:ARG:HH11 | 0.51 | 2.17 | 18 | 5 |
| 3:A:52:TRP:NE1 | 3:A:56:GLN:OE1 | 0.51 | 2.43 | 30 | 1 |
| 3:A:37:LYS:N | 3:A:37:LYS:CD | 0.51 | 2.74 | 14 | 10 |
| 1:B:8:DC:O4' | 3:A:20:ARG:NH1 | 0.51 | 2.43 | 32 | 4 |
| 3:A:62:GLN:NE2 | 3:A:63:ALA:N | 0.51 | 2.59 | 3 | 1 |
| 3:A:56:GLN:H | 3:A:56:GLN:HE21 | 0.51 | 1.49 | 16 | 1 |
| 3:A:65:HIS:CD2 | 3:A:65:HIS:N | 0.51 | 2.79 | 5 | 5 |
| 3:A:6:LYS:HZ1 | 3:A:65:HIS:CG | 0.51 | 2.23 | 10 | 1 |
| 3:A:41:TYR:CE2 | 3:A:45:MET:CE | 0.51 | 2.93 | 1 | 1 |
| 3:A:7:ARG:NH1 | 3:A:7:ARG:CG | 0.50 | 2.73 | 7 | 2 |
| 3:A:57:GLU:O | 3:A:59:GLN:N | 0.50 | 2.44 | 7 | 13 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 3:A:39:LEU:HD22 | 3:A:43:TRP:CH2 | 0.50 | 2.42 | 21 | 3 |
| 3:A:52:TRP:CE2 | 3:A:56:GLN:OE1 | 0.50 | 2.64 | 20 | 2 |
| 3:A:5:VAL:CG1 | 3:A:6:LYS:N | 0.50 | 2.74 | 35 | 15 |
| 3:A:31:ARG:O | 3:A:32:ASN:O | 0.50 | 2.30 | 15 | 4 |
| 3:A:18:ASP:N | 3:A:18:ASP:OD1 | 0.50 | 2.44 | 23 | 2 |
| 1:B:5:DA:O4' | 3:A:7:ARG:NH2 | 0.50 | 2.43 | 8 | 1 |
| 3:A:5:VAL:O | 3:A:7:ARG:NH2 | 0.50 | 2.45 | 12 | 2 |
| 3:A:6:LYS:H | 3:A:6:LYS:CD | 0.50 | 2.19 | 32 | 1 |
| 3:A:10:ASN:O | 3:A:12:PHE:N | 0.50 | 2.45 | 19 | 15 |
| 2:C:9:DG:HO5' | 2:C:10:DT:P | 0.50 | 2.30 | 3 | 6 |
| 3:A:47:THR:O | 3:A:49:ALA:N | 0.50 | 2.45 | 32 | 1 |
| 3:A:41:TYR:O | 3:A:45:MET:SD | 0.50 | 2.70 | 12 | 2 |
| 3:A:7:ARG:NH1 | 3:A:7:ARG:HG2 | 0.49 | 2.21 | 8 | 2 |
| 2:C:9:DG:N2 | 3:A:33:SER:OG | 0.49 | 2.45 | 17 | 1 |
| 3:A:17:ARG:N | 3:A:17:ARG:HE | 0.49 | 2.04 | 1 | 1 |
| 3:A:16:SER:OG | 3:A:20:ARG:CZ | 0.49 | 2.60 | 6 | 2 |
| 1:B:6:DA:C4' | 3:A:17:ARG:HH21 | 0.49 | 2.19 | 29 | 1 |
| 1:B:7:DA:O4' | 3:A:20:ARG:NH1 | 0.49 | 2.46 | 14 | 2 |
| 3:A:31:ARG:N | 3:A:31:ARG:CD | 0.49 | 2.75 | 14 | 1 |
| 3:A:34:GLU:N | 3:A:34:GLU:CD | 0.49 | 2.66 | 31 | 1 |
| 1:B:8:DC:C4' | 3:A:20:ARG:HH22 | 0.49 | 2.21 | 26 | 1 |
| 3:A:6:LYS:CD | 3:A:6:LYS:N | 0.49 | 2.76 | 32 | 1 |
| 3:A:27:ASN:N | 3:A:28:PRO:HD3 | 0.49 | 2.23 | 12 | 11 |
| 3:A:10:ASN:C | 3:A:12:PHE:N | 0.49 | 2.65 | 25 | 9 |
| 3:A:60:LYS:O | 3:A:61:LEU:C | 0.49 | 2.51 | 17 | 12 |
| 3:A:17:ARG:HH11 | 3:A:17:ARG:N | 0.49 | 2.06 | 6 | 1 |
| 1:B:6:DA:C1' | 3:A:17:ARG:NH2 | 0.49 | 2.76 | 29 | 1 |
| 1:B:4:DC:C4' | 3:A:7:ARG:HH21 | 0.48 | 2.21 | 15 | 1 |
| 3:A:41:TYR:C | 3:A:41:TYR:CD1 | 0.48 | 2.87 | 23 | 3 |
| 1:B:7:DA:O4' | 3:A:17:ARG:NH2 | 0.48 | 2.46 | 1 | 1 |
| 3:A:75:ARG:NE | 3:A:75:ARG:C | 0.48 | 2.67 | 26 | 1 |
| 3:A:31:ARG:CD | 3:A:31:ARG:N | 0.48 | 2.77 | 20 | 3 |
| 3:A:52:TRP:NE1 | 3:A:56:GLN:CD | 0.48 | 2.66 | 26 | 1 |
| 3:A:16:SER:O | 3:A:20:ARG:CB | 0.48 | 2.62 | 20 | 15 |
| 3:A:62:GLN:CD | 3:A:63:ALA:N | 0.48 | 2.66 | 16 | 2 |
| 3:A:44:LYS:C | 3:A:45:MET:SD | 0.48 | 2.92 | 17 | 19 |
| 3:A:75:ARG:HE | 3:A:75:ARG:C | 0.48 | 2.10 | 32 | 1 |
| 3:A:15:TRP:O | 3:A:19:GLN:CB | 0.48 | 2.62 | 23 | 13 |
| 3:A:71:ASN:N | 3:A:71:ASN:ND2 | 0.48 | 2.60 | 18 | 1 |
| 3:A:16:SER:O | 3:A:17:ARG:C | 0.47 | 2.51 | 8 | 25 |
| 3:A:17:ARG:N | 3:A:17:ARG:NH1 | 0.47 | 2.62 | 6 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 3:A:35:ILE:C | 3:A:35:ILE:CD1 | 0.47 | 2.82 | 8 | 3 |
| 3:A:6:LYS:NZ | 3:A:65:HIS:CD2 | 0.47 | 2.82 | 10 | 1 |
| 3:A:65:HIS:N | 3:A:65:HIS:CD2 | 0.47 | 2.80 | 24 | 3 |
| 3:A:34:GLU:C | 3:A:36:SER:N | 0.47 | 2.68 | 13 | 24 |
| 3:A:20:ARG:NH1 | 3:A:20:ARG:CG | 0.47 | 2.78 | 19 | 1 |
| 3:A:39:LEU:HD22 | 3:A:43:TRP:CZ2 | 0.47 | 2.45 | 21 | 1 |
| 3:A:7:ARG:NH2 | 3:A:74:TYR:OH | 0.47 | 2.47 | 19 | 2 |
| 3:A:62:GLN:O | 3:A:66:ARG:CG | 0.47 | 2.61 | 4 | 2 |
| 3:A:63:ALA:O | 3:A:67:GLU:CG | 0.47 | 2.63 | 26 | 8 |
| 1:B:4:DC:O3' | 3:A:7:ARG:NH2 | 0.47 | 2.47 | 15 | 1 |
| 3:A:7:ARG:O | 3:A:8:PRO:O | 0.46 | 2.33 | 4 | 4 |
| 1:B:5:DA:C4' | 3:A:7:ARG:HH21 | 0.46 | 2.23 | 8 | 1 |
| 3:A:7:ARG:N | 3:A:7:ARG:NE | 0.46 | 2.64 | 26 | 3 |
| 2:C:13:DG:H21 | 3:A:10:ASN:HD21 | 0.46 | 1.52 | 17 | 1 |
| 3:A:15:TRP:O | 3:A:16:SER:C | 0.46 | 2.54 | 4 | 19 |
| 3:A:41:TYR:CD1 | 3:A:41:TYR:C | 0.46 | 2.89 | 26 | 6 |
| 3:A:51:LYS:O | 3:A:52:TRP:C | 0.46 | 2.53 | 24 | 9 |
| 3:A:32:ASN:ND2 | 3:A:33:SER:H | 0.46 | 2.09 | 24 | 1 |
| 1:B:2:DC:N4 | 1:B:3:DA:N6 | 0.45 | 2.64 | 7 | 1 |
| 3:A:54:PHE:CE1 | 3:A:55:PHE:CE1 | 0.45 | 3.04 | 16 | 2 |
| 1:B:1:DG:C5 | 1:B:2:DC:C4 | 0.45 | 3.04 | 29 | 1 |
| 3:A:68:LYS:O | 3:A:69:TYR:CD1 | 0.45 | 2.70 | 35 | 1 |
| 2:C:9:DG:C2' | 2:C:10:DT:O5' | 0.45 | 2.64 | 3 | 35 |
| 3:A:42:GLN:O | 3:A:45:MET:C | 0.45 | 2.55 | 15 | 26 |
| 3:A:52:TRP:O | 3:A:56:GLN:OE1 | 0.45 | 2.35 | 22 | 5 |
| 3:A:63:ALA:O | 3:A:67:GLU:OE1 | 0.45 | 2.34 | 2 | 1 |
| 3:A:70:PRO:C | 3:A:72:TYR:H | 0.45 | 2.15 | 2 | 2 |
| 3:A:15:TRP:CE3 | 3:A:43:TRP:CZ2 | 0.45 | 3.05 | 21 | 4 |
| 3:A:75:ARG:NE | 3:A:75:ARG:H | 0.45 | 2.09 | 6 | 1 |
| 2:C:13:DG:N2 | 3:A:10:ASN:OD1 | 0.45 | 2.50 | 5 | 1 |
| 3:A:27:ASN:O | 3:A:30:MET:SD | 0.45 | 2.75 | 6 | 1 |
| 3:A:6:LYS:NZ | 3:A:65:HIS:CG | 0.45 | 2.85 | 10 | 1 |
| 1:B:3:DA:N3 | 3:A:74:TYR:CD2 | 0.45 | 2.85 | 22 | 1 |
| 3:A:50:GLU:CD | 3:A:50:GLU:N | 0.44 | 2.70 | 32 | 2 |
| 3:A:70:PRO:C | 3:A:72:TYR:N | 0.44 | 2.70 | 2 | 2 |
| 1:B:2:DC:C4 | 1:B:3:DA:N6 | 0.44 | 2.86 | 32 | 1 |
| 3:A:20:ARG:NH2 | 3:A:35:ILE:HD12 | 0.44 | 2.28 | 8 | 1 |
| 3:A:73:LYS:O | 3:A:74:TYR:O | 0.44 | 2.36 | 13 | 1 |
| 3:A:32:ASN:CG | 3:A:33:SER:N | 0.44 | 2.71 | 33 | 3 |
| 3:A:20:ARG:CG | 3:A:21:ARG:N | 0.44 | 2.81 | 19 | 3 |
| 1:B:8:DC:C5' | 3:A:20:ARG:HH22 | 0.44 | 2.25 | 26 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 3:A:35:ILE:HD13 | 3:A:35:ILE:O | 0.44 | 2.12 | 15 | 1 |
| 3:A:52:TRP:CZ2 | 3:A:56:GLN:OE1 | 0.44 | 2.70 | 29 | 2 |
| 1:B:1:DG:C6 | 1:B:2:DC:N4 | 0.44 | 2.85 | 29 | 1 |
| 3:A:62:GLN:NE2 | 3:A:63:ALA:CA | 0.43 | 2.81 | 3 | 1 |
| 3:A:49:ALA:HB3 | 3:A:50:GLU:OE1 | 0.43 | 2.13 | 22 | 2 |
| 3:A:60:LYS:O | 3:A:63:ALA:N | 0.43 | 2.51 | 24 | 2 |
| 1:B:8:DC:C1' | 3:A:20:ARG:NH2 | 0.43 | 2.81 | 4 | 1 |
| 3:A:54:PHE:C | 3:A:54:PHE:CD1 | 0.43 | 2.92 | 35 | 3 |
| 3:A:31:ARG:O | 3:A:32:ASN:OD1 | 0.43 | 2.36 | 3 | 1 |
| 3:A:32:ASN:CG | 3:A:33:SER:H | 0.43 | 2.16 | 16 | 2 |
| 3:A:47:THR:C | 3:A:49:ALA:N | 0.43 | 2.72 | 32 | 1 |
| 3:A:31:ARG:O | 3:A:32:ASN:CB | 0.43 | 2.66 | 14 | 1 |
| 1:B:7:DA:O3' | 3:A:20:ARG:NH1 | 0.43 | 2.51 | 31 | 2 |
| 3:A:69:TYR:N | 3:A:70:PRO:HD3 | 0.43 | 2.29 | 14 | 3 |
| 3:A:52:TRP:NE1 | 3:A:56:GLN:NE2 | 0.43 | 2.66 | 24 | 1 |
| 3:A:75:ARG:C | 3:A:75:ARG:NE | 0.43 | 2.72 | 32 | 1 |
| 1:B:8:DC:C1' | 3:A:20:ARG:HH22 | 0.43 | 2.27 | 4 | 1 |
| 3:A:32:ASN:OD1 | 3:A:33:SER:N | 0.43 | 2.52 | 16 | 2 |
| 3:A:54:PHE:CD1 | 3:A:54:PHE:C | 0.43 | 2.92 | 34 | 2 |
| 3:A:7:ARG:O | 3:A:7:ARG:CG | 0.42 | 2.66 | 5 | 1 |
| 3:A:67:GLU:OE1 | 3:A:67:GLU:N | 0.42 | 2.51 | 2 | 1 |
| 3:A:7:ARG:H | 3:A:7:ARG:CD | 0.42 | 2.27 | 6 | 1 |
| 3:A:62:GLN:O | 3:A:66:ARG:CB | 0.42 | 2.67 | 22 | 1 |
| 3:A:20:ARG:HH22 | 3:A:35:ILE:HD12 | 0.42 | 1.75 | 33 | 1 |
| 3:A:57:GLU:C | 3:A:59:GLN:N | 0.42 | 2.72 | 7 | 4 |
| 1:B:7:DA:N3 | 3:A:20:ARG:NH1 | 0.42 | 2.64 | 22 | 1 |
| 3:A:6:LYS:O | 3:A:6:LYS:CG | 0.42 | 2.66 | 15 | 1 |
| 3:A:19:GLN:HE21 | 3:A:39:LEU:HD21 | 0.42 | 1.66 | 28 | 1 |
| 1:B:6:DA:C1' | 3:A:17:ARG:HH21 | 0.42 | 2.27 | 29 | 1 |
| 3:A:20:ARG:HH11 | 3:A:20:ARG:HB3 | 0.42 | 1.74 | 10 | 3 |
| 2:C:15:DG:OP1 | 3:A:66:ARG:NH1 | 0.42 | 2.52 | 10 | 2 |
| 3:A:54:PHE:CE1 | 3:A:55:PHE:CD2 | 0.42 | 3.08 | 3 | 1 |
| 3:A:52:TRP:CE2 | 3:A:56:GLN:NE2 | 0.42 | 2.88 | 34 | 1 |
| 3:A:27:ASN:C | 3:A:29:ARG:H | 0.42 | 2.19 | 6 | 2 |
| 2:C:9:DG:O3' | 2:C:9:DG:O5' | 0.42 | 2.36 | 23 | 2 |
| 3:A:60:LYS:C | 3:A:64:MET:SD | 0.42 | 2.98 | 24 | 1 |
| 3:A:32:ASN:O | 3:A:34:GLU:N | 0.42 | 2.53 | 35 | 1 |
| 3:A:32:ASN:HD22 | 3:A:33:SER:H | 0.41 | 1.58 | 15 | 1 |
| 3:A:57:GLU:O | 3:A:58:ALA:C | 0.41 | 2.58 | 15 | 3 |
| 3:A:10:ASN:O | 3:A:11:ALA:C | 0.41 | 2.57 | 27 | 4 |
| 3:A:5:VAL:CG2 | 3:A:72:TYR:CD1 | 0.41 | 3.03 | 9 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 1:B:6:DA:C2' | 3:A:17:ARG:NH2 | 0.41 | 2.83 | 29 | 1 |
| 3:A:19:GLN:OE1 | 3:A:19:GLN:C | 0.41 | 2.59 | 19 | 2 |
| 3:A:5:VAL:CG1 | 3:A:69:TYR:CZ | 0.41 | 3.04 | 15 | 1 |
| 2:C:14:DT:C4 | 2:C:15:DG:O6 | 0.41 | 2.73 | 33 | 3 |
| 3:A:7:ARG:HH11 | 3:A:7:ARG:HG3 | 0.41 | 1.75 | 8 | 1 |
| 1:B:8:DC:C4' | 3:A:20:ARG:HH12 | 0.41 | 2.28 | 30 | 1 |
| 3:A:39:LEU:O | 3:A:40:GLY:C | 0.41 | 2.59 | 35 | 1 |
| 3:A:7:ARG:NH2 | 3:A:74:TYR:CE1 | 0.41 | 2.89 | 29 | 1 |
| 3:A:43:TRP:N | 3:A:43:TRP:CE3 | 0.41 | 2.89 | 21 | 1 |
| 3:A:54:PHE:CZ | 3:A:55:PHE:CE1 | 0.41 | 3.09 | 21 | 1 |
| 3:A:62:GLN:N | 3:A:62:GLN:OE1 | 0.41 | 2.54 | 23 | 1 |
| 3:A:62:GLN:OE1 | 3:A:62:GLN:O | 0.41 | 2.39 | 21 | 1 |
| 3:A:61:LEU:N | 3:A:61:LEU:CD2 | 0.41 | 2.84 | 29 | 1 |
| 1:B:7:DA:C1' | 3:A:20:ARG:NH1 | 0.41 | 2.84 | 14 | 1 |
| 3:A:7:ARG:H | 3:A:7:ARG:HE | 0.41 | 1.57 | 17 | 1 |
| 3:A:68:LYS:C | 3:A:69:TYR:CD1 | 0.40 | 2.95 | 6 | 1 |
| 3:A:10:ASN:N | 3:A:10:ASN:HD22 | 0.40 | 2.15 | 13 | 1 |
| 3:A:34:GLU:O | 3:A:35:ILE:C | 0.40 | 2.60 | 3 | 1 |
| 3:A:19:GLN:NE2 | 3:A:22:LYS:HZ2 | 0.40 | 2.13 | 12 | 1 |
| 3:A:47:THR:OG1 | 3:A:50:GLU:OE1 | 0.40 | 2.39 | 2 | 1 |
| 3:A:7:ARG:HD3 | 3:A:7:ARG:N | 0.40 | 2.31 | 8 | 1 |
| 3:A:20:ARG:HH11 | 3:A:20:ARG:HG2 | 0.40 | 1.76 | 13 | 2 |
| 3:A:52:TRP:N | 3:A:53:PRO:HD2 | 0.40 | 2.31 | 7 | 1 |
| 3:A:5:VAL:HG21 | 3:A:72:TYR:CE1 | 0.40 | 2.51 | 17 | 1 |

## 6.3 Torsion angles (i)

### 6.3.1 Protein backbone (i)

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 3 | A | 70/76 (92%) | 54±2 (78±3%) | 11±2 (16±3%) | 5±1 (7±2%) | 2 18 |
| All | All | 2450/2660 (92%) | 1904 (78%) | 382 (16%) | 164 (7%) | 2 18 |

All 16 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 3 | A | 53 | PRO | 34 |
| 3 | A | 17 | ARG | 25 |
| 3 | A | 70 | PRO | 25 |
| 3 | A | 35 | ILE | 16 |
| 3 | A | 32 | ASN | 13 |
| 3 | A | 8 | PRO | 11 |
| 3 | A | 31 | ARG | 10 |
| 3 | A | 51 | LYS | 7 |
| 3 | A | 58 | ALA | 7 |
| 3 | A | 74 | TYR | 5 |
| 3 | A | 71 | ASN | 3 |
| 3 | A | 25 | LEU | 3 |
| 3 | A | 61 | LEU | 2 |
| 3 | A | 16 | SER | 1 |
| 3 | A | 28 | PRO | 1 |
| 3 | A | 48 | GLU | 1 |

### 6.3.2 Protein sidechains (i)

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 3 | A | 65/70 (93%) | 56±2 (86±3%) | 9±2 (14±3%) | 7 47 |
| All | All | 2275/2450 (93%) | 1967 (86%) | 308 (14%) | 7 47 |

All 30 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 | A | 7 | ARG | 35 |
| 3 | A | 35 | ILE | 35 |
| 3 | A | 43 | TRP | 35 |
| 3 | A | 31 | ARG | 21 |
| 3 | A | 6 | LYS | 20 |
| 3 | A | 20 | ARG | 18 |
| 3 | A | 75 | ARG | 18 |
| 3 | A | 37 | LYS | 17 |
| 3 | A | 44 | LYS | 13 |
| 3 | A | 66 | ARG | 12 |

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| Mol | Chain | Res | Type | Models (Total) |
|---|---|---|---|---|
| 3 | A | 32 | ASN | 10 |
| 3 | A | 29 | ARG | 9 |
| 3 | A | 60 | LYS | 9 |
| 3 | A | 50 | GLU | 7 |
| 3 | A | 56 | GLN | 7 |
| 3 | A | 17 | ARG | 7 |
| 3 | A | 62 | GLN | 6 |
| 3 | A | 21 | ARG | 5 |
| 3 | A | 64 | MET | 5 |
| 3 | A | 22 | LYS | 4 |
| 3 | A | 18 | ASP | 3 |
| 3 | A | 59 | GLN | 2 |
| 3 | A | 38 | GLN | 2 |
| 3 | A | 19 | GLN | 2 |
| 3 | A | 67 | GLU | 1 |
| 3 | A | 10 | ASN | 1 |
| 3 | A | 30 | MET | 1 |
| 3 | A | 9 | MET | 1 |
| 3 | A | 28 | PRO | 1 |
| 3 | A | 71 | ASN | 1 |

### 6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.6 Ligand geometry (i)

There are no ligands in this entry.

## 6.7 Other polymers (i)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 7 Chemical shift validation (i)

No chemical shift data were provided