



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 04:39 PM BST

PDB ID : 1S40
Title : SOLUTION STRUCTURE OF THE CDC13 DNA-BINDING DOMAIN
COMPLEXED WITH A SINGLE-STRANDED TELOMERIC DNA 11-MER
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D.S.
Deposited on : 2004-01-14

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
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

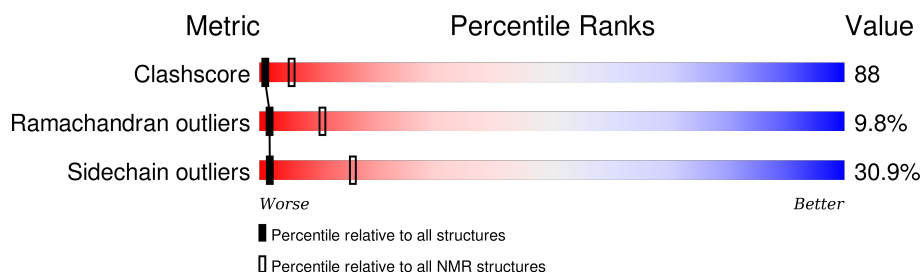
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



| Metric | Whole archive (#Entries) | NMR archive (#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore | 114402 | 11133 |
| Ramachandran outliers | 111179 | 9975 |
| Sidechain outliers | 111093 | 9958 |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | B | 11 | 100% |
| 2 | A | 199 | <div> <div>9%</div> <div>60%</div> <div>17%</div> <div>• 6%</div> <div>6%</div> </div> |

2 Ensemble composition and analysis

This entry contains 10 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:10-A:108, A:115-A:191 (176) | 0.69 | 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 and 1 single-model cluster was found.

| Cluster number | Models |
|-----------------------|---------------------|
| 1 | 1, 2, 3, 4, 5, 7, 8 |
| 2 | 6, 10 |
| Single-model clusters | 9 |

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3457 atoms, of which 1667 are hydrogens and 0 are deuteriums.

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

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|-----|----|----|----|-------|
| 1 | B | 11 | Total | C | H | N | O | P | 0 |
| | | | 358 | 110 | 127 | 43 | 68 | 10 | |

- Molecule 2 is a protein called Cell division control protein 13.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|-------|
| 2 | A | 187 | Total | C | H | N | O | S | 0 |
| | | | 3099 | 1003 | 1540 | 262 | 283 | 11 | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| A | 1 | MET | - | CLONING ARTIFACT | UNP P32797 |

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble


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

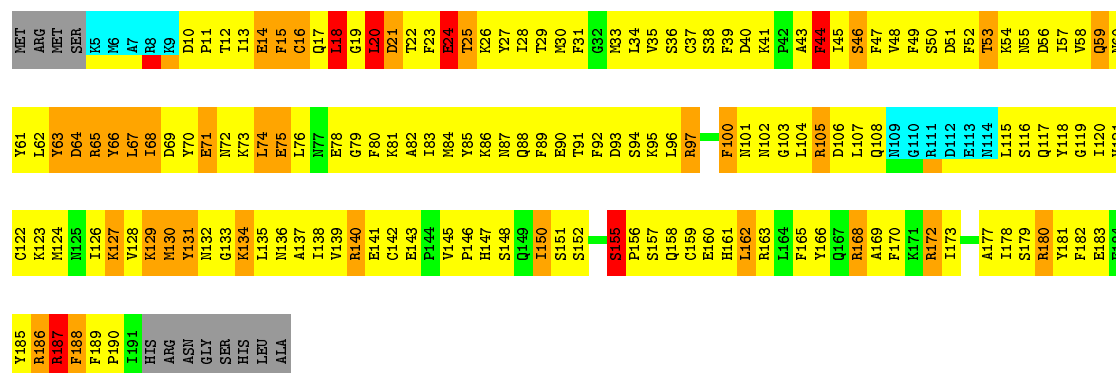
- Molecule 1: 5'-D(*GP*TP*GP*TP*GP*GP*GP*TP*GP*TP*G)-3'

Chain B:  100%

G1
T2
G3
T4
G5
G6
G7
T8
G9
T10
G11

- Molecule 2: Cell division control protein 13

Chain A:  9% 60% 17% 6% 6%



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

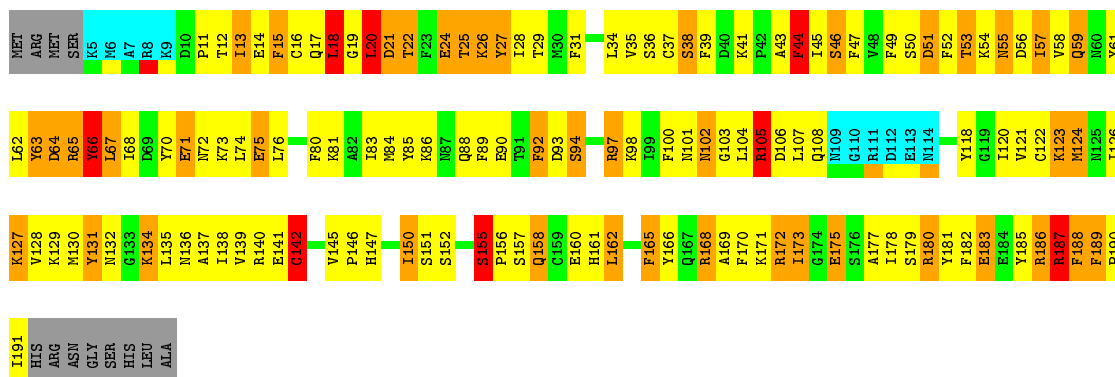
- Molecule 1: 5'-D(*GP*TP*GP*TP*GP*GP*GP*TP*GP*TP*G)-3'

Chain B:  100%

G1
T2
G3
T4
G5
G6
G7
T8
G9
T10
G11

- Molecule 2: Cell division control protein 13

Chain A: 19% 44% 22% • 6% 6%



4.2.2 Score per residue for model 2

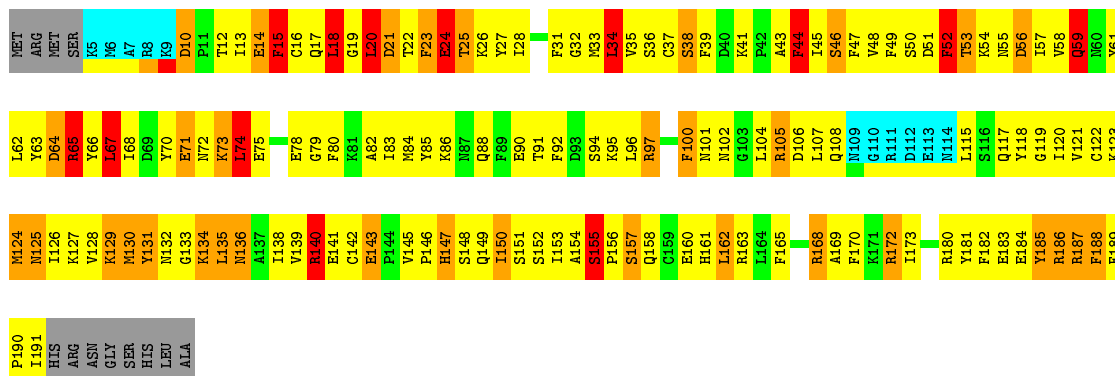
- Molecule 1: 5'-D(*GP*TP*GP*TP*GP*GP*GP*TP*GP*TP*G)-3'

Chain B: 100%

G1
T2
G3
T4
G5
G6
G7
T8
G9
T10
G11

- Molecule 2: Cell division control protein 13

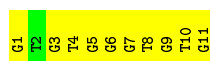
Chain A: 15% 50% 17% 7% 6% 6%



4.2.3 Score per residue for model 3 (medoid)

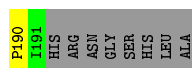
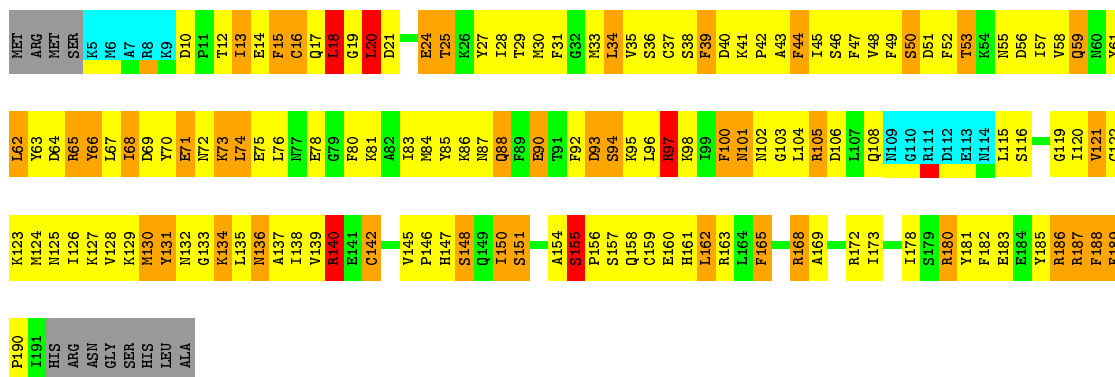
- Molecule 1: 5'-D(*GP*TP*GP*TP*GP*GP*GP*TP*GP*TP*G)-3'

Chain B: 9% 91%



- Molecule 2: Cell division control protein 13

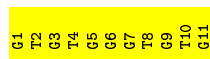
Chain A: 17% 48% 21% 6% 6%



4.2.4 Score per residue for model 4

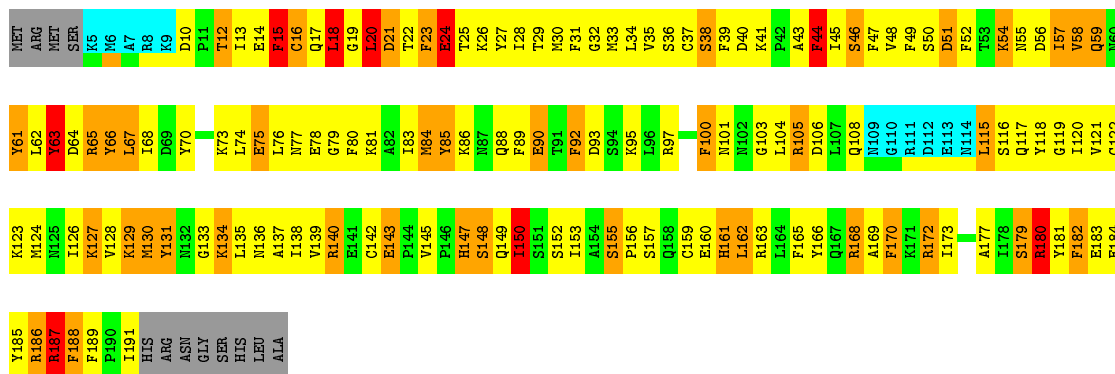
- Molecule 1: 5'-D(*GP*TP*GP*TP*GP*GP*GP*TP*GP*TP*G)-3'

Chain B: 100%



- Molecule 2: Cell division control protein 13

Chain A: 16% 47% 21% 5% 6% 6%



4.2.5 Score per residue for model 5

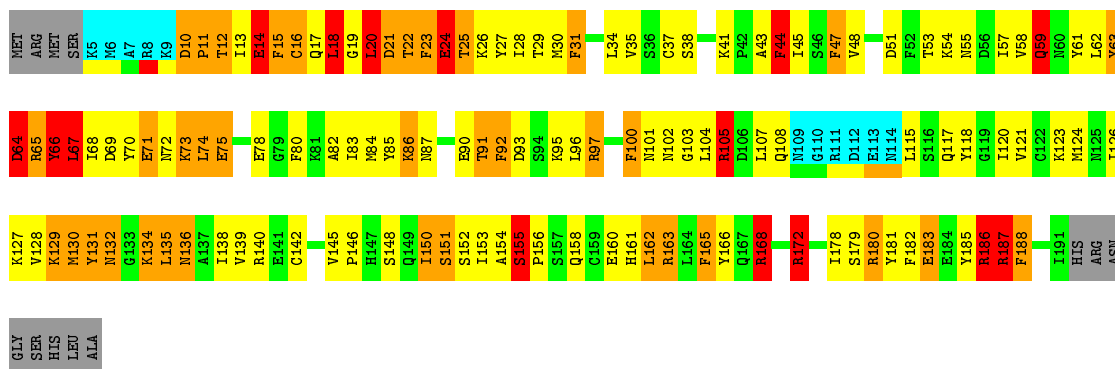
- Molecule 1: 5'-D(*GP*TP*GP*TP*GP*GP*GP*TP*GP*TP*G)-3'

Chain B: 100%

G1
T2
G3
T4
G5
G6
G7
T8
G9
T10
G11

- Molecule 2: Cell division control protein 13

Chain A: 25% 38% 19% 8% 6% 6%



4.2.6 Score per residue for model 6

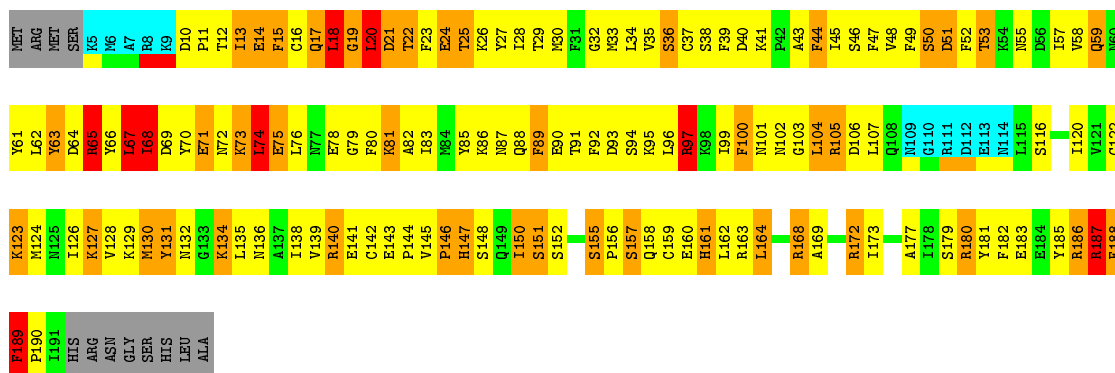
- Molecule 1: 5'-D(*GP*TP*GP*TP*GP*GP*GP*TP*GP*TP*G)-3'

Chain B: 100%

G1
T2
G3
T4
G5
G6
G7
T8
G9
T10
G11

- Molecule 2: Cell division control protein 13

Chain A: 16% 47% 22% 5% 6% 6%



4.2.7 Score per residue for model 7

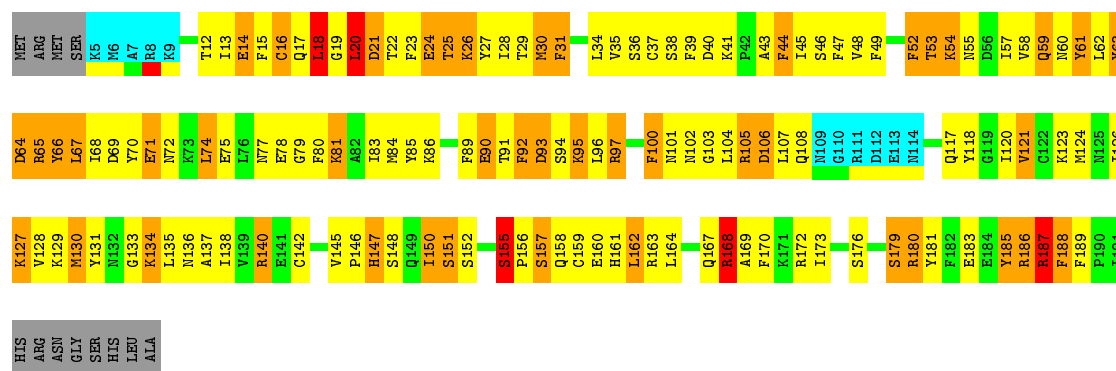
- Molecule 1: 5'-D(*GP*TP*GP*TP*GP*GP*GP*TP*GP*TP*G)-3'

Chain B: 100%

G1
T2
G3
T4
G5
G6
G7
T8
G9
T10
G11

- Molecule 2: Cell division control protein 13

Chain A: 20% 44% 23% 6% 6%



4.2.8 Score per residue for model 8

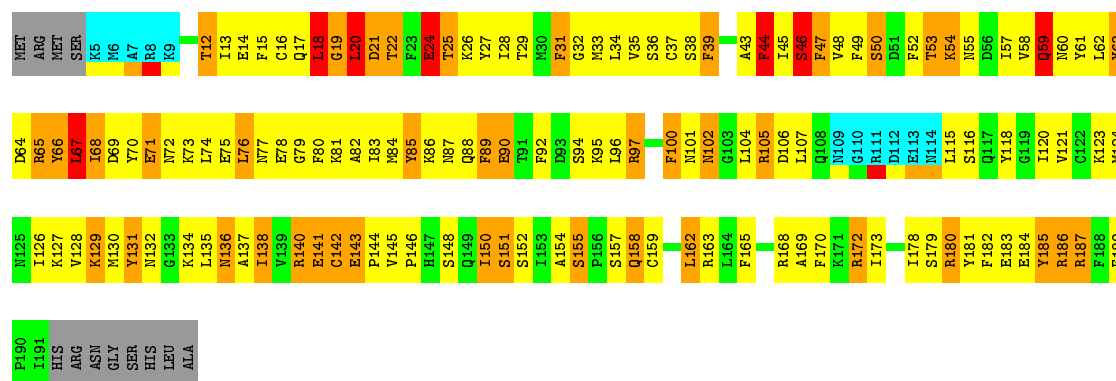
- Molecule 1: 5'-D(*GP*TP*GP*TP*GP*GP*GP*TP*GP*TP*G)-3'

Chain B: 100%

G1
T2
G3
T4
G5
G6
G7
T8
G9
T10
G11

- Molecule 2: Cell division control protein 13

Chain A: 19% 45% 21% 6% 6%



4.2.9 Score per residue for model 9

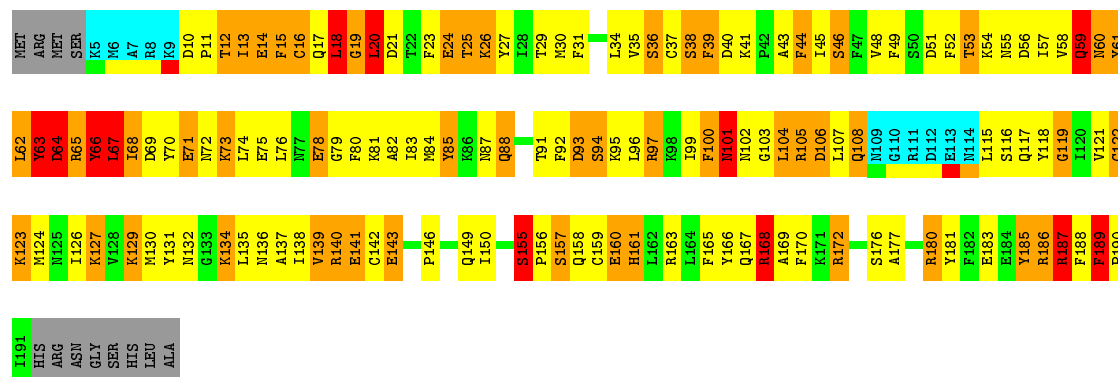
- Molecule 1: 5'-D(*GP*TP*GP*TP*GP*GP*GP*TP*GP*TP*G)-3'

Chain B: 100%

G1
T2
G3
T4
G5
G6
G7
T8
G9
T10
G11

- Molecule 2: Cell division control protein 13

Chain A: 18% 40% 25% 6% 6% 6%



4.2.10 Score per residue for model 10

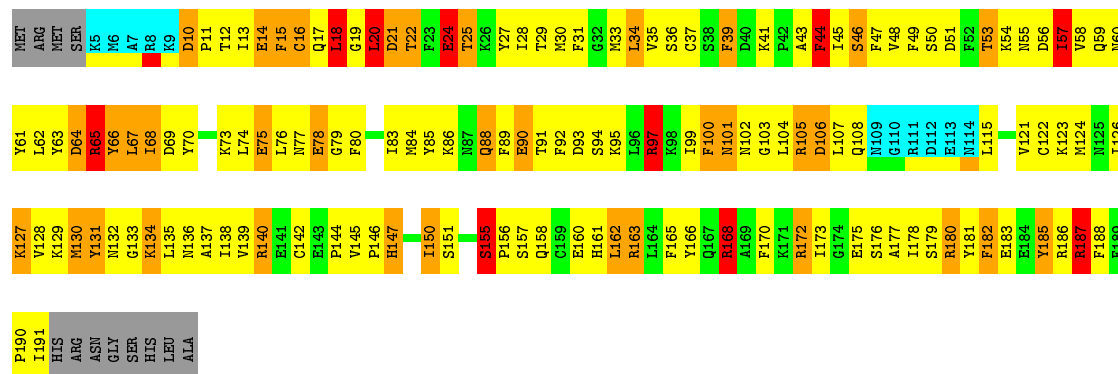
- Molecule 1: 5'-D(*GP*TP*GP*TP*GP*GP*GP*TP*GP*TP*G)-3'

Chain B: 100%

G1
T2
G3
T4
G5
G6
G7
T8
G9
T10
G11

- Molecule 2: Cell division control protein 13

Chain A: 18% 48% 18% 5% 6% 6%



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *distance geometry, simulated annealing, molecular dynamics, matrix relaxation, torsion angle dynamics*.

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with acceptable covalent geometry, structures with the lowest energy*.

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

| Software name | Classification | Version |
|---------------|--------------------|---------|
| X-PLOR | structure solution | 3.851 |
| X-PLOR | refinement | 3.851 |

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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

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 |
|-----|-------|-----------|-----------|
| 2 | A | 0.0±0.0 | 9.5±0.5 |
| All | All | 0 | 95 |

There are no bond-length outliers.

There are no bond-angle outliers.

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) |
|-----|-------|-----|------|-----------|----------------|
| 2 | A | 172 | ARG | Sidechain | 10 |
| 2 | A | 168 | ARG | Sidechain | 10 |
| 2 | A | 187 | ARG | Sidechain | 10 |
| 2 | A | 140 | ARG | Sidechain | 10 |
| 2 | A | 105 | ARG | Sidechain | 10 |
| 2 | A | 65 | ARG | Sidechain | 9 |
| 2 | A | 186 | ARG | Sidechain | 9 |
| 2 | A | 180 | ARG | Sidechain | 9 |
| 2 | A | 97 | ARG | Sidechain | 9 |
| 2 | A | 163 | ARG | Sidechain | 9 |

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 | B | 231 | 127 | 127 | 113±12 |
| 2 | A | 1469 | 1449 | 1449 | 236±15 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| All | All | 17000 | 15760 | 15760 | 2873 |

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 88.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:7:DG:H2'' | 1:B:8:DT:O5' | 1.13 | 1.38 | 4 | 5 |
| 2:A:83:ILE:HD11 | 2:A:138:ILE:HG22 | 1.11 | 1.13 | 1 | 6 |
| 2:A:13:ILE:HD11 | 2:A:28:ILE:HD13 | 1.10 | 1.17 | 10 | 4 |
| 1:B:10:DT:H1' | 1:B:11:DG:N3 | 1.02 | 1.69 | 2 | 3 |
| 1:B:9:DG:H2'' | 1:B:10:DT:O5' | 0.99 | 1.57 | 4 | 8 |
| 1:B:9:DG:O4' | 1:B:10:DT:H71 | 0.99 | 1.56 | 5 | 4 |
| 1:B:4:DT:H4' | 1:B:5:DG:O5' | 0.98 | 1.56 | 4 | 3 |
| 2:A:61:TYR:O | 2:A:76:LEU:HD13 | 0.96 | 1.61 | 1 | 1 |
| 2:A:68:ILE:HD12 | 2:A:177:ALA:HB1 | 0.95 | 1.34 | 6 | 4 |
| 1:B:10:DT:H2'' | 1:B:11:DG:O5' | 0.94 | 1.60 | 2 | 6 |
| 1:B:9:DG:N3 | 1:B:10:DT:H73 | 0.94 | 1.76 | 2 | 1 |
| 1:B:4:DT:C2' | 2:A:83:ILE:HD13 | 0.94 | 1.93 | 9 | 5 |
| 1:B:9:DG:O3' | 1:B:10:DT:H73 | 0.92 | 1.64 | 9 | 2 |
| 1:B:4:DT:H2'' | 2:A:83:ILE:HD13 | 0.92 | 1.41 | 3 | 7 |
| 2:A:57:ILE:HD13 | 2:A:135:LEU:HD23 | 0.90 | 1.44 | 5 | 1 |
| 1:B:7:DG:O3' | 1:B:8:DT:H72 | 0.89 | 1.67 | 5 | 7 |
| 1:B:8:DT:H5'' | 1:B:9:DG:N7 | 0.89 | 1.83 | 8 | 3 |
| 2:A:34:LEU:HD21 | 2:A:37:CYS:SG | 0.89 | 2.06 | 6 | 1 |
| 2:A:145:VAL:CG1 | 2:A:150:ILE:HD12 | 0.88 | 1.98 | 6 | 3 |
| 1:B:9:DG:O4' | 1:B:10:DT:H72 | 0.88 | 1.68 | 4 | 2 |
| 1:B:10:DT:H2'' | 1:B:11:DG:O4' | 0.88 | 1.67 | 4 | 1 |
| 1:B:7:DG:C2' | 1:B:8:DT:O5' | 0.87 | 2.23 | 1 | 9 |
| 2:A:128:VAL:HB | 2:A:135:LEU:HD11 | 0.87 | 1.47 | 8 | 5 |
| 2:A:13:ILE:HD11 | 2:A:28:ILE:CD1 | 0.86 | 1.99 | 4 | 3 |
| 1:B:8:DT:O3' | 1:B:9:DG:H3' | 0.86 | 1.71 | 3 | 6 |
| 1:B:9:DG:O4' | 1:B:10:DT:H73 | 0.86 | 1.70 | 3 | 2 |
| 1:B:2:DT:H2'' | 1:B:3:DG:O5' | 0.86 | 1.68 | 7 | 3 |
| 2:A:12:THR:HG21 | 2:A:158:GLN:OE1 | 0.86 | 1.70 | 8 | 1 |
| 2:A:15:PHE:O | 2:A:18:LEU:HD23 | 0.85 | 1.71 | 2 | 1 |
| 2:A:150:ILE:HD11 | 2:A:162:LEU:HD13 | 0.85 | 1.47 | 7 | 1 |
| 2:A:126:ILE:HG23 | 2:A:138:ILE:O | 0.85 | 1.72 | 9 | 10 |
| 2:A:104:LEU:HD12 | 2:A:107:LEU:HD12 | 0.84 | 1.50 | 1 | 3 |
| 2:A:76:LEU:N | 2:A:76:LEU:HD13 | 0.83 | 1.88 | 8 | 1 |
| 2:A:62:LEU:O | 2:A:62:LEU:HD13 | 0.83 | 1.73 | 1 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:A:57:ILE:O | 2:A:58:VAL:HG23 | 0.82 | 1.75 | 4 | 1 |
| 1:B:2:DT:H1' | 1:B:3:DG:O4' | 0.82 | 1.75 | 7 | 1 |
| 2:A:13:ILE:HD12 | 2:A:18:LEU:HA | 0.81 | 1.51 | 9 | 5 |
| 1:B:10:DT:O3' | 1:B:11:DG:H3' | 0.81 | 1.75 | 10 | 1 |
| 1:B:1:DG:C2' | 2:A:27:TYR:CZ | 0.81 | 2.64 | 7 | 1 |
| 2:A:83:ILE:CG1 | 2:A:138:ILE:HG22 | 0.81 | 2.06 | 9 | 2 |
| 2:A:13:ILE:HD11 | 2:A:28:ILE:HD12 | 0.80 | 1.51 | 8 | 3 |
| 1:B:3:DG:C2' | 1:B:4:DT:H72 | 0.80 | 2.06 | 7 | 2 |
| 2:A:126:ILE:HG21 | 2:A:137:ALA:HB1 | 0.80 | 1.51 | 7 | 5 |
| 1:B:4:DT:H1' | 2:A:43:ALA:O | 0.79 | 1.77 | 4 | 5 |
| 1:B:9:DG:H5'' | 2:A:61:TYR:OH | 0.79 | 1.77 | 6 | 5 |
| 1:B:1:DG:H2'' | 2:A:27:TYR:CE2 | 0.79 | 2.13 | 10 | 6 |
| 2:A:45:ILE:HD13 | 2:A:89:PHE:CG | 0.79 | 2.13 | 1 | 4 |
| 1:B:5:DG:C4 | 2:A:131:TYR:CD2 | 0.79 | 2.71 | 10 | 6 |
| 2:A:62:LEU:HD22 | 2:A:80:PHE:HA | 0.79 | 1.52 | 6 | 2 |
| 1:B:11:DG:C8 | 2:A:70:TYR:CD2 | 0.78 | 2.71 | 6 | 3 |
| 1:B:5:DG:C8 | 2:A:131:TYR:CD2 | 0.78 | 2.71 | 7 | 3 |
| 2:A:28:ILE:HD11 | 2:A:128:VAL:HG11 | 0.78 | 1.54 | 1 | 2 |
| 2:A:13:ILE:HD12 | 2:A:18:LEU:HD22 | 0.78 | 1.54 | 2 | 2 |
| 1:B:3:DG:H2'' | 1:B:4:DT:O5' | 0.77 | 1.78 | 6 | 2 |
| 1:B:1:DG:H2'' | 2:A:27:TYR:CZ | 0.77 | 2.15 | 7 | 4 |
| 2:A:14:GLU:O | 2:A:18:LEU:HD23 | 0.76 | 1.80 | 8 | 3 |
| 2:A:62:LEU:HD11 | 2:A:80:PHE:CA | 0.76 | 2.10 | 3 | 1 |
| 2:A:69:ASP:OD1 | 2:A:177:ALA:HB2 | 0.76 | 1.79 | 6 | 1 |
| 1:B:8:DT:H3' | 1:B:9:DG:N7 | 0.76 | 1.95 | 4 | 3 |
| 1:B:2:DT:H2' | 1:B:3:DG:N7 | 0.76 | 1.95 | 1 | 2 |
| 2:A:62:LEU:HB2 | 2:A:76:LEU:HD12 | 0.76 | 1.56 | 8 | 1 |
| 1:B:8:DT:H5'' | 1:B:9:DG:C8 | 0.76 | 2.15 | 9 | 10 |
| 2:A:30:MET:CB | 2:A:126:ILE:HD12 | 0.75 | 2.09 | 7 | 1 |
| 2:A:83:ILE:O | 2:A:83:ILE:HD12 | 0.75 | 1.82 | 7 | 4 |
| 2:A:18:LEU:HD11 | 2:A:57:ILE:HD13 | 0.75 | 1.59 | 10 | 1 |
| 2:A:48:VAL:HG21 | 2:A:63:TYR:O | 0.74 | 1.82 | 6 | 3 |
| 2:A:13:ILE:HD13 | 2:A:18:LEU:HD22 | 0.74 | 1.58 | 8 | 2 |
| 2:A:83:ILE:CD1 | 2:A:138:ILE:HG22 | 0.74 | 2.12 | 5 | 2 |
| 2:A:14:GLU:O | 2:A:53:THR:HG21 | 0.74 | 1.82 | 2 | 1 |
| 1:B:5:DG:C4 | 2:A:131:TYR:CE2 | 0.73 | 2.76 | 3 | 5 |
| 1:B:8:DT:C5' | 1:B:9:DG:C8 | 0.73 | 2.71 | 8 | 4 |
| 2:A:145:VAL:HG12 | 2:A:145:VAL:O | 0.73 | 1.83 | 1 | 6 |
| 2:A:83:ILE:HD11 | 2:A:138:ILE:CG2 | 0.73 | 2.05 | 3 | 4 |
| 1:B:11:DG:C8 | 2:A:70:TYR:CE2 | 0.73 | 2.77 | 10 | 5 |
| 2:A:173:ILE:HG21 | 2:A:185:TYR:OH | 0.73 | 1.83 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:8:DT:H1' | 2:A:61:TYR:CG | 0.73 | 2.18 | 1 | 10 |
| 1:B:1:DG:H2'' | 2:A:27:TYR:OH | 0.72 | 1.85 | 2 | 3 |
| 1:B:3:DG:C1' | 1:B:4:DT:H72 | 0.72 | 2.13 | 7 | 2 |
| 2:A:126:ILE:CG2 | 2:A:137:ALA:HB1 | 0.72 | 2.13 | 7 | 3 |
| 1:B:5:DG:H4' | 1:B:6:DG:N7 | 0.72 | 1.99 | 5 | 1 |
| 1:B:8:DT:C1' | 2:A:61:TYR:CD2 | 0.72 | 2.73 | 8 | 9 |
| 1:B:8:DT:H5' | 2:A:63:TYR:CE1 | 0.72 | 2.19 | 5 | 6 |
| 1:B:5:DG:C8 | 2:A:131:TYR:CD1 | 0.72 | 2.78 | 5 | 1 |
| 2:A:13:ILE:CD1 | 2:A:28:ILE:HD12 | 0.72 | 2.14 | 8 | 1 |
| 1:B:5:DG:H2' | 2:A:131:TYR:CE2 | 0.71 | 2.19 | 4 | 9 |
| 2:A:62:LEU:HD12 | 2:A:76:LEU:HA | 0.71 | 1.61 | 6 | 2 |
| 1:B:8:DT:H1' | 2:A:61:TYR:CD1 | 0.71 | 2.19 | 5 | 1 |
| 2:A:120:ILE:O | 2:A:120:ILE:HG22 | 0.71 | 1.85 | 2 | 3 |
| 1:B:1:DG:H2'' | 2:A:27:TYR:CE1 | 0.71 | 2.20 | 4 | 1 |
| 2:A:52:PHE:O | 2:A:53:THR:HG23 | 0.71 | 1.84 | 3 | 2 |
| 1:B:5:DG:C8 | 1:B:5:DG:P | 0.71 | 2.84 | 2 | 1 |
| 2:A:108:GLN:HB3 | 2:A:115:LEU:HD11 | 0.71 | 1.62 | 10 | 1 |
| 1:B:2:DT:H71 | 1:B:2:DT:OP1 | 0.71 | 1.86 | 7 | 1 |
| 1:B:9:DG:N3 | 1:B:10:DT:H72 | 0.71 | 2.00 | 5 | 3 |
| 1:B:11:DG:C2' | 2:A:70:TYR:CE2 | 0.70 | 2.74 | 5 | 6 |
| 2:A:14:GLU:HA | 2:A:18:LEU:HD23 | 0.70 | 1.62 | 7 | 1 |
| 2:A:65:ARG:CD | 2:A:74:LEU:HD21 | 0.70 | 2.16 | 1 | 1 |
| 1:B:7:DG:H1' | 2:A:63:TYR:CE2 | 0.70 | 2.22 | 3 | 6 |
| 1:B:7:DG:C8 | 2:A:63:TYR:CB | 0.70 | 2.75 | 7 | 4 |
| 1:B:5:DG:N3 | 2:A:131:TYR:CD2 | 0.70 | 2.60 | 10 | 5 |
| 2:A:83:ILE:HD12 | 2:A:83:ILE:C | 0.70 | 2.07 | 3 | 3 |
| 1:B:9:DG:O4' | 1:B:10:DT:H2' | 0.70 | 1.86 | 9 | 2 |
| 1:B:1:DG:HO5' | 1:B:1:DG:H8 | 0.70 | 1.28 | 3 | 1 |
| 2:A:48:VAL:HG21 | 2:A:64:ASP:HB2 | 0.70 | 1.61 | 9 | 2 |
| 1:B:3:DG:C8 | 1:B:4:DT:C7 | 0.70 | 2.75 | 8 | 5 |
| 1:B:8:DT:C6 | 1:B:8:DT:O5' | 0.70 | 2.44 | 5 | 5 |
| 1:B:8:DT:H6 | 1:B:8:DT:O5' | 0.70 | 1.70 | 5 | 4 |
| 2:A:35:VAL:HG12 | 2:A:65:ARG:HB2 | 0.70 | 1.62 | 7 | 2 |
| 1:B:4:DT:O2 | 2:A:43:ALA:HB1 | 0.70 | 1.85 | 1 | 1 |
| 1:B:10:DT:O3' | 1:B:11:DG:H4' | 0.70 | 1.86 | 4 | 2 |
| 1:B:8:DT:H5' | 2:A:63:TYR:CZ | 0.69 | 2.21 | 6 | 7 |
| 2:A:67:LEU:HD12 | 2:A:74:LEU:HD23 | 0.69 | 1.62 | 8 | 2 |
| 2:A:12:THR:O | 2:A:13:ILE:HG23 | 0.69 | 1.87 | 3 | 2 |
| 1:B:9:DG:C8 | 1:B:9:DG:P | 0.69 | 2.85 | 2 | 2 |
| 1:B:3:DG:N9 | 1:B:4:DT:H72 | 0.69 | 2.02 | 1 | 2 |
| 1:B:4:DT:O3' | 2:A:83:ILE:HD12 | 0.69 | 1.87 | 6 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:7:DG:O3' | 1:B:8:DT:H71 | 0.69 | 1.88 | 6 | 3 |
| 1:B:10:DT:C2 | 1:B:11:DG:N2 | 0.68 | 2.61 | 2 | 1 |
| 2:A:20:LEU:HD12 | 2:A:135:LEU:CD2 | 0.68 | 2.18 | 2 | 2 |
| 1:B:4:DT:C2' | 2:A:83:ILE:HD12 | 0.68 | 2.18 | 6 | 1 |
| 1:B:2:DT:C2' | 1:B:3:DG:N7 | 0.68 | 2.57 | 1 | 1 |
| 1:B:3:DG:H5' | 2:A:138:ILE:HD13 | 0.68 | 1.64 | 2 | 1 |
| 1:B:8:DT:C3' | 1:B:9:DG:C8 | 0.68 | 2.77 | 4 | 4 |
| 2:A:83:ILE:HG13 | 2:A:138:ILE:HG22 | 0.68 | 1.63 | 9 | 2 |
| 2:A:104:LEU:HA | 2:A:107:LEU:HD12 | 0.68 | 1.66 | 9 | 4 |
| 2:A:62:LEU:HD21 | 2:A:80:PHE:HA | 0.68 | 1.66 | 3 | 2 |
| 2:A:63:TYR:CD1 | 2:A:66:TYR:CZ | 0.68 | 2.82 | 8 | 1 |
| 1:B:7:DG:O4' | 1:B:7:DG:P | 0.68 | 2.51 | 8 | 1 |
| 2:A:74:LEU:HD12 | 2:A:75:GLU:O | 0.67 | 1.88 | 4 | 1 |
| 2:A:31:PHE:CE1 | 2:A:162:LEU:HD11 | 0.67 | 2.25 | 7 | 1 |
| 2:A:30:MET:HB2 | 2:A:126:ILE:HD12 | 0.67 | 1.65 | 7 | 1 |
| 1:B:5:DG:N3 | 2:A:136:ASN:HB2 | 0.67 | 2.05 | 10 | 5 |
| 2:A:180:ARG:CB | 2:A:181:TYR:CE1 | 0.67 | 2.77 | 4 | 6 |
| 1:B:8:DT:C5' | 2:A:63:TYR:CE2 | 0.67 | 2.77 | 4 | 3 |
| 1:B:8:DT:C1' | 2:A:61:TYR:CD1 | 0.67 | 2.77 | 5 | 1 |
| 1:B:2:DT:C2' | 1:B:3:DG:C8 | 0.67 | 2.77 | 1 | 2 |
| 1:B:8:DT:H1' | 2:A:61:TYR:CD2 | 0.67 | 2.24 | 7 | 9 |
| 1:B:1:DG:C2' | 2:A:27:TYR:CE2 | 0.66 | 2.77 | 7 | 4 |
| 2:A:58:VAL:HG21 | 2:A:133:GLY:O | 0.66 | 1.91 | 10 | 1 |
| 1:B:8:DT:C5' | 2:A:63:TYR:CE1 | 0.66 | 2.78 | 10 | 6 |
| 1:B:2:DT:H1' | 1:B:3:DG:N7 | 0.66 | 2.05 | 4 | 2 |
| 1:B:2:DT:C2 | 1:B:3:DG:C6 | 0.66 | 2.84 | 5 | 1 |
| 2:A:20:LEU:HD12 | 2:A:135:LEU:HD21 | 0.66 | 1.67 | 2 | 1 |
| 2:A:82:ALA:HB1 | 2:A:139:VAL:HG13 | 0.66 | 1.67 | 9 | 1 |
| 2:A:28:ILE:HD11 | 2:A:128:VAL:CG1 | 0.66 | 2.21 | 4 | 3 |
| 1:B:8:DT:O3' | 1:B:9:DG:C8 | 0.66 | 2.49 | 2 | 5 |
| 2:A:63:TYR:CE1 | 2:A:66:TYR:CE2 | 0.65 | 2.83 | 8 | 2 |
| 1:B:5:DG:OP2 | 2:A:83:ILE:HD13 | 0.65 | 1.91 | 4 | 2 |
| 1:B:9:DG:O4' | 1:B:10:DT:C6 | 0.65 | 2.50 | 1 | 3 |
| 1:B:6:DG:C8 | 2:A:41:LYS:CE | 0.65 | 2.79 | 2 | 1 |
| 2:A:15:PHE:N | 2:A:18:LEU:HD23 | 0.65 | 2.06 | 5 | 5 |
| 2:A:24:GLU:O | 2:A:25:THR:CB | 0.65 | 2.44 | 5 | 9 |
| 1:B:11:DG:H2' | 2:A:70:TYR:CE2 | 0.65 | 2.27 | 8 | 3 |
| 2:A:92:PHE:CE1 | 2:A:96:LEU:HD12 | 0.65 | 2.26 | 9 | 2 |
| 1:B:4:DT:O4' | 2:A:43:ALA:HB1 | 0.65 | 1.92 | 8 | 4 |
| 1:B:11:DG:C8 | 2:A:70:TYR:CZ | 0.65 | 2.85 | 10 | 4 |
| 1:B:9:DG:O3' | 2:A:66:TYR:CE2 | 0.65 | 2.49 | 4 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:A:27:TYR:O | 2:A:28:ILE:HG23 | 0.64 | 1.92 | 10 | 4 |
| 1:B:7:DG:H1' | 2:A:63:TYR:CD2 | 0.64 | 2.28 | 7 | 6 |
| 1:B:9:DG:O4' | 1:B:10:DT:C7 | 0.64 | 2.43 | 3 | 8 |
| 1:B:9:DG:N3 | 1:B:10:DT:C7 | 0.64 | 2.58 | 2 | 2 |
| 1:B:10:DT:O5' | 2:A:66:TYR:CD2 | 0.64 | 2.50 | 8 | 1 |
| 1:B:8:DT:C3' | 1:B:9:DG:N7 | 0.64 | 2.60 | 8 | 2 |
| 1:B:9:DG:P | 1:B:9:DG:C8 | 0.64 | 2.90 | 5 | 4 |
| 1:B:8:DT:O5' | 1:B:8:DT:C6 | 0.64 | 2.50 | 7 | 1 |
| 2:A:35:VAL:HG11 | 2:A:65:ARG:HG3 | 0.64 | 1.70 | 8 | 1 |
| 1:B:10:DT:H2'' | 1:B:11:DG:O3' | 0.64 | 1.92 | 6 | 2 |
| 1:B:7:DG:C3' | 1:B:8:DT:C5 | 0.64 | 2.81 | 9 | 9 |
| 2:A:48:VAL:HG21 | 2:A:64:ASP:CB | 0.64 | 2.21 | 9 | 1 |
| 2:A:57:ILE:HD12 | 2:A:135:LEU:HD22 | 0.64 | 1.67 | 10 | 1 |
| 1:B:8:DT:H5' | 2:A:63:TYR:CE2 | 0.64 | 2.28 | 8 | 3 |
| 1:B:7:DG:N2 | 2:A:41:LYS:NZ | 0.64 | 2.46 | 5 | 1 |
| 1:B:7:DG:H3' | 1:B:8:DT:C5 | 0.63 | 2.27 | 6 | 10 |
| 2:A:14:GLU:CD | 2:A:53:THR:HG21 | 0.63 | 2.12 | 3 | 1 |
| 2:A:57:ILE:HG22 | 2:A:58:VAL:N | 0.63 | 2.08 | 4 | 1 |
| 2:A:62:LEU:HD21 | 2:A:80:PHE:C | 0.63 | 2.13 | 8 | 2 |
| 1:B:9:DG:O5' | 1:B:9:DG:C8 | 0.63 | 2.52 | 10 | 3 |
| 1:B:10:DT:O3' | 2:A:66:TYR:CD2 | 0.63 | 2.51 | 1 | 2 |
| 1:B:1:DG:C1' | 2:A:27:TYR:CE1 | 0.63 | 2.82 | 1 | 1 |
| 2:A:67:LEU:CD1 | 2:A:74:LEU:HD23 | 0.63 | 2.23 | 4 | 2 |
| 1:B:9:DG:C8 | 1:B:9:DG:O5' | 0.63 | 2.52 | 9 | 4 |
| 2:A:135:LEU:C | 2:A:135:LEU:HD13 | 0.63 | 2.14 | 9 | 2 |
| 2:A:49:PHE:CE1 | 2:A:80:PHE:CE1 | 0.63 | 2.86 | 2 | 1 |
| 2:A:80:PHE:CD1 | 2:A:80:PHE:N | 0.63 | 2.67 | 1 | 7 |
| 2:A:57:ILE:HD13 | 2:A:135:LEU:HG | 0.63 | 1.69 | 9 | 2 |
| 1:B:10:DT:OP2 | 2:A:66:TYR:CG | 0.63 | 2.52 | 8 | 2 |
| 2:A:10:ASP:CB | 2:A:11:PRO:CD | 0.63 | 2.77 | 5 | 1 |
| 1:B:8:DT:O3' | 2:A:61:TYR:CZ | 0.63 | 2.52 | 8 | 7 |
| 2:A:45:ILE:HD13 | 2:A:89:PHE:CD2 | 0.63 | 2.29 | 1 | 2 |
| 2:A:27:TYR:N | 2:A:27:TYR:CD1 | 0.63 | 2.67 | 3 | 3 |
| 1:B:7:DG:O3' | 1:B:8:DT:C7 | 0.62 | 2.47 | 4 | 10 |
| 2:A:34:LEU:HD12 | 2:A:49:PHE:CZ | 0.62 | 2.28 | 3 | 1 |
| 2:A:82:ALA:HB1 | 2:A:139:VAL:CG2 | 0.62 | 2.24 | 5 | 1 |
| 2:A:44:PHE:CZ | 2:A:83:ILE:HG21 | 0.62 | 2.29 | 8 | 3 |
| 2:A:49:PHE:CB | 2:A:80:PHE:CZ | 0.62 | 2.82 | 1 | 3 |
| 2:A:65:ARG:HD3 | 2:A:74:LEU:HD21 | 0.62 | 1.70 | 1 | 1 |
| 2:A:147:HIS:O | 2:A:150:ILE:HG22 | 0.62 | 1.92 | 2 | 4 |
| 2:A:74:LEU:HD13 | 2:A:78:GLU:HB2 | 0.62 | 1.70 | 8 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:A:49:PHE:CB | 2:A:80:PHE:CE1 | 0.62 | 2.82 | 9 | 5 |
| 1:B:10:DT:O3' | 1:B:11:DG:C4' | 0.62 | 2.47 | 9 | 2 |
| 2:A:20:LEU:HD13 | 2:A:21:ASP:H | 0.62 | 1.54 | 3 | 4 |
| 2:A:126:ILE:CG1 | 2:A:139:VAL:HG22 | 0.62 | 2.24 | 4 | 1 |
| 1:B:4:DT:H2'' | 2:A:83:ILE:HD12 | 0.62 | 1.70 | 6 | 1 |
| 2:A:61:TYR:HA | 2:A:76:LEU:HD21 | 0.62 | 1.72 | 10 | 1 |
| 2:A:120:ILE:HG22 | 2:A:120:ILE:O | 0.62 | 1.94 | 4 | 1 |
| 1:B:7:DG:C8 | 2:A:63:TYR:HB2 | 0.62 | 2.29 | 3 | 4 |
| 2:A:49:PHE:CE1 | 2:A:124:MET:CE | 0.62 | 2.82 | 2 | 1 |
| 2:A:45:ILE:CG2 | 2:A:47:PHE:CE2 | 0.62 | 2.81 | 2 | 4 |
| 1:B:5:DG:C2' | 2:A:131:TYR:CE2 | 0.62 | 2.82 | 4 | 3 |
| 1:B:4:DT:H2'' | 2:A:44:PHE:CD2 | 0.62 | 2.29 | 6 | 2 |
| 1:B:7:DG:N9 | 1:B:7:DG:OP2 | 0.62 | 2.32 | 3 | 1 |
| 2:A:118:TYR:HB2 | 2:A:120:ILE:HD11 | 0.62 | 1.70 | 1 | 1 |
| 1:B:7:DG:N9 | 2:A:63:TYR:CD2 | 0.62 | 2.68 | 7 | 3 |
| 1:B:3:DG:H2' | 1:B:4:DT:H73 | 0.62 | 1.72 | 2 | 1 |
| 2:A:50:SER:OG | 2:A:74:LEU:HD11 | 0.62 | 1.94 | 10 | 1 |
| 1:B:5:DG:C8 | 2:A:131:TYR:CE2 | 0.62 | 2.87 | 4 | 4 |
| 2:A:169:ALA:HB1 | 2:A:173:ILE:HD11 | 0.62 | 1.70 | 8 | 2 |
| 2:A:83:ILE:O | 2:A:139:VAL:HG23 | 0.61 | 1.95 | 3 | 3 |
| 2:A:28:ILE:CD1 | 2:A:128:VAL:HG11 | 0.61 | 2.24 | 1 | 1 |
| 2:A:182:PHE:CE2 | 2:A:183:GLU:HG2 | 0.61 | 2.30 | 3 | 1 |
| 1:B:8:DT:H2'' | 2:A:61:TYR:CD2 | 0.61 | 2.31 | 7 | 8 |
| 2:A:180:ARG:HB2 | 2:A:181:TYR:CD1 | 0.61 | 2.30 | 4 | 9 |
| 1:B:5:DG:N9 | 2:A:131:TYR:CE1 | 0.61 | 2.69 | 5 | 1 |
| 1:B:7:DG:N7 | 2:A:63:TYR:CB | 0.61 | 2.63 | 7 | 2 |
| 1:B:5:DG:O4' | 1:B:6:DG:H5'' | 0.61 | 1.94 | 9 | 1 |
| 1:B:9:DG:C1' | 1:B:10:DT:H3' | 0.61 | 2.25 | 5 | 4 |
| 1:B:10:DT:O3' | 2:A:66:TYR:CD1 | 0.61 | 2.54 | 6 | 1 |
| 2:A:50:SER:CB | 2:A:74:LEU:HD11 | 0.61 | 2.26 | 10 | 1 |
| 2:A:68:ILE:HD11 | 2:A:117:GLN:HG2 | 0.61 | 1.73 | 5 | 1 |
| 1:B:9:DG:O3' | 1:B:10:DT:C7 | 0.61 | 2.47 | 9 | 2 |
| 2:A:34:LEU:N | 2:A:49:PHE:CD1 | 0.61 | 2.68 | 3 | 2 |
| 1:B:7:DG:C6 | 2:A:64:ASP:OD1 | 0.61 | 2.54 | 7 | 1 |
| 1:B:9:DG:H2'' | 1:B:10:DT:H3' | 0.61 | 1.71 | 2 | 6 |
| 2:A:69:ASP:CG | 2:A:177:ALA:HB2 | 0.61 | 2.15 | 6 | 1 |
| 1:B:10:DT:O2 | 1:B:11:DG:C2 | 0.61 | 2.54 | 5 | 2 |
| 1:B:11:DG:C8 | 2:A:70:TYR:OH | 0.61 | 2.52 | 1 | 3 |
| 2:A:34:LEU:HD11 | 2:A:36:SER:O | 0.61 | 1.95 | 4 | 2 |
| 1:B:5:DG:H3' | 2:A:131:TYR:CE2 | 0.61 | 2.30 | 4 | 1 |
| 2:A:80:PHE:N | 2:A:80:PHE:CD1 | 0.60 | 2.69 | 9 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:A:134:LYS:N | 2:A:134:LYS:CD | 0.60 | 2.64 | 5 | 3 |
| 2:A:74:LEU:HD23 | 2:A:75:GLU:N | 0.60 | 2.10 | 2 | 2 |
| 2:A:182:PHE:CE2 | 2:A:191:ILE:CD1 | 0.60 | 2.85 | 2 | 1 |
| 1:B:3:DG:H2'' | 1:B:4:DT:H73 | 0.60 | 1.73 | 10 | 1 |
| 2:A:57:ILE:HD13 | 2:A:135:LEU:HD13 | 0.60 | 1.71 | 3 | 1 |
| 2:A:59:GLN:HG3 | 2:A:135:LEU:HD23 | 0.60 | 1.72 | 3 | 1 |
| 2:A:67:LEU:HD12 | 2:A:74:LEU:CG | 0.60 | 2.26 | 6 | 1 |
| 1:B:7:DG:H2'' | 1:B:8:DT:H5' | 0.60 | 1.73 | 10 | 6 |
| 2:A:180:ARG:HB2 | 2:A:181:TYR:CE1 | 0.60 | 2.32 | 10 | 9 |
| 2:A:57:ILE:HG21 | 2:A:135:LEU:HB2 | 0.60 | 1.72 | 4 | 4 |
| 1:B:11:DG:N7 | 2:A:70:TYR:OH | 0.60 | 2.34 | 10 | 3 |
| 1:B:5:DG:N9 | 2:A:131:TYR:CE2 | 0.60 | 2.69 | 6 | 6 |
| 1:B:5:DG:C8 | 1:B:5:DG:H5' | 0.60 | 2.32 | 9 | 3 |
| 1:B:7:DG:C1' | 2:A:63:TYR:CD2 | 0.60 | 2.84 | 7 | 4 |
| 1:B:8:DT:O5' | 1:B:8:DT:H6 | 0.60 | 1.79 | 7 | 1 |
| 1:B:7:DG:C2' | 1:B:8:DT:C6 | 0.60 | 2.85 | 1 | 4 |
| 2:A:71:GLU:CG | 2:A:72:ASN:N | 0.60 | 2.65 | 5 | 6 |
| 2:A:67:LEU:HD11 | 2:A:74:LEU:HD23 | 0.60 | 1.73 | 1 | 1 |
| 2:A:13:ILE:HD11 | 2:A:28:ILE:HG21 | 0.60 | 1.73 | 7 | 1 |
| 2:A:20:LEU:HD21 | 2:A:25:THR:HA | 0.59 | 1.74 | 9 | 1 |
| 1:B:9:DG:P | 2:A:61:TYR:OH | 0.59 | 2.60 | 3 | 4 |
| 1:B:6:DG:C8 | 1:B:6:DG:O5' | 0.59 | 2.55 | 3 | 1 |
| 2:A:67:LEU:HD11 | 2:A:74:LEU:HD12 | 0.59 | 1.74 | 3 | 1 |
| 1:B:8:DT:C5' | 1:B:9:DG:N7 | 0.59 | 2.63 | 8 | 1 |
| 1:B:10:DT:H1' | 1:B:11:DG:O3' | 0.59 | 1.97 | 3 | 3 |
| 1:B:3:DG:C8 | 1:B:4:DT:H72 | 0.59 | 2.31 | 8 | 4 |
| 1:B:10:DT:OP2 | 2:A:66:TYR:CE2 | 0.59 | 2.55 | 7 | 1 |
| 1:B:5:DG:C1' | 2:A:131:TYR:CE2 | 0.59 | 2.85 | 7 | 1 |
| 2:A:179:SER:O | 2:A:182:PHE:CE2 | 0.59 | 2.56 | 10 | 2 |
| 1:B:8:DT:O3' | 2:A:61:TYR:CE2 | 0.59 | 2.56 | 1 | 8 |
| 1:B:10:DT:OP2 | 2:A:66:TYR:CD2 | 0.59 | 2.55 | 7 | 5 |
| 1:B:11:DG:OP1 | 2:A:66:TYR:CZ | 0.59 | 2.55 | 6 | 2 |
| 1:B:11:DG:OP1 | 2:A:66:TYR:CE1 | 0.59 | 2.56 | 2 | 2 |
| 2:A:76:LEU:N | 2:A:76:LEU:CD1 | 0.59 | 2.59 | 8 | 1 |
| 1:B:10:DT:O3' | 1:B:11:DG:C3' | 0.59 | 2.49 | 10 | 1 |
| 1:B:7:DG:C2' | 1:B:8:DT:C5' | 0.59 | 2.81 | 5 | 3 |
| 2:A:15:PHE:CE2 | 2:A:78:GLU:O | 0.59 | 2.56 | 3 | 5 |
| 1:B:5:DG:OP2 | 2:A:44:PHE:CD2 | 0.59 | 2.55 | 4 | 1 |
| 2:A:126:ILE:HA | 2:A:138:ILE:O | 0.59 | 1.98 | 10 | 9 |
| 2:A:14:GLU:O | 2:A:16:CYS:N | 0.59 | 2.36 | 10 | 10 |
| 1:B:7:DG:H3' | 1:B:8:DT:C4 | 0.59 | 2.33 | 9 | 5 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:A:12:THR:HG23 | 2:A:29:THR:HB | 0.59 | 1.74 | 5 | 5 |
| 2:A:14:GLU:N | 2:A:17:GLN:HB2 | 0.59 | 2.13 | 2 | 2 |
| 1:B:9:DG:O3' | 2:A:66:TYR:CZ | 0.59 | 2.56 | 8 | 1 |
| 2:A:44:PHE:N | 2:A:44:PHE:CD1 | 0.58 | 2.67 | 1 | 1 |
| 2:A:135:LEU:HD13 | 2:A:135:LEU:C | 0.58 | 2.18 | 6 | 2 |
| 1:B:6:DG:C8 | 2:A:41:LYS:HE2 | 0.58 | 2.33 | 2 | 1 |
| 1:B:8:DT:C2' | 2:A:61:TYR:CD2 | 0.58 | 2.87 | 7 | 9 |
| 2:A:45:ILE:O | 2:A:47:PHE:CD2 | 0.58 | 2.56 | 1 | 5 |
| 2:A:15:PHE:CA | 2:A:18:LEU:HD23 | 0.58 | 2.29 | 9 | 3 |
| 2:A:63:TYR:CD1 | 2:A:66:TYR:CE2 | 0.58 | 2.91 | 8 | 2 |
| 1:B:5:DG:C3' | 2:A:131:TYR:CE2 | 0.58 | 2.86 | 4 | 1 |
| 1:B:7:DG:C4 | 1:B:7:DG:OP2 | 0.58 | 2.56 | 3 | 1 |
| 1:B:7:DG:OP1 | 1:B:8:DT:C4 | 0.58 | 2.56 | 3 | 1 |
| 1:B:4:DT:O3' | 2:A:83:ILE:CD1 | 0.58 | 2.52 | 2 | 4 |
| 1:B:10:DT:O3' | 2:A:66:TYR:CE2 | 0.58 | 2.56 | 1 | 1 |
| 2:A:180:ARG:HB3 | 2:A:181:TYR:CE1 | 0.58 | 2.32 | 5 | 3 |
| 1:B:7:DG:C8 | 2:A:63:TYR:CG | 0.58 | 2.91 | 2 | 4 |
| 2:A:38:SER:O | 2:A:45:ILE:HG23 | 0.58 | 1.98 | 6 | 2 |
| 2:A:96:LEU:HD21 | 2:A:120:ILE:CG2 | 0.58 | 2.29 | 6 | 1 |
| 1:B:2:DT:C2' | 1:B:3:DG:O5' | 0.58 | 2.49 | 7 | 1 |
| 2:A:49:PHE:HB2 | 2:A:80:PHE:CZ | 0.58 | 2.33 | 1 | 6 |
| 2:A:74:LEU:C | 2:A:74:LEU:HD12 | 0.58 | 2.18 | 1 | 3 |
| 1:B:2:DT:C2' | 1:B:3:DG:OP2 | 0.58 | 2.51 | 2 | 1 |
| 2:A:180:ARG:HB2 | 2:A:181:TYR:CE2 | 0.58 | 2.34 | 9 | 1 |
| 1:B:3:DG:C2' | 1:B:4:DT:C7 | 0.58 | 2.81 | 7 | 2 |
| 1:B:7:DG:H8 | 1:B:8:DT:O4' | 0.58 | 1.80 | 5 | 2 |
| 1:B:2:DT:OP1 | 1:B:2:DT:C7 | 0.58 | 2.51 | 7 | 1 |
| 2:A:186:ARG:O | 2:A:187:ARG:C | 0.58 | 2.42 | 7 | 9 |
| 1:B:4:DT:O2 | 2:A:43:ALA:CB | 0.58 | 2.52 | 1 | 1 |
| 1:B:5:DG:C8 | 1:B:5:DG:O5' | 0.58 | 2.56 | 6 | 1 |
| 2:A:31:PHE:CD2 | 2:A:162:LEU:HD11 | 0.58 | 2.33 | 8 | 1 |
| 2:A:130:MET:CE | 2:A:134:LYS:O | 0.58 | 2.52 | 3 | 5 |
| 2:A:134:LYS:CD | 2:A:134:LYS:N | 0.58 | 2.65 | 4 | 1 |
| 1:B:4:DT:C5' | 1:B:5:DG:O5' | 0.58 | 2.52 | 5 | 1 |
| 2:A:68:ILE:HD12 | 2:A:177:ALA:CB | 0.58 | 2.22 | 6 | 1 |
| 1:B:5:DG:OP1 | 1:B:5:DG:C8 | 0.58 | 2.57 | 4 | 2 |
| 2:A:131:TYR:O | 2:A:131:TYR:CD2 | 0.58 | 2.56 | 5 | 1 |
| 2:A:131:TYR:O | 2:A:131:TYR:CG | 0.58 | 2.56 | 5 | 1 |
| 1:B:3:DG:C2' | 1:B:4:DT:OP1 | 0.58 | 2.52 | 5 | 2 |
| 1:B:2:DT:C4' | 1:B:3:DG:OP1 | 0.58 | 2.52 | 6 | 2 |
| 2:A:55:ASN:ND2 | 2:A:59:GLN:NE2 | 0.58 | 2.51 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:A:27:TYR:CD1 | 2:A:127:LYS:CG | 0.58 | 2.86 | 2 | 1 |
| 2:A:15:PHE:CZ | 2:A:79:GLY:O | 0.57 | 2.57 | 10 | 1 |
| 1:B:8:DT:O5' | 2:A:63:TYR:CE2 | 0.57 | 2.57 | 4 | 3 |
| 2:A:15:PHE:CZ | 2:A:78:GLU:O | 0.57 | 2.57 | 9 | 2 |
| 2:A:15:PHE:CE2 | 2:A:51:ASP:OD2 | 0.57 | 2.57 | 1 | 2 |
| 2:A:105:ARG:CG | 2:A:106:ASP:N | 0.57 | 2.66 | 7 | 1 |
| 2:A:80:PHE:CE2 | 2:A:126:ILE:HD13 | 0.57 | 2.34 | 2 | 1 |
| 1:B:10:DT:O5' | 2:A:66:TYR:CE2 | 0.57 | 2.57 | 8 | 1 |
| 1:B:4:DT:C6 | 1:B:4:DT:O5' | 0.57 | 2.57 | 10 | 1 |
| 2:A:155:SER:CB | 2:A:156:PRO:CD | 0.57 | 2.82 | 10 | 9 |
| 2:A:121:VAL:HG11 | 2:A:162:LEU:HD21 | 0.57 | 1.75 | 4 | 3 |
| 1:B:8:DT:H2'' | 2:A:61:TYR:CE2 | 0.57 | 2.33 | 10 | 10 |
| 1:B:8:DT:H4' | 2:A:63:TYR:CE1 | 0.57 | 2.35 | 3 | 6 |
| 1:B:7:DG:O6 | 2:A:81:LYS:CE | 0.57 | 2.52 | 7 | 3 |
| 2:A:57:ILE:HG21 | 2:A:135:LEU:HD22 | 0.57 | 1.75 | 3 | 1 |
| 1:B:9:DG:OP2 | 2:A:61:TYR:CZ | 0.57 | 2.56 | 3 | 2 |
| 1:B:11:DG:P | 1:B:11:DG:H3' | 0.57 | 2.40 | 10 | 1 |
| 1:B:9:DG:C2' | 1:B:10:DT:O5' | 0.57 | 2.48 | 2 | 7 |
| 1:B:11:DG:H2'' | 2:A:70:TYR:CE2 | 0.57 | 2.34 | 5 | 4 |
| 2:A:10:ASP:N | 2:A:11:PRO:CD | 0.57 | 2.67 | 9 | 2 |
| 1:B:8:DT:H2'' | 2:A:61:TYR:CG | 0.57 | 2.34 | 5 | 7 |
| 2:A:13:ILE:CD1 | 2:A:18:LEU:HD22 | 0.57 | 2.28 | 4 | 1 |
| 1:B:5:DG:O5' | 2:A:44:PHE:CE2 | 0.57 | 2.57 | 4 | 1 |
| 1:B:2:DT:H2'' | 1:B:3:DG:C8 | 0.57 | 2.34 | 1 | 3 |
| 2:A:14:GLU:HB3 | 2:A:53:THR:HG21 | 0.57 | 1.75 | 1 | 1 |
| 1:B:9:DG:OP1 | 1:B:9:DG:N7 | 0.57 | 2.37 | 2 | 1 |
| 2:A:182:PHE:CZ | 2:A:191:ILE:CD1 | 0.57 | 2.88 | 2 | 1 |
| 2:A:127:LYS:CB | 2:A:138:ILE:HD11 | 0.57 | 2.30 | 2 | 3 |
| 1:B:9:DG:O4' | 1:B:10:DT:C2' | 0.57 | 2.53 | 9 | 1 |
| 1:B:7:DG:N2 | 2:A:41:LYS:CE | 0.57 | 2.67 | 5 | 1 |
| 1:B:10:DT:P | 2:A:64:ASP:HB2 | 0.57 | 2.39 | 1 | 1 |
| 1:B:5:DG:C5 | 2:A:131:TYR:CG | 0.57 | 2.92 | 7 | 1 |
| 2:A:49:PHE:HB2 | 2:A:80:PHE:CE1 | 0.57 | 2.35 | 9 | 6 |
| 2:A:121:VAL:HG21 | 2:A:166:TYR:OH | 0.57 | 1.98 | 9 | 1 |
| 2:A:127:LYS:HB3 | 2:A:138:ILE:HD11 | 0.57 | 1.75 | 9 | 3 |
| 1:B:8:DT:H5' | 2:A:63:TYR:OH | 0.57 | 2.00 | 9 | 1 |
| 2:A:15:PHE:CE1 | 2:A:51:ASP:OD1 | 0.57 | 2.57 | 9 | 1 |
| 2:A:37:CYS:SG | 2:A:47:PHE:CE1 | 0.57 | 2.98 | 1 | 2 |
| 1:B:7:DG:N3 | 1:B:7:DG:OP1 | 0.57 | 2.38 | 10 | 1 |
| 1:B:5:DG:OP2 | 2:A:83:ILE:CG1 | 0.57 | 2.52 | 4 | 2 |
| 1:B:2:DT:H5' | 2:A:27:TYR:OH | 0.57 | 2.00 | 8 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:A:30:MET:SD | 2:A:80:PHE:CE1 | 0.57 | 2.98 | 7 | 1 |
| 2:A:65:ARG:NH2 | 2:A:76:LEU:CD2 | 0.57 | 2.68 | 3 | 1 |
| 2:A:154:ALA:CB | 2:A:158:GLN:NE2 | 0.57 | 2.67 | 3 | 1 |
| 2:A:48:VAL:HG11 | 2:A:62:LEU:O | 0.57 | 2.00 | 6 | 1 |
| 2:A:39:PHE:CD1 | 2:A:40:ASP:N | 0.57 | 2.73 | 4 | 1 |
| 2:A:27:TYR:CZ | 2:A:127:LYS:CD | 0.57 | 2.88 | 3 | 1 |
| 2:A:35:VAL:HG12 | 2:A:65:ARG:CB | 0.57 | 2.30 | 7 | 1 |
| 2:A:127:LYS:HB2 | 2:A:138:ILE:HD11 | 0.56 | 1.77 | 5 | 2 |
| 1:B:3:DG:OP2 | 2:A:138:ILE:HG21 | 0.56 | 2.00 | 1 | 1 |
| 2:A:74:LEU:HD23 | 2:A:75:GLU:H | 0.56 | 1.59 | 2 | 1 |
| 2:A:182:PHE:O | 2:A:191:ILE:HD11 | 0.56 | 1.99 | 4 | 1 |
| 2:A:44:PHE:CD1 | 2:A:44:PHE:N | 0.56 | 2.73 | 5 | 1 |
| 2:A:126:ILE:CG2 | 2:A:138:ILE:O | 0.56 | 2.53 | 4 | 7 |
| 2:A:45:ILE:HD13 | 2:A:89:PHE:CB | 0.56 | 2.30 | 1 | 1 |
| 1:B:2:DT:H71 | 2:A:127:LYS:NZ | 0.56 | 2.16 | 6 | 1 |
| 2:A:58:VAL:O | 2:A:59:GLN:C | 0.56 | 2.44 | 3 | 6 |
| 2:A:49:PHE:CE1 | 2:A:80:PHE:CZ | 0.56 | 2.93 | 2 | 1 |
| 1:B:10:DT:C2' | 1:B:11:DG:O5' | 0.56 | 2.54 | 8 | 3 |
| 1:B:7:DG:N7 | 2:A:63:TYR:HB2 | 0.56 | 2.15 | 3 | 4 |
| 2:A:182:PHE:CD2 | 2:A:183:GLU:N | 0.56 | 2.73 | 1 | 3 |
| 2:A:25:THR:OG1 | 2:A:129:LYS:CB | 0.56 | 2.53 | 2 | 1 |
| 2:A:66:TYR:CD1 | 2:A:66:TYR:N | 0.56 | 2.74 | 9 | 3 |
| 2:A:29:THR:HG22 | 2:A:31:PHE:CE1 | 0.56 | 2.35 | 1 | 2 |
| 2:A:131:TYR:C | 2:A:131:TYR:CD1 | 0.56 | 2.79 | 1 | 1 |
| 2:A:35:VAL:HG11 | 2:A:65:ARG:HE | 0.56 | 1.60 | 1 | 1 |
| 2:A:15:PHE:CZ | 2:A:51:ASP:OD2 | 0.56 | 2.59 | 1 | 2 |
| 2:A:15:PHE:CD2 | 2:A:53:THR:OG1 | 0.56 | 2.56 | 3 | 2 |
| 1:B:10:DT:O2 | 1:B:11:DG:N3 | 0.56 | 2.39 | 2 | 1 |
| 2:A:85:TYR:CD1 | 2:A:87:ASN:ND2 | 0.56 | 2.74 | 9 | 1 |
| 2:A:104:LEU:HG | 2:A:115:LEU:HD11 | 0.56 | 1.76 | 4 | 1 |
| 2:A:45:ILE:HG22 | 2:A:47:PHE:CE2 | 0.56 | 2.35 | 2 | 2 |
| 1:B:11:DG:H2' | 2:A:70:TYR:CE1 | 0.56 | 2.36 | 7 | 1 |
| 1:B:10:DT:P | 2:A:66:TYR:CE2 | 0.56 | 2.99 | 8 | 1 |
| 1:B:10:DT:C2' | 1:B:11:DG:O3' | 0.56 | 2.54 | 10 | 2 |
| 2:A:31:PHE:N | 2:A:31:PHE:CD1 | 0.56 | 2.74 | 9 | 3 |
| 2:A:27:TYR:CD1 | 2:A:127:LYS:HD2 | 0.56 | 2.36 | 5 | 1 |
| 2:A:83:ILE:C | 2:A:83:ILE:HD12 | 0.56 | 2.22 | 7 | 2 |
| 1:B:9:DG:C3' | 2:A:61:TYR:OH | 0.56 | 2.54 | 7 | 1 |
| 1:B:5:DG:H2' | 2:A:131:TYR:CD2 | 0.55 | 2.36 | 3 | 6 |
| 1:B:7:DG:H2'' | 1:B:8:DT:C5' | 0.55 | 2.30 | 7 | 6 |
| 2:A:189:PHE:CB | 2:A:190:PRO:CD | 0.55 | 2.84 | 9 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:A:67:LEU:HD12 | 2:A:74:LEU:HD12 | 0.55 | 1.76 | 5 | 2 |
| 2:A:27:TYR:CZ | 2:A:127:LYS:HD2 | 0.55 | 2.36 | 3 | 1 |
| 1:B:2:DT:H2' | 1:B:3:DG:C8 | 0.55 | 2.35 | 7 | 1 |
| 1:B:10:DT:C1' | 1:B:11:DG:O3' | 0.55 | 2.55 | 8 | 3 |
| 2:A:186:ARG:O | 2:A:188:PHE:N | 0.55 | 2.40 | 4 | 7 |
| 2:A:164:LEU:HD23 | 2:A:167:GLN:OE1 | 0.55 | 2.01 | 7 | 1 |
| 2:A:154:ALA:HB3 | 2:A:159:CYS:SG | 0.55 | 2.41 | 8 | 1 |
| 2:A:167:GLN:CG | 2:A:168:ARG:N | 0.55 | 2.69 | 7 | 1 |
| 2:A:65:ARG:C | 2:A:66:TYR:CD2 | 0.55 | 2.80 | 2 | 1 |
| 2:A:14:GLU:OE1 | 2:A:161:HIS:CE1 | 0.55 | 2.59 | 5 | 1 |
| 1:B:3:DG:H1' | 1:B:4:DT:H72 | 0.55 | 1.75 | 7 | 1 |
| 2:A:35:VAL:HG23 | 2:A:49:PHE:HA | 0.55 | 1.78 | 2 | 1 |
| 1:B:8:DT:H1' | 2:A:61:TYR:CB | 0.55 | 2.32 | 3 | 9 |
| 1:B:6:DG:H2' | 1:B:7:DG:N2 | 0.55 | 2.17 | 5 | 1 |
| 2:A:118:TYR:CB | 2:A:120:ILE:HD11 | 0.55 | 2.31 | 1 | 1 |
| 1:B:4:DT:O5' | 1:B:5:DG:OP1 | 0.55 | 2.25 | 3 | 1 |
| 2:A:38:SER:C | 2:A:45:ILE:HG23 | 0.55 | 2.22 | 6 | 1 |
| 2:A:80:PHE:CE2 | 2:A:82:ALA:HB2 | 0.55 | 2.37 | 2 | 1 |
| 2:A:31:PHE:CZ | 2:A:123:LYS:HB3 | 0.55 | 2.36 | 4 | 3 |
| 2:A:91:THR:O | 2:A:95:LYS:CE | 0.55 | 2.54 | 5 | 2 |
| 2:A:129:LYS:CG | 2:A:130:MET:N | 0.55 | 2.69 | 7 | 3 |
| 1:B:4:DT:O2 | 2:A:43:ALA:CA | 0.55 | 2.55 | 1 | 1 |
| 2:A:108:GLN:HB3 | 2:A:115:LEU:HD21 | 0.55 | 1.77 | 2 | 1 |
| 2:A:127:LYS:CB | 2:A:138:ILE:CG1 | 0.55 | 2.84 | 10 | 2 |
| 2:A:22:THR:HG22 | 2:A:23:PHE:N | 0.55 | 2.17 | 4 | 3 |
| 1:B:9:DG:H5'' | 2:A:61:TYR:HH | 0.55 | 1.61 | 5 | 2 |
| 1:B:2:DT:C2 | 1:B:3:DG:C2 | 0.55 | 2.95 | 7 | 1 |
| 2:A:37:CYS:HB3 | 2:A:47:PHE:CE1 | 0.55 | 2.37 | 2 | 3 |
| 2:A:127:LYS:HG2 | 2:A:138:ILE:HD11 | 0.55 | 1.78 | 3 | 2 |
| 2:A:74:LEU:CD1 | 2:A:75:GLU:O | 0.55 | 2.55 | 4 | 2 |
| 1:B:5:DG:O6 | 2:A:135:LEU:O | 0.55 | 2.25 | 4 | 3 |
| 2:A:10:ASP:HB3 | 2:A:11:PRO:CD | 0.55 | 2.32 | 5 | 1 |
| 1:B:3:DG:H3' | 1:B:3:DG:P | 0.55 | 2.42 | 1 | 1 |
| 2:A:118:TYR:O | 2:A:118:TYR:CD1 | 0.55 | 2.59 | 8 | 1 |
| 2:A:62:LEU:HD11 | 2:A:79:GLY:O | 0.55 | 2.02 | 8 | 3 |
| 1:B:1:DG:C4' | 2:A:27:TYR:CE1 | 0.55 | 2.90 | 3 | 1 |
| 2:A:27:TYR:O | 2:A:28:ILE:CG2 | 0.54 | 2.55 | 2 | 5 |
| 1:B:5:DG:N9 | 2:A:131:TYR:CD2 | 0.54 | 2.75 | 7 | 6 |
| 2:A:18:LEU:CD1 | 2:A:57:ILE:HD12 | 0.54 | 2.32 | 7 | 1 |
| 1:B:2:DT:C6 | 1:B:3:DG:C6 | 0.54 | 2.95 | 7 | 1 |
| 2:A:21:ASP:CB | 2:A:24:GLU:HB2 | 0.54 | 2.33 | 10 | 8 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:A:60:ASN:O | 2:A:76:LEU:CD2 | 0.54 | 2.55 | 10 | 1 |
| 1:B:8:DT:H2'' | 2:A:61:TYR:CD1 | 0.54 | 2.37 | 5 | 8 |
| 2:A:32:GLY:CA | 2:A:50:SER:O | 0.54 | 2.55 | 6 | 2 |
| 2:A:44:PHE:CD2 | 2:A:83:ILE:HB | 0.54 | 2.37 | 5 | 2 |
| 1:B:5:DG:C1' | 2:A:131:TYR:CE1 | 0.54 | 2.90 | 5 | 1 |
| 1:B:10:DT:C3' | 2:A:66:TYR:CD2 | 0.54 | 2.91 | 3 | 1 |
| 2:A:44:PHE:CE1 | 2:A:83:ILE:CG2 | 0.54 | 2.91 | 6 | 1 |
| 1:B:5:DG:C1' | 2:A:131:TYR:CD2 | 0.54 | 2.91 | 2 | 5 |
| 2:A:15:PHE:N | 2:A:15:PHE:CD1 | 0.54 | 2.72 | 1 | 2 |
| 2:A:62:LEU:HD11 | 2:A:80:PHE:HA | 0.54 | 1.76 | 3 | 1 |
| 1:B:7:DG:O6 | 2:A:81:LYS:CD | 0.54 | 2.55 | 3 | 1 |
| 1:B:11:DG:C8 | 2:A:70:TYR:CE1 | 0.54 | 2.95 | 7 | 1 |
| 1:B:9:DG:C2' | 1:B:10:DT:H3' | 0.54 | 2.32 | 2 | 5 |
| 2:A:68:ILE:O | 2:A:70:TYR:CD1 | 0.54 | 2.61 | 7 | 3 |
| 2:A:150:ILE:HD12 | 2:A:162:LEU:HD13 | 0.54 | 1.79 | 3 | 1 |
| 2:A:160:GLU:O | 2:A:164:LEU:HD12 | 0.54 | 2.02 | 6 | 1 |
| 2:A:83:ILE:O | 2:A:83:ILE:CD1 | 0.54 | 2.55 | 7 | 1 |
| 1:B:7:DG:OP2 | 1:B:7:DG:C4 | 0.54 | 2.61 | 2 | 1 |
| 1:B:7:DG:C6 | 2:A:81:LYS:HE2 | 0.54 | 2.38 | 9 | 1 |
| 2:A:155:SER:CB | 2:A:156:PRO:HD2 | 0.54 | 2.33 | 2 | 6 |
| 1:B:1:DG:O4' | 2:A:27:TYR:OH | 0.54 | 2.25 | 1 | 1 |
| 2:A:92:PHE:CZ | 2:A:96:LEU:HD12 | 0.54 | 2.38 | 7 | 2 |
| 2:A:127:LYS:HB3 | 2:A:138:ILE:CG1 | 0.54 | 2.32 | 9 | 3 |
| 2:A:92:PHE:CD1 | 2:A:142:CYS:SG | 0.54 | 2.99 | 1 | 1 |
| 1:B:7:DG:C2' | 1:B:8:DT:H5' | 0.54 | 2.32 | 10 | 3 |
| 2:A:147:HIS:NE2 | 2:A:163:ARG:NH1 | 0.54 | 2.55 | 10 | 1 |
| 2:A:91:THR:O | 2:A:95:LYS:CG | 0.54 | 2.56 | 7 | 4 |
| 2:A:15:PHE:CZ | 2:A:55:ASN:ND2 | 0.54 | 2.75 | 4 | 1 |
| 2:A:45:ILE:HG13 | 2:A:89:PHE:CG | 0.54 | 2.38 | 4 | 2 |
| 1:B:6:DG:O6 | 2:A:43:ALA:CB | 0.54 | 2.55 | 5 | 1 |
| 2:A:65:ARG:CG | 2:A:74:LEU:HD21 | 0.54 | 2.31 | 1 | 1 |
| 1:B:9:DG:C5' | 1:B:10:DT:H71 | 0.54 | 2.32 | 1 | 1 |
| 1:B:3:DG:C1' | 1:B:4:DT:C7 | 0.54 | 2.86 | 7 | 1 |
| 1:B:7:DG:C8 | 1:B:7:DG:OP1 | 0.54 | 2.60 | 8 | 1 |
| 2:A:89:PHE:C | 2:A:89:PHE:CD1 | 0.54 | 2.81 | 8 | 1 |
| 1:B:5:DG:C4' | 1:B:6:DG:O5' | 0.54 | 2.55 | 1 | 3 |
| 2:A:62:LEU:O | 2:A:64:ASP:N | 0.54 | 2.41 | 4 | 1 |
| 1:B:5:DG:OP2 | 2:A:83:ILE:CD1 | 0.54 | 2.56 | 4 | 2 |
| 2:A:20:LEU:CD1 | 2:A:135:LEU:HD21 | 0.54 | 2.33 | 2 | 1 |
| 2:A:183:GLU:O | 2:A:186:ARG:CG | 0.54 | 2.56 | 10 | 5 |
| 1:B:10:DT:H72 | 1:B:10:DT:OP1 | 0.54 | 2.01 | 9 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:A:129:LYS:HG2 | 2:A:130:MET:N | 0.54 | 2.18 | 4 | 3 |
| 2:A:37:CYS:SG | 2:A:45:ILE:CG2 | 0.54 | 2.96 | 3 | 3 |
| 2:A:63:TYR:O | 2:A:76:LEU:HD22 | 0.54 | 2.02 | 1 | 1 |
| 2:A:45:ILE:HD11 | 2:A:89:PHE:CD2 | 0.54 | 2.38 | 7 | 1 |
| 1:B:5:DG:N3 | 2:A:131:TYR:CG | 0.54 | 2.75 | 2 | 1 |
| 2:A:15:PHE:CE2 | 2:A:79:GLY:O | 0.54 | 2.61 | 10 | 2 |
| 1:B:8:DT:C5' | 2:A:63:TYR:CZ | 0.54 | 2.91 | 6 | 2 |
| 2:A:76:LEU:HD23 | 2:A:76:LEU:N | 0.54 | 2.18 | 1 | 2 |
| 2:A:162:LEU:O | 2:A:166:TYR:CD2 | 0.54 | 2.61 | 5 | 2 |
| 2:A:24:GLU:O | 2:A:25:THR:OG1 | 0.53 | 2.26 | 2 | 9 |
| 2:A:86:LYS:O | 2:A:90:GLU:CG | 0.53 | 2.56 | 3 | 8 |
| 1:B:10:DT:C1' | 1:B:11:DG:N3 | 0.53 | 2.60 | 2 | 2 |
| 2:A:33:MET:O | 2:A:50:SER:N | 0.53 | 2.42 | 4 | 1 |
| 2:A:27:TYR:CD1 | 2:A:127:LYS:CD | 0.53 | 2.91 | 5 | 1 |
| 2:A:72:ASN:OD1 | 2:A:73:LYS:N | 0.53 | 2.41 | 1 | 2 |
| 2:A:21:ASP:CB | 2:A:24:GLU:OE1 | 0.53 | 2.56 | 3 | 1 |
| 2:A:119:GLY:O | 2:A:121:VAL:N | 0.53 | 2.41 | 3 | 1 |
| 2:A:127:LYS:HE2 | 2:A:138:ILE:HD12 | 0.53 | 1.78 | 8 | 1 |
| 2:A:26:LYS:C | 2:A:27:TYR:CD1 | 0.53 | 2.81 | 6 | 4 |
| 2:A:69:ASP:O | 2:A:71:GLU:N | 0.53 | 2.37 | 5 | 1 |
| 1:B:11:DG:H3' | 2:A:70:TYR:CE2 | 0.53 | 2.39 | 3 | 2 |
| 2:A:63:TYR:O | 2:A:64:ASP:CB | 0.53 | 2.56 | 6 | 1 |
| 1:B:3:DG:H2' | 1:B:4:DT:C7 | 0.53 | 2.33 | 7 | 4 |
| 2:A:35:VAL:HG11 | 2:A:64:ASP:OD1 | 0.53 | 2.04 | 4 | 1 |
| 2:A:181:TYR:CD1 | 2:A:181:TYR:N | 0.53 | 2.77 | 5 | 5 |
| 2:A:31:PHE:CZ | 2:A:123:LYS:HG3 | 0.53 | 2.38 | 1 | 1 |
| 2:A:160:GLU:CG | 2:A:161:HIS:N | 0.53 | 2.71 | 5 | 8 |
| 1:B:6:DG:C8 | 1:B:7:DG:C5 | 0.53 | 2.96 | 9 | 1 |
| 2:A:13:ILE:CG2 | 2:A:17:GLN:O | 0.53 | 2.57 | 8 | 4 |
| 2:A:49:PHE:CE1 | 2:A:122:CYS:SG | 0.53 | 3.02 | 3 | 1 |
| 2:A:182:PHE:CE2 | 2:A:183:GLU:CG | 0.53 | 2.91 | 3 | 1 |
| 2:A:47:PHE:O | 2:A:82:ALA:HB3 | 0.53 | 2.03 | 6 | 1 |
| 2:A:58:VAL:CG2 | 2:A:133:GLY:O | 0.53 | 2.56 | 10 | 1 |
| 2:A:43:ALA:O | 2:A:44:PHE:CB | 0.53 | 2.57 | 4 | 7 |
| 1:B:9:DG:H2'' | 1:B:10:DT:C5' | 0.53 | 2.32 | 4 | 1 |
| 2:A:34:LEU:CD1 | 2:A:36:SER:O | 0.53 | 2.56 | 1 | 2 |
| 1:B:9:DG:N7 | 1:B:9:DG:OP1 | 0.53 | 2.42 | 6 | 3 |
| 2:A:100:PHE:O | 2:A:102:ASN:ND2 | 0.53 | 2.42 | 1 | 3 |
| 2:A:92:PHE:CD1 | 2:A:93:ASP:N | 0.53 | 2.77 | 7 | 1 |
| 1:B:1:DG:O5' | 1:B:2:DT:C7 | 0.53 | 2.56 | 9 | 1 |
| 1:B:9:DG:H3' | 1:B:9:DG:P | 0.53 | 2.44 | 9 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:A:97:ARG:O | 2:A:101:ASN:N | 0.53 | 2.42 | 4 | 7 |
| 2:A:27:TYR:C | 2:A:28:ILE:HG23 | 0.53 | 2.24 | 5 | 5 |
| 1:B:5:DG:H4' | 1:B:6:DG:C8 | 0.53 | 2.38 | 5 | 1 |
| 2:A:105:ARG:HG3 | 2:A:106:ASP:N | 0.53 | 2.18 | 7 | 1 |
| 2:A:154:ALA:HB1 | 2:A:158:GLN:OE1 | 0.53 | 2.04 | 2 | 1 |
| 2:A:169:ALA:HB1 | 2:A:173:ILE:CD1 | 0.53 | 2.33 | 8 | 1 |
| 2:A:181:TYR:N | 2:A:181:TYR:CD1 | 0.53 | 2.76 | 3 | 4 |
| 1:B:2:DT:H2'' | 1:B:3:DG:C5' | 0.53 | 2.34 | 9 | 1 |
| 2:A:92:PHE:CE1 | 2:A:96:LEU:CD1 | 0.53 | 2.91 | 9 | 1 |
| 2:A:85:TYR:CG | 2:A:87:ASN:ND2 | 0.53 | 2.77 | 9 | 1 |
| 2:A:48:VAL:HG11 | 2:A:64:ASP:OD2 | 0.53 | 2.03 | 4 | 1 |
| 1:B:10:DT:C2' | 1:B:11:DG:OP2 | 0.53 | 2.56 | 4 | 2 |
| 2:A:30:MET:SD | 2:A:80:PHE:CE2 | 0.53 | 3.01 | 4 | 1 |
| 2:A:147:HIS:O | 2:A:148:SER:CB | 0.53 | 2.56 | 3 | 2 |
| 2:A:121:VAL:HG11 | 2:A:166:TYR:OH | 0.53 | 2.04 | 5 | 1 |
| 2:A:149:GLN:CD | 2:A:153:ILE:HD11 | 0.53 | 2.23 | 2 | 1 |
| 2:A:39:PHE:CE1 | 2:A:45:ILE:CG1 | 0.53 | 2.91 | 8 | 1 |
| 2:A:61:TYR:CD2 | 2:A:63:TYR:HA | 0.53 | 2.39 | 1 | 1 |
| 2:A:131:TYR:O | 2:A:132:ASN:CB | 0.53 | 2.57 | 10 | 7 |
| 1:B:11:DG:H2' | 2:A:70:TYR:CD2 | 0.53 | 2.38 | 10 | 2 |
| 1:B:8:DT:H2'' | 2:A:61:TYR:CZ | 0.53 | 2.39 | 1 | 10 |
| 2:A:31:PHE:CZ | 2:A:123:LYS:HB2 | 0.53 | 2.38 | 5 | 2 |
| 1:B:10:DT:O3' | 2:A:66:TYR:CE1 | 0.53 | 2.62 | 6 | 1 |
| 2:A:74:LEU:HD21 | 2:A:78:GLU:OE1 | 0.53 | 2.04 | 2 | 2 |
| 1:B:10:DT:P | 2:A:66:TYR:CD2 | 0.53 | 3.02 | 8 | 1 |
| 1:B:9:DG:P | 1:B:9:DG:H3' | 0.53 | 2.44 | 10 | 3 |
| 2:A:156:PRO:O | 2:A:157:SER:CB | 0.53 | 2.56 | 7 | 6 |
| 2:A:189:PHE:CG | 2:A:190:PRO:HD2 | 0.53 | 2.39 | 6 | 3 |
| 2:A:13:ILE:O | 2:A:14:GLU:CB | 0.53 | 2.55 | 7 | 1 |
| 2:A:55:ASN:OD1 | 2:A:57:ILE:N | 0.53 | 2.42 | 2 | 1 |
| 1:B:2:DT:C6 | 1:B:3:DG:N7 | 0.52 | 2.77 | 10 | 1 |
| 2:A:130:MET:HA | 2:A:134:LYS:O | 0.52 | 2.04 | 4 | 10 |
| 2:A:34:LEU:HD12 | 2:A:35:VAL:N | 0.52 | 2.20 | 1 | 2 |
| 2:A:117:GLN:C | 2:A:118:TYR:CD1 | 0.52 | 2.82 | 4 | 1 |
| 2:A:24:GLU:OE2 | 2:A:26:LYS:NZ | 0.52 | 2.42 | 6 | 1 |
| 1:B:6:DG:OP1 | 1:B:6:DG:N9 | 0.52 | 2.42 | 6 | 1 |
| 2:A:180:ARG:HB2 | 2:A:181:TYR:CD2 | 0.52 | 2.39 | 9 | 1 |
| 2:A:100:PHE:CZ | 2:A:118:TYR:CD2 | 0.52 | 2.97 | 9 | 1 |
| 2:A:57:ILE:O | 2:A:58:VAL:CG2 | 0.52 | 2.53 | 4 | 1 |
| 2:A:12:THR:O | 2:A:13:ILE:CG2 | 0.52 | 2.56 | 3 | 3 |
| 1:B:5:DG:OP1 | 1:B:6:DG:O6 | 0.52 | 2.27 | 3 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:A:118:TYR:CE1 | 2:A:184:GLU:O | 0.52 | 2.63 | 2 | 1 |
| 2:A:31:PHE:CE2 | 2:A:123:LYS:HD2 | 0.52 | 2.39 | 10 | 2 |
| 1:B:2:DT:C5 | 1:B:3:DG:N1 | 0.52 | 2.77 | 7 | 1 |
| 1:B:5:DG:O5' | 2:A:136:ASN:ND2 | 0.52 | 2.43 | 6 | 2 |
| 2:A:134:LYS:N | 2:A:134:LYS:HD3 | 0.52 | 2.20 | 7 | 1 |
| 2:A:52:PHE:CD1 | 2:A:52:PHE:C | 0.52 | 2.81 | 7 | 1 |
| 2:A:58:VAL:CB | 2:A:133:GLY:O | 0.52 | 2.58 | 10 | 1 |
| 2:A:65:ARG:NE | 2:A:74:LEU:O | 0.52 | 2.43 | 5 | 1 |
| 2:A:62:LEU:HD11 | 2:A:80:PHE:N | 0.52 | 2.19 | 3 | 1 |
| 1:B:7:DG:C8 | 2:A:63:TYR:CD2 | 0.52 | 2.98 | 6 | 3 |
| 1:B:4:DT:C2' | 2:A:44:PHE:CD2 | 0.52 | 2.93 | 6 | 1 |
| 1:B:5:DG:P | 2:A:83:ILE:HG12 | 0.52 | 2.45 | 1 | 2 |
| 2:A:57:ILE:CD1 | 2:A:135:LEU:HD23 | 0.52 | 2.27 | 5 | 1 |
| 1:B:10:DT:H3' | 2:A:66:TYR:CD2 | 0.52 | 2.40 | 3 | 1 |
| 1:B:11:DG:N9 | 2:A:70:TYR:CE2 | 0.52 | 2.78 | 6 | 2 |
| 1:B:2:DT:H71 | 2:A:127:LYS:HE2 | 0.52 | 1.80 | 2 | 1 |
| 2:A:44:PHE:CD1 | 2:A:44:PHE:C | 0.52 | 2.83 | 9 | 4 |
| 2:A:49:PHE:HB3 | 2:A:80:PHE:CE1 | 0.52 | 2.40 | 9 | 1 |
| 2:A:60:ASN:OD1 | 2:A:134:LYS:CG | 0.52 | 2.58 | 9 | 1 |
| 2:A:87:ASN:OD1 | 2:A:88:GLN:N | 0.52 | 2.42 | 9 | 1 |
| 2:A:139:VAL:HG12 | 2:A:141:GLU:O | 0.52 | 2.04 | 1 | 3 |
| 2:A:145:VAL:HG13 | 2:A:150:ILE:HD12 | 0.52 | 1.77 | 6 | 1 |
| 2:A:131:TYR:CD1 | 2:A:131:TYR:O | 0.52 | 2.63 | 7 | 1 |
| 2:A:14:GLU:HA | 2:A:18:LEU:CD2 | 0.52 | 2.32 | 7 | 1 |
| 1:B:5:DG:OP2 | 2:A:136:ASN:OD1 | 0.52 | 2.28 | 10 | 2 |
| 2:A:61:TYR:O | 2:A:63:TYR:N | 0.52 | 2.41 | 10 | 2 |
| 2:A:131:TYR:N | 2:A:134:LYS:O | 0.52 | 2.43 | 4 | 2 |
| 2:A:37:CYS:HB2 | 2:A:104:LEU:HD23 | 0.52 | 1.81 | 7 | 1 |
| 2:A:17:GLN:O | 2:A:18:LEU:O | 0.52 | 2.27 | 2 | 9 |
| 1:B:11:DG:N2 | 2:A:70:TYR:O | 0.52 | 2.43 | 5 | 1 |
| 1:B:5:DG:C2 | 2:A:129:LYS:HE3 | 0.52 | 2.40 | 2 | 2 |
| 1:B:10:DT:C6 | 1:B:10:DT:H5' | 0.52 | 2.40 | 8 | 1 |
| 2:A:65:ARG:O | 2:A:67:LEU:N | 0.52 | 2.43 | 9 | 3 |
| 2:A:14:GLU:C | 2:A:18:LEU:HD23 | 0.52 | 2.26 | 4 | 1 |
| 2:A:62:LEU:HD21 | 2:A:80:PHE:CA | 0.52 | 2.35 | 1 | 2 |
| 2:A:38:SER:O | 2:A:45:ILE:CG2 | 0.52 | 2.58 | 6 | 2 |
| 1:B:1:DG:H2' | 2:A:27:TYR:CZ | 0.52 | 2.39 | 7 | 1 |
| 2:A:45:ILE:CD1 | 2:A:89:PHE:CD2 | 0.52 | 2.93 | 7 | 1 |
| 2:A:129:LYS:CE | 2:A:136:ASN:OD1 | 0.52 | 2.57 | 8 | 1 |
| 2:A:31:PHE:CD2 | 2:A:123:LYS:HB3 | 0.51 | 2.41 | 9 | 1 |
| 2:A:126:ILE:CG1 | 2:A:138:ILE:O | 0.51 | 2.58 | 4 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:6:DG:H1' | 1:B:7:DG:O5' | 0.51 | 2.06 | 1 | 1 |
| 1:B:9:DG:O5' | 2:A:61:TYR:OH | 0.51 | 2.27 | 3 | 1 |
| 1:B:3:DG:C1' | 1:B:4:DT:OP1 | 0.51 | 2.58 | 6 | 1 |
| 2:A:100:PHE:CD1 | 2:A:107:LEU:HD21 | 0.51 | 2.40 | 7 | 2 |
| 2:A:187:ARG:HD3 | 2:A:188:PHE:CE2 | 0.51 | 2.40 | 2 | 1 |
| 2:A:39:PHE:CD1 | 2:A:39:PHE:C | 0.51 | 2.82 | 10 | 1 |
| 1:B:9:DG:OP2 | 2:A:61:TYR:OH | 0.51 | 2.28 | 9 | 5 |
| 2:A:157:SER:OG | 2:A:158:GLN:N | 0.51 | 2.43 | 9 | 3 |
| 2:A:72:ASN:O | 2:A:73:LYS:C | 0.51 | 2.48 | 9 | 3 |
| 2:A:62:LEU:N | 2:A:62:LEU:HD23 | 0.51 | 2.20 | 4 | 1 |
| 2:A:67:LEU:CD1 | 2:A:74:LEU:HD12 | 0.51 | 2.35 | 5 | 2 |
| 1:B:8:DT:C2' | 2:A:61:TYR:CD1 | 0.51 | 2.93 | 5 | 1 |
| 2:A:15:PHE:CD1 | 2:A:15:PHE:N | 0.51 | 2.74 | 8 | 1 |
| 1:B:8:DT:H2'' | 2:A:61:TYR:CE1 | 0.51 | 2.40 | 1 | 7 |
| 1:B:1:DG:O4' | 2:A:27:TYR:CE1 | 0.51 | 2.62 | 1 | 2 |
| 2:A:76:LEU:H | 2:A:76:LEU:HD22 | 0.51 | 1.65 | 8 | 1 |
| 1:B:10:DT:O4' | 1:B:11:DG:O3' | 0.51 | 2.28 | 8 | 1 |
| 1:B:9:DG:H4' | 1:B:10:DT:C6 | 0.51 | 2.41 | 10 | 2 |
| 1:B:1:DG:C1' | 2:A:27:TYR:CE2 | 0.51 | 2.93 | 9 | 1 |
| 2:A:187:ARG:CG | 2:A:188:PHE:N | 0.51 | 2.71 | 1 | 3 |
| 2:A:63:TYR:CD1 | 2:A:66:TYR:CD2 | 0.51 | 2.98 | 4 | 1 |
| 2:A:120:ILE:O | 2:A:120:ILE:CG2 | 0.51 | 2.57 | 2 | 2 |
| 2:A:38:SER:HB2 | 2:A:46:SER:CB | 0.51 | 2.36 | 4 | 1 |
| 2:A:127:LYS:HB2 | 2:A:138:ILE:CD1 | 0.51 | 2.36 | 2 | 3 |
| 1:B:10:DT:H1' | 1:B:11:DG:C3' | 0.51 | 2.35 | 3 | 1 |
| 2:A:57:ILE:CG2 | 2:A:58:VAL:N | 0.51 | 2.74 | 9 | 6 |
| 2:A:135:LEU:HD13 | 2:A:136:ASN:N | 0.51 | 2.20 | 2 | 3 |
| 2:A:165:PHE:C | 2:A:165:PHE:CD1 | 0.51 | 2.83 | 3 | 3 |
| 2:A:129:LYS:O | 2:A:135:LEU:HD22 | 0.51 | 2.04 | 2 | 1 |
| 2:A:14:GLU:HG3 | 2:A:53:THR:HG21 | 0.51 | 1.82 | 9 | 1 |
| 2:A:10:ASP:CB | 2:A:11:PRO:HD2 | 0.51 | 2.34 | 5 | 1 |
| 2:A:182:PHE:CD1 | 2:A:183:GLU:N | 0.51 | 2.79 | 5 | 1 |
| 2:A:20:LEU:HD23 | 2:A:26:LYS:CE | 0.51 | 2.35 | 7 | 2 |
| 2:A:15:PHE:CE2 | 2:A:51:ASP:OD1 | 0.51 | 2.63 | 1 | 1 |
| 2:A:182:PHE:CZ | 2:A:191:ILE:HD12 | 0.51 | 2.40 | 2 | 1 |
| 2:A:10:ASP:N | 2:A:11:PRO:HD3 | 0.51 | 2.21 | 9 | 3 |
| 2:A:189:PHE:CB | 2:A:190:PRO:HD3 | 0.51 | 2.35 | 9 | 1 |
| 2:A:156:PRO:O | 2:A:158:GLN:N | 0.51 | 2.44 | 9 | 5 |
| 2:A:67:LEU:HD11 | 2:A:74:LEU:CD2 | 0.51 | 2.36 | 1 | 1 |
| 2:A:128:VAL:CG1 | 2:A:135:LEU:HD11 | 0.51 | 2.36 | 6 | 1 |
| 2:A:15:PHE:CZ | 2:A:80:PHE:CD1 | 0.51 | 2.98 | 8 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:10:DT:O2 | 1:B:11:DG:O3' | 0.51 | 2.28 | 8 | 1 |
| 2:A:123:LYS:C | 2:A:124:MET:CG | 0.51 | 2.78 | 4 | 6 |
| 2:A:29:THR:CG2 | 2:A:123:LYS:CG | 0.51 | 2.89 | 7 | 2 |
| 2:A:69:ASP:OD2 | 2:A:177:ALA:HB2 | 0.51 | 2.05 | 6 | 1 |
| 2:A:31:PHE:CZ | 2:A:162:LEU:HD11 | 0.51 | 2.40 | 7 | 1 |
| 1:B:3:DG:O5' | 1:B:3:DG:C8 | 0.51 | 2.64 | 2 | 1 |
| 2:A:182:PHE:CE2 | 2:A:191:ILE:HD11 | 0.51 | 2.41 | 2 | 1 |
| 2:A:92:PHE:CZ | 2:A:96:LEU:CD1 | 0.51 | 2.93 | 8 | 2 |
| 2:A:143:GLU:OE2 | 2:A:153:ILE:CG2 | 0.51 | 2.58 | 2 | 1 |
| 2:A:18:LEU:CD1 | 2:A:57:ILE:HD13 | 0.51 | 2.35 | 10 | 1 |
| 1:B:10:DT:O4' | 1:B:11:DG:H1' | 0.51 | 2.06 | 9 | 1 |
| 2:A:71:GLU:HG3 | 2:A:72:ASN:N | 0.51 | 2.21 | 8 | 3 |
| 1:B:6:DG:C8 | 1:B:6:DG:OP1 | 0.51 | 2.64 | 6 | 1 |
| 2:A:130:MET:HE3 | 2:A:134:LYS:O | 0.51 | 2.05 | 2 | 2 |
| 2:A:21:ASP:CB | 2:A:24:GLU:CD | 0.51 | 2.80 | 4 | 1 |
| 1:B:5:DG:C2 | 2:A:81:LYS:HD2 | 0.51 | 2.41 | 1 | 1 |
| 2:A:147:HIS:CD2 | 2:A:147:HIS:O | 0.51 | 2.64 | 6 | 1 |
| 1:B:6:DG:H3' | 1:B:7:DG:C2 | 0.51 | 2.41 | 2 | 1 |
| 2:A:62:LEU:HD21 | 2:A:81:LYS:N | 0.51 | 2.21 | 8 | 1 |
| 1:B:2:DT:C6 | 1:B:2:DT:H5'' | 0.50 | 2.41 | 10 | 2 |
| 2:A:13:ILE:CB | 2:A:17:GLN:HB3 | 0.50 | 2.36 | 4 | 4 |
| 1:B:2:DT:C2' | 1:B:3:DG:H5'' | 0.50 | 2.35 | 9 | 1 |
| 2:A:57:ILE:HD13 | 2:A:135:LEU:CG | 0.50 | 2.35 | 9 | 1 |
| 1:B:5:DG:H5'' | 2:A:44:PHE:CE2 | 0.50 | 2.41 | 5 | 1 |
| 1:B:1:DG:C1' | 2:A:27:TYR:HE1 | 0.50 | 2.19 | 1 | 1 |
| 2:A:24:GLU:OE1 | 2:A:25:THR:N | 0.50 | 2.43 | 10 | 1 |
| 2:A:19:GLY:O | 2:A:20:LEU:O | 0.50 | 2.29 | 7 | 10 |
| 2:A:135:LEU:C | 2:A:135:LEU:CD1 | 0.50 | 2.80 | 9 | 3 |
| 2:A:65:ARG:O | 2:A:66:TYR:C | 0.50 | 2.47 | 1 | 5 |
| 2:A:145:VAL:CG1 | 2:A:145:VAL:O | 0.50 | 2.56 | 1 | 2 |
| 1:B:7:DG:P | 1:B:7:DG:O4' | 0.50 | 2.69 | 7 | 1 |
| 2:A:31:PHE:CE2 | 2:A:123:LYS:HG3 | 0.50 | 2.41 | 7 | 1 |
| 2:A:167:GLN:HG3 | 2:A:168:ARG:N | 0.50 | 2.20 | 7 | 1 |
| 2:A:13:ILE:HB | 2:A:17:GLN:CB | 0.50 | 2.37 | 2 | 1 |
| 1:B:1:DG:C2' | 2:A:27:TYR:HE2 | 0.50 | 2.19 | 8 | 1 |
| 2:A:44:PHE:CE2 | 2:A:83:ILE:CD1 | 0.50 | 2.95 | 8 | 1 |
| 2:A:39:PHE:CZ | 2:A:45:ILE:HG12 | 0.50 | 2.41 | 8 | 1 |
| 2:A:57:ILE:HD12 | 2:A:135:LEU:CD2 | 0.50 | 2.36 | 10 | 1 |
| 2:A:57:ILE:HG22 | 2:A:59:GLN:H | 0.50 | 1.66 | 5 | 2 |
| 1:B:4:DT:O2 | 2:A:43:ALA:O | 0.50 | 2.28 | 1 | 2 |
| 2:A:85:TYR:CE2 | 2:A:87:ASN:HB2 | 0.50 | 2.42 | 3 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:A:62:LEU:O | 2:A:63:TYR:O | 0.50 | 2.29 | 6 | 1 |
| 2:A:121:VAL:O | 2:A:145:VAL:N | 0.50 | 2.44 | 8 | 2 |
| 2:A:92:PHE:HA | 2:A:95:LYS:CE | 0.50 | 2.37 | 5 | 2 |
| 2:A:71:GLU:HG2 | 2:A:72:ASN:N | 0.50 | 2.21 | 2 | 2 |
| 1:B:3:DG:O3' | 1:B:5:DG:OP2 | 0.50 | 2.30 | 2 | 2 |
| 2:A:66:TYR:O | 2:A:67:LEU:O | 0.50 | 2.30 | 2 | 4 |
| 2:A:37:CYS:CB | 2:A:47:PHE:CE1 | 0.50 | 2.94 | 10 | 2 |
| 2:A:150:ILE:HG23 | 2:A:151:SER:N | 0.50 | 2.22 | 3 | 8 |
| 2:A:58:VAL:O | 2:A:59:GLN:O | 0.50 | 2.28 | 8 | 7 |
| 2:A:48:VAL:HG11 | 2:A:64:ASP:HB3 | 0.50 | 1.83 | 4 | 1 |
| 1:B:9:DG:P | 2:A:61:TYR:CZ | 0.50 | 3.05 | 3 | 1 |
| 1:B:1:DG:O3' | 2:A:27:TYR:OH | 0.50 | 2.29 | 9 | 2 |
| 1:B:4:DT:OP2 | 1:B:5:DG:OP1 | 0.50 | 2.28 | 9 | 2 |
| 2:A:31:PHE:CE2 | 2:A:123:LYS:HB3 | 0.50 | 2.42 | 9 | 1 |
| 2:A:36:SER:OG | 2:A:64:ASP:CB | 0.50 | 2.59 | 4 | 1 |
| 1:B:10:DT:O2 | 1:B:11:DG:N2 | 0.50 | 2.45 | 5 | 1 |
| 1:B:10:DT:P | 2:A:64:ASP:CB | 0.50 | 3.00 | 1 | 1 |
| 1:B:7:DG:O4' | 1:B:7:DG:OP2 | 0.50 | 2.29 | 8 | 2 |
| 2:A:39:PHE:N | 2:A:39:PHE:CD1 | 0.50 | 2.80 | 2 | 1 |
| 2:A:63:TYR:HA | 2:A:66:TYR:CE1 | 0.50 | 2.42 | 8 | 1 |
| 2:A:84:MET:O | 2:A:85:TYR:C | 0.50 | 2.49 | 3 | 9 |
| 2:A:40:ASP:OD1 | 2:A:40:ASP:N | 0.50 | 2.43 | 9 | 1 |
| 1:B:3:DG:H2' | 1:B:4:DT:C6 | 0.50 | 2.42 | 1 | 1 |
| 2:A:27:TYR:CD1 | 2:A:127:LYS:HG2 | 0.50 | 2.42 | 2 | 1 |
| 2:A:15:PHE:CE2 | 2:A:55:ASN:ND2 | 0.50 | 2.80 | 4 | 1 |
| 1:B:2:DT:H1' | 1:B:3:DG:C5 | 0.50 | 2.42 | 5 | 2 |
| 1:B:2:DT:C5' | 1:B:3:DG:OP1 | 0.50 | 2.59 | 1 | 1 |
| 2:A:25:THR:HG22 | 2:A:25:THR:O | 0.50 | 2.07 | 2 | 1 |
| 2:A:188:PHE:O | 2:A:189:PHE:CB | 0.50 | 2.60 | 2 | 1 |
| 2:A:81:LYS:HG3 | 2:A:82:ALA:N | 0.50 | 2.22 | 9 | 1 |
| 2:A:129:LYS:HE2 | 2:A:136:ASN:ND2 | 0.50 | 2.22 | 4 | 1 |
| 2:A:31:PHE:CZ | 2:A:123:LYS:HD3 | 0.50 | 2.42 | 3 | 1 |
| 2:A:19:GLY:O | 2:A:24:GLU:OE2 | 0.50 | 2.30 | 3 | 1 |
| 2:A:65:ARG:O | 2:A:66:TYR:O | 0.50 | 2.30 | 8 | 1 |
| 2:A:74:LEU:HD22 | 2:A:78:GLU:OE1 | 0.50 | 2.07 | 8 | 1 |
| 1:B:3:DG:C2' | 1:B:4:DT:H73 | 0.49 | 2.37 | 10 | 1 |
| 1:B:7:DG:H2' | 1:B:8:DT:C2 | 0.49 | 2.42 | 9 | 1 |
| 1:B:9:DG:H2'' | 1:B:10:DT:C3' | 0.49 | 2.36 | 2 | 3 |
| 1:B:1:DG:H4' | 2:A:27:TYR:CE1 | 0.49 | 2.41 | 3 | 1 |
| 1:B:7:DG:OP1 | 1:B:7:DG:O4' | 0.49 | 2.30 | 6 | 1 |
| 2:A:96:LEU:HD22 | 2:A:100:PHE:CD2 | 0.49 | 2.41 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:A:66:TYR:O | 2:A:67:LEU:C | 0.49 | 2.49 | 8 | 1 |
| 2:A:50:SER:HB2 | 2:A:74:LEU:HD11 | 0.49 | 1.83 | 10 | 1 |
| 2:A:49:PHE:CE2 | 2:A:124:MET:SD | 0.49 | 3.05 | 4 | 1 |
| 2:A:92:PHE:CD1 | 2:A:92:PHE:C | 0.49 | 2.85 | 5 | 1 |
| 2:A:155:SER:N | 2:A:156:PRO:HD2 | 0.49 | 2.23 | 3 | 2 |
| 1:B:9:DG:P | 2:A:61:TYR:HH | 0.49 | 2.29 | 3 | 1 |
| 2:A:154:ALA:O | 2:A:155:SER:CB | 0.49 | 2.59 | 3 | 1 |
| 2:A:31:PHE:CD2 | 2:A:123:LYS:HG3 | 0.49 | 2.42 | 7 | 1 |
| 2:A:117:GLN:HG3 | 2:A:181:TYR:CD2 | 0.49 | 2.41 | 7 | 1 |
| 1:B:8:DT:C2' | 2:A:61:TYR:CE2 | 0.49 | 2.96 | 10 | 9 |
| 2:A:39:PHE:O | 2:A:39:PHE:CD1 | 0.49 | 2.65 | 10 | 1 |
| 2:A:27:TYR:CD1 | 2:A:27:TYR:N | 0.49 | 2.77 | 5 | 1 |
| 2:A:58:VAL:C | 2:A:59:GLN:CG | 0.49 | 2.81 | 6 | 2 |
| 1:B:10:DT:C2 | 1:B:11:DG:C2 | 0.49 | 3.00 | 2 | 2 |
| 1:B:11:DG:OP1 | 1:B:11:DG:H4' | 0.49 | 2.07 | 2 | 1 |
| 2:A:32:GLY:HA3 | 2:A:49:PHE:CD1 | 0.49 | 2.42 | 2 | 1 |
| 2:A:178:ILE:HD13 | 2:A:185:TYR:CE2 | 0.49 | 2.42 | 10 | 1 |
| 2:A:127:LYS:HB3 | 2:A:138:ILE:CD1 | 0.49 | 2.37 | 9 | 1 |
| 1:B:9:DG:C4' | 1:B:10:DT:H2' | 0.49 | 2.37 | 9 | 1 |
| 1:B:2:DT:C2 | 1:B:3:DG:O6 | 0.49 | 2.66 | 5 | 1 |
| 1:B:4:DT:C1' | 2:A:44:PHE:CD2 | 0.49 | 2.95 | 6 | 2 |
| 1:B:4:DT:O5' | 1:B:5:DG:P | 0.49 | 2.70 | 3 | 1 |
| 1:B:9:DG:H3' | 2:A:61:TYR:OH | 0.49 | 2.08 | 7 | 1 |
| 1:B:11:DG:OP1 | 2:A:64:ASP:O | 0.49 | 2.30 | 7 | 1 |
| 2:A:33:MET:O | 2:A:34:LEU:O | 0.49 | 2.31 | 2 | 1 |
| 2:A:155:SER:CB | 2:A:156:PRO:HD3 | 0.49 | 2.37 | 1 | 3 |
| 2:A:37:CYS:SG | 2:A:45:ILE:HG22 | 0.49 | 2.48 | 5 | 2 |
| 2:A:143:GLU:OE1 | 2:A:153:ILE:CG2 | 0.49 | 2.60 | 4 | 1 |
| 2:A:18:LEU:HD12 | 2:A:57:ILE:HD12 | 0.49 | 1.84 | 5 | 2 |
| 1:B:6:DG:C1' | 1:B:7:DG:P | 0.49 | 3.01 | 1 | 1 |
| 2:A:31:PHE:CE2 | 2:A:123:LYS:HB2 | 0.49 | 2.43 | 7 | 2 |
| 2:A:92:PHE:CZ | 2:A:96:LEU:HD11 | 0.49 | 2.42 | 2 | 1 |
| 2:A:159:CYS:SG | 2:A:160:GLU:N | 0.49 | 2.85 | 3 | 3 |
| 1:B:1:DG:C1' | 2:A:27:TYR:OH | 0.49 | 2.59 | 1 | 1 |
| 1:B:10:DT:H4' | 2:A:66:TYR:CD2 | 0.49 | 2.42 | 1 | 1 |
| 2:A:59:GLN:NE2 | 2:A:76:LEU:O | 0.49 | 2.45 | 6 | 1 |
| 1:B:4:DT:H2'' | 1:B:5:DG:OP2 | 0.49 | 2.07 | 1 | 2 |
| 1:B:9:DG:O3' | 2:A:61:TYR:OH | 0.49 | 2.31 | 7 | 1 |
| 2:A:52:PHE:CZ | 2:A:168:ARG:CD | 0.49 | 2.95 | 2 | 1 |
| 2:A:50:SER:CB | 2:A:79:GLY:CA | 0.49 | 2.91 | 2 | 1 |
| 2:A:180:ARG:CB | 2:A:181:TYR:CD1 | 0.49 | 2.96 | 5 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:6:DG:N2 | 2:A:136:ASN:OD1 | 0.49 | 2.46 | 9 | 1 |
| 1:B:5:DG:H3' | 2:A:131:TYR:CZ | 0.49 | 2.42 | 4 | 1 |
| 2:A:21:ASP:HB2 | 2:A:24:GLU:CG | 0.49 | 2.38 | 2 | 3 |
| 2:A:52:PHE:C | 2:A:52:PHE:CD1 | 0.49 | 2.83 | 2 | 2 |
| 2:A:130:MET:HE2 | 2:A:134:LYS:O | 0.49 | 2.06 | 8 | 1 |
| 2:A:20:LEU:HD22 | 2:A:24:GLU:HB3 | 0.49 | 1.85 | 5 | 3 |
| 2:A:129:LYS:HG3 | 2:A:136:ASN:HB3 | 0.49 | 1.85 | 5 | 4 |
| 2:A:141:GLU:O | 2:A:142:CYS:C | 0.49 | 2.52 | 9 | 1 |
| 2:A:186:ARG:O | 2:A:189:PHE:O | 0.49 | 2.31 | 4 | 2 |
| 2:A:147:HIS:O | 2:A:149:GLN:N | 0.49 | 2.46 | 4 | 1 |
| 1:B:8:DT:O5' | 2:A:63:TYR:HE1 | 0.49 | 1.90 | 1 | 1 |
| 2:A:127:LYS:CB | 2:A:138:ILE:CD1 | 0.49 | 2.91 | 2 | 1 |
| 1:B:6:DG:H2'' | 2:A:41:LYS:CE | 0.49 | 2.38 | 9 | 2 |
| 2:A:48:VAL:CG1 | 2:A:64:ASP:HB3 | 0.49 | 2.38 | 4 | 1 |
| 1:B:5:DG:C4 | 2:A:131:TYR:CE1 | 0.49 | 3.01 | 5 | 1 |
| 2:A:64:ASP:HA | 2:A:66:TYR:CE1 | 0.49 | 2.42 | 5 | 1 |
| 2:A:150:ILE:CD1 | 2:A:162:LEU:HD13 | 0.49 | 2.30 | 7 | 1 |
| 2:A:164:LEU:CD2 | 2:A:167:GLN:OE1 | 0.49 | 2.60 | 7 | 1 |
| 1:B:8:DT:C1' | 2:A:61:TYR:CG | 0.48 | 2.95 | 1 | 4 |
| 2:A:20:LEU:HG | 2:A:128:VAL:CG2 | 0.48 | 2.38 | 5 | 1 |
| 2:A:27:TYR:CE2 | 2:A:127:LYS:HD2 | 0.48 | 2.43 | 3 | 1 |
| 2:A:61:TYR:CE2 | 2:A:66:TYR:OH | 0.48 | 2.56 | 7 | 1 |
| 1:B:5:DG:N2 | 2:A:131:TYR:HA | 0.48 | 2.23 | 2 | 1 |
| 2:A:68:ILE:O | 2:A:69:ASP:C | 0.48 | 2.52 | 8 | 3 |
| 2:A:48:VAL:CB | 2:A:64:ASP:HB3 | 0.48 | 2.37 | 4 | 2 |
| 2:A:15:PHE:CD2 | 2:A:55:ASN:OD1 | 0.48 | 2.66 | 9 | 1 |
| 2:A:129:LYS:CE | 2:A:136:ASN:ND2 | 0.48 | 2.76 | 4 | 1 |
| 2:A:135:LEU:CD1 | 2:A:135:LEU:C | 0.48 | 2.81 | 6 | 1 |
| 2:A:63:TYR:O | 2:A:65:ARG:N | 0.48 | 2.47 | 9 | 1 |
| 2:A:35:VAL:CG1 | 2:A:64:ASP:OD1 | 0.48 | 2.61 | 4 | 1 |
| 2:A:100:PHE:O | 2:A:101:ASN:HB3 | 0.48 | 2.08 | 7 | 7 |
| 2:A:45:ILE:O | 2:A:47:PHE:CE2 | 0.48 | 2.67 | 5 | 1 |
| 2:A:29:THR:HG21 | 2:A:123:LYS:HD2 | 0.48 | 1.85 | 7 | 2 |
| 2:A:10:ASP:OD1 | 2:A:10:ASP:N | 0.48 | 2.44 | 3 | 1 |
| 2:A:52:PHE:CD1 | 2:A:52:PHE:O | 0.48 | 2.66 | 7 | 1 |
| 2:A:43:ALA:O | 2:A:44:PHE:HB3 | 0.48 | 2.09 | 6 | 10 |
| 2:A:127:LYS:CB | 2:A:138:ILE:HG13 | 0.48 | 2.39 | 9 | 1 |
| 1:B:4:DT:C2' | 2:A:83:ILE:CD1 | 0.48 | 2.90 | 6 | 2 |
| 2:A:85:TYR:O | 2:A:88:GLN:N | 0.48 | 2.47 | 3 | 3 |
| 1:B:5:DG:OP2 | 2:A:83:ILE:HG21 | 0.48 | 2.08 | 4 | 1 |
| 1:B:5:DG:H2'' | 1:B:6:DG:C5' | 0.48 | 2.39 | 5 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:2:DT:H4' | 1:B:3:DG:OP1 | 0.48 | 2.08 | 1 | 1 |
| 1:B:9:DG:O4' | 1:B:10:DT:C5 | 0.48 | 2.67 | 1 | 1 |
| 1:B:7:DG:H2' | 1:B:8:DT:N1 | 0.48 | 2.23 | 9 | 2 |
| 2:A:72:ASN:O | 2:A:73:LYS:O | 0.48 | 2.31 | 2 | 2 |
| 2:A:118:TYR:CE2 | 2:A:184:GLU:HB3 | 0.48 | 2.44 | 4 | 1 |
| 1:B:4:DT:C5' | 1:B:5:DG:OP1 | 0.48 | 2.62 | 7 | 2 |
| 1:B:4:DT:C4' | 1:B:5:DG:OP1 | 0.48 | 2.60 | 8 | 1 |
| 1:B:9:DG:C1' | 1:B:10:DT:H2' | 0.48 | 2.38 | 9 | 2 |
| 1:B:10:DT:C7 | 1:B:10:DT:OP1 | 0.48 | 2.61 | 9 | 1 |
| 1:B:11:DG:P | 2:A:63:TYR:OH | 0.48 | 2.71 | 4 | 1 |
| 2:A:45:ILE:N | 2:A:45:ILE:HD12 | 0.48 | 2.23 | 5 | 1 |
| 2:A:49:PHE:HB3 | 2:A:80:PHE:CZ | 0.48 | 2.43 | 1 | 1 |
| 2:A:120:ILE:O | 2:A:121:VAL:O | 0.48 | 2.32 | 3 | 2 |
| 1:B:7:DG:N7 | 2:A:63:TYR:HB3 | 0.48 | 2.23 | 7 | 1 |
| 1:B:2:DT:C7 | 2:A:127:LYS:HE2 | 0.48 | 2.38 | 2 | 1 |
| 2:A:27:TYR:CD1 | 2:A:127:LYS:HG3 | 0.48 | 2.43 | 2 | 1 |
| 2:A:53:THR:O | 2:A:77:ASN:O | 0.48 | 2.31 | 10 | 1 |
| 2:A:62:LEU:HG | 2:A:76:LEU:HD23 | 0.48 | 1.85 | 10 | 1 |
| 1:B:4:DT:H5'' | 1:B:5:DG:H3' | 0.48 | 1.86 | 9 | 1 |
| 1:B:5:DG:C2' | 2:A:131:TYR:HE2 | 0.48 | 2.21 | 7 | 3 |
| 2:A:66:TYR:O | 2:A:67:LEU:CB | 0.48 | 2.61 | 6 | 2 |
| 2:A:58:VAL:CG1 | 2:A:134:LYS:HA | 0.48 | 2.39 | 3 | 4 |
| 2:A:67:LEU:HD12 | 2:A:74:LEU:HG | 0.48 | 1.84 | 6 | 1 |
| 2:A:66:TYR:N | 2:A:66:TYR:CD1 | 0.48 | 2.78 | 8 | 1 |
| 2:A:65:ARG:O | 2:A:67:LEU:HD23 | 0.48 | 2.09 | 9 | 1 |
| 2:A:64:ASP:O | 2:A:65:ARG:C | 0.48 | 2.52 | 1 | 1 |
| 1:B:1:DG:H1' | 2:A:27:TYR:CE1 | 0.48 | 2.43 | 1 | 1 |
| 2:A:128:VAL:CB | 2:A:135:LEU:HD11 | 0.48 | 2.39 | 6 | 1 |
| 1:B:6:DG:H2' | 2:A:41:LYS:CE | 0.48 | 2.39 | 7 | 2 |
| 2:A:188:PHE:CD1 | 2:A:188:PHE:C | 0.48 | 2.84 | 7 | 1 |
| 2:A:39:PHE:C | 2:A:39:PHE:CD1 | 0.48 | 2.87 | 7 | 1 |
| 2:A:52:PHE:CG | 2:A:52:PHE:O | 0.48 | 2.66 | 2 | 1 |
| 2:A:62:LEU:O | 2:A:63:TYR:CB | 0.48 | 2.60 | 8 | 1 |
| 2:A:100:PHE:O | 2:A:102:ASN:OD1 | 0.48 | 2.31 | 8 | 1 |
| 2:A:15:PHE:CD2 | 2:A:55:ASN:HB2 | 0.48 | 2.43 | 5 | 2 |
| 1:B:8:DT:C4' | 2:A:63:TYR:CE1 | 0.48 | 2.97 | 3 | 4 |
| 2:A:129:LYS:N | 2:A:136:ASN:O | 0.48 | 2.46 | 4 | 2 |
| 1:B:6:DG:C2' | 1:B:7:DG:N2 | 0.48 | 2.77 | 5 | 1 |
| 2:A:83:ILE:CD1 | 2:A:83:ILE:C | 0.48 | 2.80 | 3 | 1 |
| 2:A:125:ASN:O | 2:A:140:ARG:N | 0.48 | 2.44 | 3 | 1 |
| 2:A:13:ILE:CB | 2:A:17:GLN:HB2 | 0.48 | 2.38 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:A:36:SER:HB3 | 2:A:65:ARG:CG | 0.48 | 2.39 | 7 | 1 |
| 1:B:5:DG:C2' | 2:A:131:TYR:CD2 | 0.48 | 2.97 | 3 | 5 |
| 2:A:43:ALA:C | 2:A:44:PHE:CG | 0.48 | 2.85 | 4 | 3 |
| 2:A:31:PHE:CZ | 2:A:123:LYS:CB | 0.48 | 2.96 | 4 | 1 |
| 2:A:128:VAL:HB | 2:A:135:LEU:HD21 | 0.48 | 1.86 | 6 | 1 |
| 2:A:67:LEU:HD12 | 2:A:74:LEU:CD1 | 0.48 | 2.38 | 6 | 1 |
| 1:B:7:DG:O6 | 2:A:81:LYS:HD3 | 0.47 | 2.09 | 9 | 1 |
| 1:B:7:DG:H22 | 2:A:46:SER:CB | 0.47 | 2.21 | 9 | 1 |
| 1:B:8:DT:C4' | 1:B:9:DG:C8 | 0.47 | 2.96 | 8 | 2 |
| 2:A:30:MET:SD | 2:A:80:PHE:CD2 | 0.47 | 3.07 | 4 | 1 |
| 2:A:183:GLU:HG3 | 2:A:184:GLU:N | 0.47 | 2.24 | 4 | 1 |
| 2:A:62:LEU:CD2 | 2:A:80:PHE:HA | 0.47 | 2.40 | 2 | 3 |
| 2:A:67:LEU:HD11 | 2:A:74:LEU:CD1 | 0.47 | 2.39 | 3 | 1 |
| 2:A:49:PHE:CE1 | 2:A:124:MET:HE1 | 0.47 | 2.43 | 2 | 1 |
| 2:A:36:SER:HB2 | 2:A:64:ASP:O | 0.47 | 2.10 | 2 | 3 |
| 2:A:48:VAL:CG2 | 2:A:64:ASP:CB | 0.47 | 2.92 | 9 | 2 |
| 2:A:70:TYR:CD1 | 2:A:70:TYR:N | 0.47 | 2.82 | 1 | 4 |
| 2:A:39:PHE:CE1 | 2:A:45:ILE:HG12 | 0.47 | 2.43 | 9 | 2 |
| 2:A:133:GLY:C | 2:A:134:LYS:CD | 0.47 | 2.82 | 4 | 1 |
| 1:B:11:DG:H2'' | 2:A:70:TYR:CD2 | 0.47 | 2.44 | 1 | 1 |
| 2:A:51:ASP:OD1 | 2:A:78:GLU:O | 0.47 | 2.32 | 6 | 1 |
| 2:A:155:SER:OG | 2:A:158:GLN:NE2 | 0.47 | 2.47 | 7 | 1 |
| 2:A:117:GLN:HG2 | 2:A:181:TYR:CG | 0.47 | 2.45 | 2 | 1 |
| 1:B:4:DT:H73 | 2:A:85:TYR:OH | 0.47 | 2.09 | 10 | 1 |
| 2:A:36:SER:OG | 2:A:64:ASP:O | 0.47 | 2.32 | 6 | 3 |
| 2:A:86:LYS:O | 2:A:90:GLU:HG2 | 0.47 | 2.08 | 4 | 9 |
| 1:B:4:DT:H2' | 2:A:83:ILE:HD13 | 0.47 | 1.80 | 9 | 1 |
| 2:A:48:VAL:HG11 | 2:A:64:ASP:CB | 0.47 | 2.39 | 4 | 1 |
| 2:A:52:PHE:O | 2:A:53:THR:OG1 | 0.47 | 2.32 | 1 | 2 |
| 2:A:15:PHE:HB3 | 2:A:55:ASN:N | 0.47 | 2.25 | 8 | 3 |
| 2:A:13:ILE:O | 2:A:14:GLU:HG2 | 0.47 | 2.10 | 7 | 1 |
| 1:B:2:DT:H2' | 1:B:3:DG:C5 | 0.47 | 2.43 | 7 | 1 |
| 2:A:121:VAL:HG12 | 2:A:145:VAL:HB | 0.47 | 1.86 | 8 | 1 |
| 2:A:24:GLU:OE1 | 2:A:24:GLU:CA | 0.47 | 2.62 | 10 | 1 |
| 2:A:45:ILE:O | 2:A:46:SER:C | 0.47 | 2.53 | 1 | 5 |
| 2:A:122:CYS:SG | 2:A:143:GLU:O | 0.47 | 2.72 | 6 | 3 |
| 1:B:5:DG:H2'' | 1:B:6:DG:OP2 | 0.47 | 2.09 | 4 | 2 |
| 2:A:15:PHE:O | 2:A:54:LYS:O | 0.47 | 2.32 | 8 | 3 |
| 2:A:38:SER:CB | 2:A:46:SER:HB2 | 0.47 | 2.40 | 4 | 1 |
| 1:B:5:DG:H5'' | 2:A:44:PHE:CZ | 0.47 | 2.44 | 5 | 1 |
| 1:B:9:DG:C4' | 1:B:10:DT:O5' | 0.47 | 2.62 | 5 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:A:61:TYR:CE2 | 2:A:63:TYR:HA | 0.47 | 2.44 | 1 | 1 |
| 2:A:31:PHE:CE1 | 2:A:123:LYS:HB2 | 0.47 | 2.45 | 3 | 1 |
| 2:A:15:PHE:CZ | 2:A:51:ASP:CG | 0.47 | 2.88 | 6 | 1 |
| 2:A:25:THR:OG1 | 2:A:129:LYS:HB2 | 0.47 | 2.09 | 2 | 1 |
| 1:B:7:DG:H2' | 1:B:8:DT:C5' | 0.47 | 2.40 | 5 | 2 |
| 2:A:131:TYR:CD2 | 2:A:134:LYS:HB2 | 0.47 | 2.44 | 5 | 1 |
| 1:B:7:DG:C5 | 2:A:63:TYR:HB2 | 0.47 | 2.44 | 5 | 1 |
| 2:A:64:ASP:O | 2:A:65:ARG:CG | 0.47 | 2.62 | 1 | 1 |
| 2:A:150:ILE:O | 2:A:154:ALA:N | 0.47 | 2.47 | 3 | 1 |
| 2:A:24:GLU:OE2 | 2:A:26:LYS:CE | 0.47 | 2.63 | 6 | 1 |
| 2:A:45:ILE:CG2 | 2:A:47:PHE:CE1 | 0.47 | 2.98 | 7 | 1 |
| 1:B:3:DG:OP2 | 2:A:138:ILE:HD11 | 0.47 | 2.09 | 2 | 2 |
| 1:B:4:DT:H4' | 1:B:5:DG:OP1 | 0.47 | 2.10 | 8 | 2 |
| 2:A:187:ARG:O | 2:A:188:PHE:O | 0.47 | 2.33 | 2 | 1 |
| 2:A:15:PHE:CE1 | 2:A:80:PHE:HB3 | 0.47 | 2.44 | 10 | 1 |
| 2:A:129:LYS:CG | 2:A:136:ASN:HB3 | 0.47 | 2.39 | 6 | 5 |
| 2:A:188:PHE:CG | 2:A:188:PHE:O | 0.47 | 2.68 | 10 | 1 |
| 2:A:36:SER:CB | 2:A:64:ASP:O | 0.47 | 2.62 | 2 | 3 |
| 2:A:132:ASN:OD1 | 2:A:132:ASN:O | 0.47 | 2.33 | 9 | 1 |
| 2:A:68:ILE:CD1 | 2:A:117:GLN:HG2 | 0.47 | 2.38 | 5 | 1 |
| 2:A:38:SER:O | 2:A:45:ILE:HA | 0.47 | 2.10 | 6 | 2 |
| 1:B:4:DT:H5'' | 1:B:5:DG:OP1 | 0.47 | 2.09 | 7 | 1 |
| 2:A:44:PHE:CE2 | 2:A:83:ILE:HG21 | 0.47 | 2.45 | 10 | 1 |
| 1:B:5:DG:H5'' | 1:B:6:DG:N3 | 0.47 | 2.25 | 9 | 1 |
| 1:B:7:DG:O6 | 2:A:81:LYS:HE2 | 0.47 | 2.09 | 9 | 3 |
| 2:A:63:TYR:O | 2:A:64:ASP:C | 0.47 | 2.52 | 8 | 4 |
| 2:A:73:LYS:O | 2:A:74:LEU:C | 0.47 | 2.52 | 2 | 4 |
| 2:A:63:TYR:O | 2:A:64:ASP:CG | 0.47 | 2.53 | 4 | 2 |
| 2:A:74:LEU:O | 2:A:74:LEU:HD12 | 0.47 | 2.09 | 4 | 1 |
| 2:A:14:GLU:O | 2:A:17:GLN:N | 0.47 | 2.48 | 4 | 2 |
| 1:B:2:DT:C1' | 1:B:3:DG:C4 | 0.47 | 2.97 | 7 | 1 |
| 1:B:6:DG:C8 | 2:A:41:LYS:HE3 | 0.47 | 2.45 | 7 | 1 |
| 2:A:13:ILE:CA | 2:A:17:GLN:HB2 | 0.47 | 2.38 | 7 | 2 |
| 2:A:33:MET:O | 2:A:119:GLY:O | 0.47 | 2.32 | 2 | 1 |
| 2:A:183:GLU:O | 2:A:186:ARG:HG2 | 0.47 | 2.10 | 4 | 5 |
| 2:A:91:THR:O | 2:A:95:LYS:HG2 | 0.47 | 2.10 | 10 | 4 |
| 1:B:5:DG:N7 | 2:A:136:ASN:HB2 | 0.47 | 2.25 | 9 | 1 |
| 2:A:126:ILE:HG12 | 2:A:139:VAL:HG22 | 0.47 | 1.87 | 4 | 1 |
| 2:A:63:TYR:O | 2:A:66:TYR:OH | 0.47 | 2.33 | 5 | 1 |
| 1:B:11:DG:H2'' | 2:A:70:TYR:CZ | 0.47 | 2.45 | 5 | 2 |
| 2:A:96:LEU:HD13 | 2:A:104:LEU:CD1 | 0.47 | 2.39 | 3 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:5:DG:N2 | 2:A:130:MET:O | 0.47 | 2.48 | 8 | 1 |
| 2:A:92:PHE:CD1 | 2:A:142:CYS:HB2 | 0.47 | 2.44 | 3 | 2 |
| 1:B:6:DG:O6 | 2:A:43:ALA:HB1 | 0.47 | 2.09 | 5 | 1 |
| 2:A:10:ASP:HB3 | 2:A:11:PRO:HD2 | 0.47 | 1.84 | 5 | 1 |
| 2:A:169:ALA:O | 2:A:173:ILE:HB | 0.47 | 2.10 | 1 | 2 |
| 1:B:11:DG:C2' | 2:A:70:TYR:CE1 | 0.47 | 2.98 | 7 | 1 |
| 2:A:117:GLN:N | 2:A:117:GLN:OE1 | 0.47 | 2.47 | 9 | 1 |
| 2:A:67:LEU:O | 2:A:68:ILE:C | 0.47 | 2.53 | 6 | 4 |
| 2:A:48:VAL:CG2 | 2:A:81:LYS:CD | 0.47 | 2.92 | 6 | 1 |
| 1:B:9:DG:C5 | 1:B:9:DG:OP1 | 0.47 | 2.67 | 8 | 1 |
| 2:A:15:PHE:CE2 | 2:A:55:ASN:HB2 | 0.46 | 2.45 | 5 | 3 |
| 2:A:102:ASN:CG | 2:A:106:ASP:CB | 0.46 | 2.84 | 9 | 1 |
| 2:A:48:VAL:HG11 | 2:A:64:ASP:CG | 0.46 | 2.30 | 4 | 1 |
| 2:A:129:LYS:O | 2:A:136:ASN:N | 0.46 | 2.41 | 4 | 1 |
| 2:A:67:LEU:HD23 | 2:A:68:ILE:H | 0.46 | 1.69 | 2 | 1 |
| 2:A:51:ASP:OD1 | 2:A:161:HIS:CE1 | 0.46 | 2.69 | 2 | 1 |
| 2:A:104:LEU:O | 2:A:107:LEU:N | 0.46 | 2.43 | 2 | 1 |
| 2:A:179:SER:O | 2:A:182:PHE:CD2 | 0.46 | 2.68 | 10 | 1 |
| 2:A:183:GLU:O | 2:A:186:ARG:HG3 | 0.46 | 2.10 | 9 | 5 |
| 2:A:31:PHE:CE2 | 2:A:123:LYS:HG2 | 0.46 | 2.46 | 10 | 1 |
| 2:A:97:ARG:CG | 2:A:102:ASN:O | 0.46 | 2.63 | 10 | 2 |
| 2:A:189:PHE:CD2 | 2:A:190:PRO:HD2 | 0.46 | 2.45 | 1 | 2 |
| 2:A:57:ILE:CD1 | 2:A:135:LEU:HD13 | 0.46 | 2.40 | 3 | 1 |
| 2:A:128:VAL:HG12 | 2:A:135:LEU:HD11 | 0.46 | 1.85 | 6 | 1 |
| 2:A:35:VAL:HB | 2:A:48:VAL:HG12 | 0.46 | 1.86 | 7 | 1 |
| 2:A:117:GLN:HG3 | 2:A:181:TYR:CG | 0.46 | 2.45 | 7 | 1 |
| 2:A:67:LEU:HD23 | 2:A:68:ILE:N | 0.46 | 2.25 | 2 | 1 |
| 1:B:5:DG:C1' | 2:A:131:TYR:HD2 | 0.46 | 2.24 | 8 | 5 |
| 2:A:187:ARG:HG3 | 2:A:188:PHE:N | 0.46 | 2.25 | 4 | 1 |
| 2:A:69:ASP:O | 2:A:70:TYR:HB2 | 0.46 | 2.09 | 5 | 1 |
| 1:B:6:DG:C4' | 1:B:7:DG:OP1 | 0.46 | 2.63 | 1 | 1 |
| 1:B:10:DT:H1' | 1:B:11:DG:H3' | 0.46 | 1.87 | 3 | 1 |
| 1:B:9:DG:N9 | 1:B:9:DG:O5' | 0.46 | 2.48 | 2 | 1 |
| 2:A:123:LYS:HD2 | 2:A:143:GLU:CG | 0.46 | 2.41 | 8 | 1 |
| 2:A:96:LEU:CD1 | 2:A:104:LEU:HD11 | 0.46 | 2.39 | 8 | 1 |
| 1:B:6:DG:C1' | 1:B:7:DG:OP1 | 0.46 | 2.63 | 1 | 1 |
| 2:A:102:ASN:HB2 | 2:A:106:ASP:CB | 0.46 | 2.40 | 8 | 4 |
| 2:A:119:GLY:O | 2:A:120:ILE:HB | 0.46 | 2.10 | 3 | 1 |
| 2:A:14:GLU:HG3 | 2:A:30:MET:CE | 0.46 | 2.40 | 7 | 1 |
| 2:A:186:ARG:HA | 2:A:189:PHE:O | 0.46 | 2.09 | 8 | 1 |
| 2:A:83:ILE:O | 2:A:139:VAL:N | 0.46 | 2.48 | 2 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:7:DG:C3' | 1:B:8:DT:H72 | 0.46 | 2.40 | 10 | 2 |
| 1:B:4:DT:O3' | 2:A:83:ILE:HG12 | 0.46 | 2.10 | 9 | 1 |
| 1:B:9:DG:C1' | 1:B:10:DT:C2' | 0.46 | 2.93 | 9 | 1 |
| 2:A:58:VAL:CG1 | 2:A:59:GLN:N | 0.46 | 2.79 | 7 | 4 |
| 1:B:8:DT:C4' | 2:A:61:TYR:CE2 | 0.46 | 2.98 | 1 | 4 |
| 1:B:5:DG:OP2 | 2:A:83:ILE:CB | 0.46 | 2.63 | 4 | 1 |
| 2:A:62:LEU:O | 2:A:62:LEU:CD1 | 0.46 | 2.56 | 1 | 1 |
| 2:A:48:VAL:HG22 | 2:A:81:LYS:HA | 0.46 | 1.86 | 6 | 1 |
| 2:A:14:GLU:CA | 2:A:18:LEU:HD23 | 0.46 | 2.38 | 7 | 1 |
| 2:A:63:TYR:CE2 | 2:A:66:TYR:OH | 0.46 | 2.67 | 10 | 1 |
| 2:A:117:GLN:HB2 | 2:A:181:TYR:CD2 | 0.46 | 2.44 | 9 | 1 |
| 2:A:65:ARG:HG3 | 2:A:66:TYR:N | 0.46 | 2.25 | 5 | 1 |
| 2:A:102:ASN:CB | 2:A:106:ASP:CB | 0.46 | 2.93 | 1 | 1 |
| 2:A:49:PHE:CZ | 2:A:122:CYS:SG | 0.46 | 3.09 | 3 | 1 |
| 2:A:23:PHE:O | 2:A:24:GLU:O | 0.46 | 2.33 | 2 | 1 |
| 2:A:32:GLY:HA2 | 2:A:50:SER:O | 0.46 | 2.11 | 8 | 1 |
| 1:B:5:DG:OP2 | 2:A:138:ILE:CG2 | 0.46 | 2.64 | 10 | 1 |
| 1:B:3:DG:H2'' | 1:B:4:DT:OP1 | 0.46 | 2.10 | 2 | 5 |
| 2:A:91:THR:O | 2:A:95:LYS:HE2 | 0.46 | 2.11 | 5 | 2 |
| 1:B:10:DT:O3' | 2:A:63:TYR:OH | 0.46 | 2.33 | 4 | 1 |
| 1:B:5:DG:H4' | 1:B:6:DG:C5 | 0.46 | 2.45 | 5 | 1 |
| 2:A:47:PHE:CE1 | 2:A:104:LEU:HD23 | 0.46 | 2.46 | 3 | 1 |
| 2:A:64:ASP:OD1 | 2:A:64:ASP:N | 0.46 | 2.48 | 7 | 1 |
| 2:A:34:LEU:HA | 2:A:49:PHE:HB3 | 0.46 | 1.87 | 2 | 1 |
| 2:A:58:VAL:HB | 2:A:134:LYS:HA | 0.46 | 1.86 | 10 | 1 |
| 2:A:44:PHE:CZ | 2:A:83:ILE:CG2 | 0.46 | 2.98 | 10 | 1 |
| 1:B:8:DT:C4' | 2:A:63:TYR:CE2 | 0.46 | 2.99 | 9 | 1 |
| 2:A:92:PHE:C | 2:A:92:PHE:CD1 | 0.46 | 2.89 | 4 | 1 |
| 2:A:15:PHE:CE2 | 2:A:51:ASP:CG | 0.46 | 2.89 | 1 | 1 |
| 1:B:7:DG:OP1 | 1:B:8:DT:O4 | 0.46 | 2.34 | 3 | 1 |
| 2:A:99:ILE:CD1 | 2:A:144:PRO:HB2 | 0.46 | 2.40 | 6 | 1 |
| 2:A:13:ILE:HB | 2:A:17:GLN:HB2 | 0.46 | 1.88 | 7 | 1 |
| 2:A:62:LEU:O | 2:A:63:TYR:C | 0.46 | 2.54 | 7 | 1 |
| 2:A:101:ASN:ND2 | 2:A:101:ASN:O | 0.46 | 2.49 | 2 | 1 |
| 2:A:65:ARG:HG2 | 2:A:66:TYR:N | 0.46 | 2.24 | 8 | 1 |
| 2:A:92:PHE:CD1 | 2:A:142:CYS:HB3 | 0.46 | 2.45 | 5 | 1 |
| 1:B:8:DT:O5' | 2:A:63:TYR:CE1 | 0.46 | 2.69 | 1 | 1 |
| 2:A:178:ILE:O | 2:A:182:PHE:CA | 0.46 | 2.64 | 8 | 3 |
| 2:A:127:LYS:O | 2:A:138:ILE:HG12 | 0.46 | 2.10 | 3 | 2 |
| 2:A:42:PRO:O | 2:A:86:LYS:NZ | 0.46 | 2.44 | 3 | 1 |
| 2:A:187:ARG:O | 2:A:188:PHE:CB | 0.46 | 2.62 | 3 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:A:13:ILE:HB | 2:A:17:GLN:O | 0.46 | 2.11 | 5 | 6 |
| 2:A:126:ILE:HG12 | 2:A:138:ILE:O | 0.46 | 2.11 | 4 | 3 |
| 2:A:50:SER:HB3 | 2:A:65:ARG:NH1 | 0.46 | 2.25 | 1 | 1 |
| 2:A:31:PHE:CE1 | 2:A:123:LYS:HD3 | 0.46 | 2.46 | 3 | 1 |
| 2:A:190:PRO:O | 2:A:191:ILE:C | 0.45 | 2.54 | 10 | 2 |
| 2:A:35:VAL:O | 2:A:36:SER:OG | 0.45 | 2.33 | 10 | 3 |
| 2:A:97:ARG:HG2 | 2:A:102:ASN:O | 0.45 | 2.11 | 9 | 5 |
| 2:A:131:TYR:CB | 2:A:136:ASN:HB2 | 0.45 | 2.40 | 5 | 2 |
| 2:A:183:GLU:HA | 2:A:186:ARG:HG2 | 0.45 | 1.88 | 5 | 4 |
| 2:A:182:PHE:CG | 2:A:183:GLU:N | 0.45 | 2.83 | 6 | 2 |
| 2:A:29:THR:HA | 2:A:124:MET:O | 0.45 | 2.11 | 3 | 5 |
| 2:A:31:PHE:CE2 | 2:A:123:LYS:CG | 0.45 | 2.99 | 7 | 2 |
| 1:B:5:DG:H5'' | 1:B:6:DG:C2 | 0.45 | 2.46 | 9 | 1 |
| 2:A:14:GLU:CG | 2:A:14:GLU:O | 0.45 | 2.65 | 9 | 1 |
| 2:A:60:ASN:O | 2:A:62:LEU:N | 0.45 | 2.49 | 9 | 1 |
| 2:A:126:ILE:CB | 2:A:138:ILE:O | 0.45 | 2.65 | 4 | 1 |
| 2:A:14:GLU:O | 2:A:15:PHE:C | 0.45 | 2.54 | 4 | 3 |
| 2:A:177:ALA:HA | 2:A:180:ARG:CG | 0.45 | 2.41 | 4 | 1 |
| 2:A:118:TYR:N | 2:A:118:TYR:CD1 | 0.45 | 2.84 | 4 | 1 |
| 2:A:20:LEU:HD13 | 2:A:21:ASP:N | 0.45 | 2.25 | 3 | 2 |
| 2:A:61:TYR:O | 2:A:76:LEU:CD2 | 0.45 | 2.65 | 6 | 1 |
| 2:A:49:PHE:CZ | 2:A:124:MET:SD | 0.45 | 3.10 | 2 | 1 |
| 2:A:25:THR:HA | 2:A:128:VAL:O | 0.45 | 2.12 | 10 | 3 |
| 2:A:39:PHE:O | 2:A:39:PHE:CG | 0.45 | 2.68 | 10 | 1 |
| 2:A:38:SER:CB | 2:A:46:SER:HB3 | 0.45 | 2.41 | 9 | 1 |
| 2:A:48:VAL:CG2 | 2:A:81:LYS:HD2 | 0.45 | 2.42 | 6 | 1 |
| 2:A:85:TYR:CD2 | 2:A:87:ASN:HB2 | 0.45 | 2.46 | 6 | 1 |
| 2:A:30:MET:SD | 2:A:80:PHE:CZ | 0.45 | 3.09 | 7 | 1 |
| 2:A:37:CYS:O | 2:A:37:CYS:SG | 0.45 | 2.74 | 8 | 1 |
| 1:B:3:DG:H1' | 1:B:4:DT:H73 | 0.45 | 1.88 | 10 | 1 |
| 1:B:5:DG:C4 | 2:A:136:ASN:HB2 | 0.45 | 2.46 | 8 | 2 |
| 2:A:121:VAL:HG21 | 2:A:165:PHE:CE1 | 0.45 | 2.46 | 10 | 1 |
| 1:B:10:DT:OP1 | 2:A:73:LYS:HB2 | 0.45 | 2.11 | 5 | 1 |
| 2:A:89:PHE:CD1 | 2:A:89:PHE:C | 0.45 | 2.90 | 1 | 1 |
| 2:A:55:ASN:OD1 | 2:A:55:ASN:C | 0.45 | 2.55 | 2 | 1 |
| 2:A:22:THR:O | 2:A:130:MET:HB2 | 0.45 | 2.12 | 2 | 3 |
| 2:A:44:PHE:CE1 | 2:A:83:ILE:HG22 | 0.45 | 2.46 | 6 | 2 |
| 1:B:10:DT:OP1 | 2:A:65:ARG:NH1 | 0.45 | 2.50 | 10 | 1 |
| 1:B:5:DG:C2' | 1:B:6:DG:OP2 | 0.45 | 2.65 | 4 | 1 |
| 2:A:92:PHE:CE2 | 2:A:104:LEU:HD22 | 0.45 | 2.46 | 5 | 1 |
| 2:A:50:SER:CB | 2:A:65:ARG:NH1 | 0.45 | 2.79 | 1 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:10:DT:OP1 | 2:A:73:LYS:CD | 0.45 | 2.64 | 1 | 1 |
| 1:B:6:DG:O4' | 1:B:7:DG:OP1 | 0.45 | 2.35 | 1 | 1 |
| 1:B:1:DG:H2' | 2:A:27:TYR:CE2 | 0.45 | 2.47 | 7 | 1 |
| 2:A:61:TYR:CD2 | 2:A:66:TYR:OH | 0.45 | 2.65 | 7 | 1 |
| 2:A:77:ASN:OD1 | 2:A:77:ASN:N | 0.45 | 2.48 | 10 | 1 |
| 2:A:129:LYS:O | 2:A:135:LEU:HA | 0.45 | 2.12 | 8 | 4 |
| 2:A:61:TYR:O | 2:A:62:LEU:HB2 | 0.45 | 2.11 | 10 | 1 |
| 2:A:14:GLU:OE2 | 2:A:161:HIS:NE2 | 0.45 | 2.50 | 9 | 1 |
| 2:A:24:GLU:O | 2:A:25:THR:HB | 0.45 | 2.08 | 5 | 5 |
| 1:B:11:DG:C3' | 2:A:70:TYR:CE2 | 0.45 | 3.00 | 3 | 2 |
| 2:A:84:MET:CG | 2:A:84:MET:O | 0.45 | 2.64 | 3 | 1 |
| 2:A:135:LEU:C | 2:A:135:LEU:HD12 | 0.45 | 2.30 | 7 | 1 |
| 2:A:36:SER:HB2 | 2:A:64:ASP:CB | 0.45 | 2.42 | 10 | 1 |
| 2:A:186:ARG:HB2 | 2:A:189:PHE:O | 0.45 | 2.12 | 9 | 2 |
| 2:A:39:PHE:CG | 2:A:40:ASP:N | 0.45 | 2.85 | 4 | 1 |
| 1:B:5:DG:C4' | 1:B:6:DG:N7 | 0.45 | 2.76 | 5 | 1 |
| 1:B:7:DG:H1' | 2:A:63:TYR:CE1 | 0.45 | 2.47 | 1 | 1 |
| 1:B:6:DG:H2' | 2:A:41:LYS:HE3 | 0.45 | 1.88 | 7 | 1 |
| 1:B:11:DG:P | 2:A:66:TYR:CE1 | 0.45 | 3.10 | 2 | 1 |
| 2:A:61:TYR:O | 2:A:62:LEU:CB | 0.45 | 2.64 | 10 | 1 |
| 1:B:7:DG:H2'' | 1:B:8:DT:OP1 | 0.45 | 2.11 | 6 | 4 |
| 1:B:8:DT:O5' | 2:A:63:TYR:HE2 | 0.45 | 1.93 | 9 | 2 |
| 2:A:180:ARG:C | 2:A:181:TYR:CG | 0.45 | 2.89 | 5 | 1 |
| 2:A:97:ARG:O | 2:A:101:ASN:CA | 0.45 | 2.65 | 5 | 1 |
| 2:A:62:LEU:HD12 | 2:A:76:LEU:CA | 0.45 | 2.38 | 6 | 1 |
| 2:A:145:VAL:O | 2:A:145:VAL:HG12 | 0.45 | 2.12 | 7 | 1 |
| 2:A:185:TYR:CD1 | 2:A:185:TYR:C | 0.45 | 2.89 | 2 | 1 |
| 2:A:35:VAL:HG21 | 2:A:50:SER:OG | 0.45 | 2.10 | 8 | 1 |
| 1:B:9:DG:H8 | 1:B:9:DG:O5' | 0.45 | 1.93 | 9 | 1 |
| 1:B:10:DT:H2' | 1:B:11:DG:OP2 | 0.45 | 2.12 | 4 | 1 |
| 1:B:8:DT:C3' | 2:A:61:TYR:CE2 | 0.45 | 2.99 | 1 | 4 |
| 2:A:15:PHE:CE2 | 2:A:55:ASN:CG | 0.45 | 2.90 | 4 | 1 |
| 1:B:9:DG:C5' | 2:A:61:TYR:OH | 0.45 | 2.65 | 5 | 1 |
| 1:B:5:DG:N2 | 1:B:7:DG:O6 | 0.45 | 2.50 | 5 | 2 |
| 1:B:10:DT:OP1 | 2:A:73:LYS:CG | 0.45 | 2.65 | 1 | 1 |
| 2:A:12:THR:C | 2:A:13:ILE:HG23 | 0.45 | 2.31 | 6 | 2 |
| 2:A:35:VAL:C | 2:A:36:SER:OG | 0.45 | 2.55 | 6 | 1 |
| 2:A:96:LEU:HD21 | 2:A:120:ILE:HG21 | 0.45 | 1.89 | 6 | 1 |
| 2:A:14:GLU:CG | 2:A:161:HIS:CE1 | 0.45 | 3.00 | 2 | 1 |
| 1:B:3:DG:H5' | 2:A:138:ILE:CD1 | 0.45 | 2.41 | 2 | 1 |
| 1:B:5:DG:P | 2:A:136:ASN:OD1 | 0.45 | 2.75 | 10 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:A:61:TYR:CA | 2:A:76:LEU:HD21 | 0.45 | 2.41 | 10 | 1 |
| 2:A:188:PHE:CD2 | 2:A:188:PHE:O | 0.45 | 2.70 | 10 | 1 |
| 2:A:123:LYS:C | 2:A:124:MET:HG3 | 0.45 | 2.32 | 5 | 4 |
| 1:B:5:DG:C2' | 1:B:6:DG:OP1 | 0.45 | 2.64 | 8 | 1 |
| 2:A:22:THR:HA | 2:A:130:MET:CG | 0.44 | 2.42 | 7 | 2 |
| 2:A:101:ASN:O | 2:A:102:ASN:OD1 | 0.44 | 2.35 | 5 | 2 |
| 2:A:27:TYR:CE2 | 2:A:127:LYS:CD | 0.44 | 3.00 | 3 | 1 |
| 2:A:186:ARG:O | 2:A:189:PHE:N | 0.44 | 2.50 | 3 | 1 |
| 2:A:63:TYR:O | 2:A:64:ASP:HB2 | 0.44 | 2.11 | 6 | 1 |
| 2:A:27:TYR:CE1 | 2:A:127:LYS:HG2 | 0.44 | 2.46 | 2 | 1 |
| 2:A:131:TYR:CD1 | 2:A:131:TYR:C | 0.44 | 2.90 | 9 | 2 |
| 2:A:55:ASN:HB2 | 2:A:77:ASN:CA | 0.44 | 2.43 | 4 | 1 |
| 1:B:10:DT:OP1 | 2:A:73:LYS:CB | 0.44 | 2.65 | 5 | 1 |
| 2:A:26:LYS:HG2 | 2:A:128:VAL:CG2 | 0.44 | 2.43 | 7 | 1 |
| 1:B:11:DG:OP2 | 2:A:63:TYR:CE1 | 0.44 | 2.70 | 7 | 1 |
| 2:A:141:GLU:HG3 | 2:A:142:CYS:N | 0.44 | 2.27 | 2 | 1 |
| 2:A:143:GLU:O | 2:A:143:GLU:HG3 | 0.44 | 2.12 | 8 | 1 |
| 2:A:126:ILE:CA | 2:A:138:ILE:O | 0.44 | 2.64 | 10 | 2 |
| 2:A:60:ASN:OD1 | 2:A:134:LYS:HG2 | 0.44 | 2.12 | 9 | 1 |
| 1:B:9:DG:C1' | 1:B:10:DT:H71 | 0.44 | 2.42 | 6 | 1 |
| 1:B:5:DG:C1' | 2:A:136:ASN:HB2 | 0.44 | 2.42 | 8 | 2 |
| 1:B:4:DT:P | 1:B:5:DG:OP1 | 0.44 | 2.76 | 7 | 1 |
| 2:A:55:ASN:OD1 | 2:A:56:ASP:N | 0.44 | 2.51 | 2 | 1 |
| 2:A:10:ASP:O | 2:A:10:ASP:OD1 | 0.44 | 2.34 | 2 | 1 |
| 1:B:10:DT:C1' | 1:B:11:DG:HO3' | 0.44 | 2.25 | 8 | 1 |
| 2:A:143:GLU:OE1 | 2:A:144:PRO:N | 0.44 | 2.50 | 8 | 1 |
| 2:A:57:ILE:CD1 | 2:A:135:LEU:HD22 | 0.44 | 2.39 | 10 | 1 |
| 2:A:21:ASP:O | 2:A:24:GLU:HB2 | 0.44 | 2.12 | 7 | 4 |
| 2:A:122:CYS:CB | 2:A:144:PRO:HA | 0.44 | 2.43 | 10 | 1 |
| 2:A:68:ILE:HG22 | 2:A:69:ASP:N | 0.44 | 2.26 | 9 | 2 |
| 1:B:10:DT:OP1 | 2:A:73:LYS:HD3 | 0.44 | 2.12 | 1 | 1 |
| 1:B:1:DG:H5' | 1:B:2:DT:C4 | 0.44 | 2.47 | 1 | 1 |
| 1:B:2:DT:O3' | 1:B:3:DG:C8 | 0.44 | 2.70 | 1 | 1 |
| 2:A:52:PHE:O | 2:A:53:THR:O | 0.44 | 2.35 | 1 | 1 |
| 2:A:130:MET:CE | 2:A:133:GLY:O | 0.44 | 2.66 | 7 | 1 |
| 2:A:14:GLU:HG3 | 2:A:161:HIS:CE1 | 0.44 | 2.48 | 2 | 1 |
| 2:A:15:PHE:HB3 | 2:A:55:ASN:CA | 0.44 | 2.42 | 8 | 1 |
| 2:A:57:ILE:CD1 | 2:A:135:LEU:HG | 0.44 | 2.40 | 9 | 1 |
| 1:B:5:DG:C3' | 2:A:131:TYR:HE2 | 0.44 | 2.25 | 4 | 1 |
| 1:B:4:DT:H2'' | 2:A:44:PHE:HD2 | 0.44 | 1.72 | 5 | 1 |
| 2:A:131:TYR:O | 2:A:132:ASN:HB2 | 0.44 | 2.13 | 3 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:A:175:GLU:HA | 2:A:178:ILE:HD12 | 0.44 | 1.90 | 1 | 1 |
| 2:A:33:MET:HG3 | 2:A:119:GLY:O | 0.44 | 2.11 | 3 | 1 |
| 2:A:35:VAL:CG2 | 2:A:50:SER:HB2 | 0.44 | 2.43 | 8 | 1 |
| 2:A:123:LYS:CD | 2:A:143:GLU:HG2 | 0.44 | 2.43 | 8 | 1 |
| 2:A:55:ASN:CB | 2:A:77:ASN:HA | 0.44 | 2.42 | 10 | 1 |
| 2:A:102:ASN:HB3 | 2:A:106:ASP:CB | 0.44 | 2.43 | 10 | 1 |
| 2:A:119:GLY:CA | 2:A:185:TYR:CE1 | 0.44 | 3.00 | 9 | 1 |
| 2:A:45:ILE:HG13 | 2:A:89:PHE:CB | 0.44 | 2.42 | 4 | 2 |
| 1:B:10:DT:O4' | 1:B:11:DG:N3 | 0.44 | 2.49 | 5 | 1 |
| 2:A:183:GLU:HA | 2:A:186:ARG:CD | 0.44 | 2.43 | 1 | 2 |
| 2:A:101:ASN:C | 2:A:102:ASN:OD1 | 0.44 | 2.56 | 1 | 2 |
| 1:B:5:DG:N9 | 2:A:136:ASN:OD1 | 0.44 | 2.50 | 3 | 1 |
| 2:A:47:PHE:O | 2:A:82:ALA:N | 0.44 | 2.51 | 6 | 1 |
| 1:B:2:DT:O4' | 1:B:3:DG:H5' | 0.44 | 2.13 | 7 | 1 |
| 2:A:104:LEU:HA | 2:A:107:LEU:CD1 | 0.44 | 2.42 | 8 | 2 |
| 2:A:62:LEU:HD23 | 2:A:62:LEU:N | 0.44 | 2.26 | 2 | 1 |
| 2:A:35:VAL:CG1 | 2:A:65:ARG:HG3 | 0.44 | 2.40 | 8 | 1 |
| 2:A:143:GLU:OE1 | 2:A:144:PRO:CD | 0.44 | 2.66 | 8 | 1 |
| 2:A:71:GLU:OE1 | 2:A:71:GLU:O | 0.44 | 2.35 | 8 | 1 |
| 2:A:51:ASP:HA | 2:A:165:PHE:CE1 | 0.44 | 2.48 | 4 | 1 |
| 1:B:11:DG:N9 | 2:A:70:TYR:CD2 | 0.44 | 2.86 | 5 | 1 |
| 2:A:163:ARG:HD2 | 2:A:163:ARG:N | 0.44 | 2.28 | 5 | 1 |
| 2:A:65:ARG:HD3 | 2:A:74:LEU:CD2 | 0.44 | 2.43 | 1 | 1 |
| 2:A:121:VAL:C | 2:A:122:CYS:SG | 0.44 | 2.96 | 1 | 1 |
| 2:A:155:SER:N | 2:A:156:PRO:CD | 0.44 | 2.81 | 3 | 1 |
| 2:A:147:HIS:O | 2:A:148:SER:HB2 | 0.44 | 2.11 | 3 | 1 |
| 2:A:146:PRO:O | 2:A:147:HIS:HB2 | 0.44 | 2.13 | 6 | 1 |
| 2:A:100:PHE:O | 2:A:101:ASN:HB2 | 0.44 | 2.13 | 10 | 3 |
| 2:A:51:ASP:O | 2:A:51:ASP:CG | 0.44 | 2.57 | 10 | 1 |
| 1:B:7:DG:C3' | 1:B:8:DT:C6 | 0.44 | 3.00 | 1 | 2 |
| 2:A:14:GLU:OE2 | 2:A:51:ASP:OD2 | 0.44 | 2.36 | 5 | 1 |
| 1:B:9:DG:H4' | 1:B:10:DT:O5' | 0.44 | 2.12 | 6 | 2 |
| 1:B:7:DG:H2'' | 1:B:8:DT:O4' | 0.44 | 2.13 | 1 | 1 |
| 1:B:2:DT:C2 | 1:B:3:DG:N3 | 0.44 | 2.86 | 7 | 1 |
| 2:A:119:GLY:O | 2:A:120:ILE:C | 0.44 | 2.56 | 2 | 1 |
| 2:A:87:ASN:HA | 2:A:90:GLU:HG3 | 0.44 | 1.88 | 8 | 1 |
| 2:A:58:VAL:O | 2:A:59:GLN:CG | 0.44 | 2.66 | 1 | 1 |
| 2:A:131:TYR:HB3 | 2:A:134:LYS:CG | 0.44 | 2.43 | 3 | 1 |
| 2:A:130:MET:HE1 | 2:A:134:LYS:O | 0.44 | 2.11 | 6 | 1 |
| 2:A:45:ILE:HG22 | 2:A:47:PHE:CE1 | 0.44 | 2.48 | 7 | 1 |
| 1:B:6:DG:O5' | 1:B:6:DG:C8 | 0.44 | 2.71 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:7:DG:C2' | 1:B:7:DG:OP1 | 0.44 | 2.66 | 8 | 1 |
| 2:A:168:ARG:O | 2:A:172:ARG:N | 0.43 | 2.47 | 10 | 1 |
| 1:B:5:DG:C8 | 1:B:5:DG:C5' | 0.43 | 3.00 | 9 | 2 |
| 2:A:45:ILE:HG21 | 2:A:47:PHE:CE2 | 0.43 | 2.48 | 4 | 1 |
| 2:A:169:ALA:O | 2:A:173:ILE:CG1 | 0.43 | 2.66 | 8 | 3 |
| 1:B:9:DG:H5' | 1:B:10:DT:H71 | 0.43 | 1.90 | 1 | 1 |
| 1:B:10:DT:H2'' | 1:B:11:DG:OP2 | 0.43 | 2.13 | 6 | 1 |
| 2:A:52:PHE:CZ | 2:A:168:ARG:HD2 | 0.43 | 2.48 | 2 | 1 |
| 2:A:14:GLU:HA | 2:A:30:MET:CE | 0.43 | 2.43 | 5 | 2 |
| 1:B:5:DG:H4' | 1:B:6:DG:O5' | 0.43 | 2.13 | 9 | 1 |
| 2:A:15:PHE:CE1 | 2:A:51:ASP:CG | 0.43 | 2.92 | 9 | 1 |
| 2:A:118:TYR:OH | 2:A:184:GLU:CD | 0.43 | 2.57 | 4 | 1 |
| 2:A:33:MET:N | 2:A:50:SER:O | 0.43 | 2.50 | 4 | 2 |
| 1:B:6:DG:H1' | 1:B:7:DG:P | 0.43 | 2.53 | 1 | 1 |
| 2:A:77:ASN:N | 2:A:77:ASN:OD1 | 0.43 | 2.48 | 7 | 1 |
| 2:A:48:VAL:HG11 | 2:A:65:ARG:HB2 | 0.43 | 1.89 | 8 | 1 |
| 2:A:71:GLU:HG3 | 2:A:72:ASN:OD1 | 0.43 | 2.14 | 8 | 1 |
| 2:A:108:GLN:HA | 2:A:115:LEU:HD21 | 0.43 | 1.90 | 9 | 1 |
| 2:A:67:LEU:CD1 | 2:A:74:LEU:CD1 | 0.43 | 2.96 | 5 | 1 |
| 1:B:9:DG:P | 1:B:9:DG:N7 | 0.43 | 2.91 | 2 | 1 |
| 2:A:50:SER:HB2 | 2:A:79:GLY:CA | 0.43 | 2.43 | 2 | 1 |
| 2:A:21:ASP:O | 2:A:22:THR:C | 0.43 | 2.55 | 6 | 4 |
| 2:A:28:ILE:O | 2:A:126:ILE:N | 0.43 | 2.52 | 2 | 3 |
| 2:A:173:ILE:HD13 | 2:A:185:TYR:OH | 0.43 | 2.13 | 10 | 1 |
| 2:A:186:ARG:HB3 | 2:A:191:ILE:CG1 | 0.43 | 2.43 | 4 | 2 |
| 2:A:101:ASN:O | 2:A:102:ASN:CG | 0.43 | 2.57 | 10 | 2 |
| 2:A:75:GLU:CG | 2:A:78:GLU:OE1 | 0.43 | 2.66 | 10 | 1 |
| 2:A:35:VAL:CG1 | 2:A:74:LEU:HD12 | 0.43 | 2.43 | 9 | 1 |
| 1:B:4:DT:H5'' | 1:B:5:DG:O5' | 0.43 | 2.13 | 5 | 1 |
| 2:A:127:LYS:HB2 | 2:A:138:ILE:CG1 | 0.43 | 2.43 | 8 | 2 |
| 1:B:3:DG:H2' | 1:B:4:DT:C5 | 0.43 | 2.49 | 1 | 1 |
| 2:A:84:MET:HG2 | 2:A:84:MET:O | 0.43 | 2.12 | 1 | 1 |
| 2:A:15:PHE:HB2 | 2:A:53:THR:OG1 | 0.43 | 2.13 | 2 | 1 |
| 2:A:15:PHE:CZ | 2:A:55:ASN:OD1 | 0.43 | 2.72 | 10 | 1 |
| 2:A:95:LYS:O | 2:A:99:ILE:HG13 | 0.43 | 2.14 | 10 | 2 |
| 1:B:1:DG:O5' | 1:B:2:DT:C5 | 0.43 | 2.71 | 9 | 1 |
| 2:A:48:VAL:CG2 | 2:A:64:ASP:HB2 | 0.43 | 2.43 | 5 | 1 |
| 1:B:10:DT:O4' | 1:B:11:DG:N2 | 0.43 | 2.52 | 5 | 1 |
| 2:A:48:VAL:HG22 | 2:A:81:LYS:HB2 | 0.43 | 1.89 | 3 | 1 |
| 2:A:54:LYS:O | 2:A:54:LYS:HG3 | 0.43 | 2.14 | 2 | 1 |
| 2:A:177:ALA:HA | 2:A:180:ARG:HG2 | 0.43 | 1.89 | 4 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:A:129:LYS:CE | 2:A:136:ASN:CG | 0.43 | 2.86 | 4 | 1 |
| 1:B:8:DT:O3' | 1:B:9:DG:H8 | 0.43 | 1.97 | 7 | 2 |
| 2:A:154:ALA:HB1 | 2:A:158:GLN:HB3 | 0.43 | 1.91 | 5 | 1 |
| 2:A:143:GLU:CD | 2:A:144:PRO:O | 0.43 | 2.56 | 8 | 1 |
| 2:A:37:CYS:HA | 2:A:46:SER:O | 0.43 | 2.14 | 1 | 2 |
| 2:A:40:ASP:O | 2:A:41:LYS:C | 0.43 | 2.56 | 4 | 1 |
| 1:B:4:DT:P | 1:B:4:DT:H3' | 0.43 | 2.53 | 5 | 1 |
| 2:A:127:LYS:HB2 | 2:A:138:ILE:HG13 | 0.43 | 1.91 | 2 | 2 |
| 2:A:31:PHE:CZ | 2:A:158:GLN:NE2 | 0.43 | 2.86 | 3 | 1 |
| 2:A:58:VAL:C | 2:A:59:GLN:HG2 | 0.43 | 2.33 | 6 | 1 |
| 1:B:9:DG:H4' | 1:B:10:DT:OP1 | 0.43 | 2.14 | 7 | 2 |
| 2:A:15:PHE:CD1 | 2:A:30:MET:HE3 | 0.43 | 2.48 | 9 | 1 |
| 1:B:2:DT:H1' | 1:B:3:DG:C4 | 0.43 | 2.48 | 5 | 1 |
| 2:A:139:VAL:CG1 | 2:A:141:GLU:O | 0.43 | 2.67 | 2 | 2 |
| 2:A:28:ILE:HD12 | 2:A:30:MET:HG2 | 0.43 | 1.89 | 6 | 1 |
| 2:A:25:THR:HG23 | 2:A:127:LYS:NZ | 0.43 | 2.28 | 7 | 1 |
| 2:A:48:VAL:HG21 | 2:A:64:ASP:OD1 | 0.43 | 2.14 | 8 | 1 |
| 1:B:8:DT:O4' | 2:A:61:TYR:CD2 | 0.43 | 2.72 | 10 | 2 |
| 2:A:70:TYR:N | 2:A:70:TYR:CD1 | 0.43 | 2.87 | 10 | 1 |
| 2:A:103:GLY:O | 2:A:104:LEU:C | 0.43 | 2.58 | 10 | 8 |
| 1:B:10:DT:OP2 | 2:A:63:TYR:CE1 | 0.43 | 2.71 | 9 | 1 |
| 2:A:15:PHE:CZ | 2:A:51:ASP:OD1 | 0.43 | 2.72 | 9 | 1 |
| 2:A:141:GLU:O | 2:A:141:GLU:CD | 0.43 | 2.56 | 9 | 1 |
| 2:A:105:ARG:O | 2:A:108:GLN:HG2 | 0.43 | 2.14 | 1 | 2 |
| 2:A:165:PHE:CD1 | 2:A:166:TYR:N | 0.43 | 2.87 | 1 | 1 |
| 2:A:178:ILE:O | 2:A:182:PHE:N | 0.43 | 2.51 | 8 | 2 |
| 2:A:44:PHE:CE2 | 2:A:83:ILE:HD12 | 0.43 | 2.49 | 8 | 1 |
| 2:A:123:LYS:HD2 | 2:A:143:GLU:HG2 | 0.43 | 1.89 | 8 | 1 |
| 2:A:143:GLU:OE1 | 2:A:144:PRO:HD2 | 0.43 | 2.13 | 8 | 1 |
| 1:B:4:DT:H4' | 2:A:44:PHE:CE2 | 0.43 | 2.49 | 5 | 1 |
| 2:A:91:THR:O | 2:A:95:LYS:HE3 | 0.43 | 2.14 | 5 | 1 |
| 2:A:187:ARG:HG2 | 2:A:188:PHE:N | 0.43 | 2.29 | 5 | 1 |
| 2:A:38:SER:N | 2:A:46:SER:O | 0.43 | 2.52 | 1 | 1 |
| 2:A:37:CYS:HB2 | 2:A:47:PHE:CE1 | 0.43 | 2.49 | 1 | 1 |
| 2:A:13:ILE:HD12 | 2:A:30:MET:SD | 0.43 | 2.54 | 3 | 1 |
| 2:A:146:PRO:O | 2:A:147:HIS:CB | 0.43 | 2.66 | 3 | 1 |
| 2:A:52:PHE:O | 2:A:53:THR:C | 0.43 | 2.56 | 6 | 2 |
| 2:A:14:GLU:O | 2:A:15:PHE:HB2 | 0.43 | 2.13 | 7 | 1 |
| 1:B:10:DT:C6 | 1:B:10:DT:C3' | 0.43 | 3.02 | 2 | 1 |
| 2:A:51:ASP:OD1 | 2:A:52:PHE:N | 0.43 | 2.52 | 2 | 1 |
| 2:A:100:PHE:HB3 | 2:A:102:ASN:ND2 | 0.43 | 2.29 | 8 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:A:127:LYS:HB3 | 2:A:138:ILE:HG12 | 0.42 | 1.90 | 10 | 1 |
| 2:A:127:LYS:O | 2:A:137:ALA:HA | 0.42 | 2.14 | 10 | 3 |
| 2:A:20:LEU:HD12 | 2:A:135:LEU:HD23 | 0.42 | 1.90 | 9 | 1 |
| 2:A:13:ILE:O | 2:A:14:GLU:HB2 | 0.42 | 2.13 | 4 | 1 |
| 1:B:4:DT:C1' | 2:A:44:PHE:HD2 | 0.42 | 2.26 | 4 | 1 |
| 2:A:70:TYR:O | 2:A:71:GLU:C | 0.42 | 2.57 | 5 | 1 |
| 2:A:120:ILE:O | 2:A:121:VAL:C | 0.42 | 2.57 | 2 | 3 |
| 1:B:11:DG:C2' | 2:A:70:TYR:CD2 | 0.42 | 3.02 | 1 | 1 |
| 1:B:5:DG:OP1 | 2:A:83:ILE:HG12 | 0.42 | 2.13 | 1 | 1 |
| 1:B:5:DG:OP2 | 2:A:83:ILE:HG12 | 0.42 | 2.13 | 1 | 1 |
| 2:A:150:ILE:HG23 | 2:A:151:SER:H | 0.42 | 1.73 | 1 | 1 |
| 2:A:76:LEU:N | 2:A:76:LEU:HD23 | 0.42 | 2.29 | 3 | 1 |
| 1:B:7:DG:N7 | 2:A:81:LYS:HE3 | 0.42 | 2.29 | 7 | 1 |
| 2:A:51:ASP:C | 2:A:51:ASP:OD1 | 0.42 | 2.57 | 2 | 1 |
| 2:A:96:LEU:O | 2:A:100:PHE:N | 0.42 | 2.51 | 2 | 1 |
| 2:A:145:VAL:HG11 | 2:A:150:ILE:HD12 | 0.42 | 1.91 | 8 | 1 |
| 2:A:178:ILE:CD1 | 2:A:185:TYR:CZ | 0.42 | 3.02 | 10 | 1 |
| 2:A:94:SER:OG | 2:A:95:LYS:N | 0.42 | 2.52 | 9 | 1 |
| 2:A:20:LEU:HD21 | 2:A:25:THR:CA | 0.42 | 2.42 | 9 | 1 |
| 2:A:117:GLN:HA | 2:A:185:TYR:CE2 | 0.42 | 2.48 | 9 | 1 |
| 1:B:5:DG:O6 | 2:A:136:ASN:HA | 0.42 | 2.14 | 7 | 2 |
| 1:B:5:DG:N2 | 2:A:81:LYS:HD2 | 0.42 | 2.28 | 1 | 1 |
| 1:B:5:DG:O4' | 1:B:6:DG:O5' | 0.42 | 2.37 | 1 | 1 |
| 2:A:62:LEU:O | 2:A:65:ARG:HB3 | 0.42 | 2.14 | 3 | 1 |
| 2:A:52:PHE:O | 2:A:53:THR:CG2 | 0.42 | 2.62 | 3 | 1 |
| 1:B:2:DT:O4' | 1:B:3:DG:OP1 | 0.42 | 2.37 | 6 | 1 |
| 1:B:9:DG:C8 | 1:B:9:DG:OP1 | 0.42 | 2.72 | 6 | 1 |
| 2:A:14:GLU:CG | 2:A:30:MET:HE2 | 0.42 | 2.44 | 7 | 1 |
| 2:A:15:PHE:CB | 2:A:53:THR:HB | 0.42 | 2.44 | 7 | 1 |
| 1:B:2:DT:C5 | 1:B:3:DG:C6 | 0.42 | 3.07 | 7 | 1 |
| 1:B:2:DT:C1' | 1:B:3:DG:O4' | 0.42 | 2.59 | 7 | 1 |
| 1:B:2:DT:C4' | 1:B:3:DG:N7 | 0.42 | 2.83 | 2 | 1 |
| 2:A:21:ASP:HB2 | 2:A:24:GLU:CD | 0.42 | 2.34 | 4 | 3 |
| 2:A:87:ASN:OD1 | 2:A:88:GLN:NE2 | 0.42 | 2.52 | 9 | 1 |
| 2:A:14:GLU:OE1 | 2:A:161:HIS:ND1 | 0.42 | 2.53 | 5 | 1 |
| 2:A:24:GLU:OE1 | 2:A:26:LYS:HE2 | 0.42 | 2.14 | 1 | 1 |
| 1:B:9:DG:C5' | 1:B:10:DT:C7 | 0.42 | 2.98 | 1 | 1 |
| 1:B:9:DG:C4' | 1:B:10:DT:H71 | 0.42 | 2.42 | 1 | 1 |
| 2:A:62:LEU:HD22 | 2:A:62:LEU:O | 0.42 | 2.14 | 1 | 1 |
| 2:A:48:VAL:CG2 | 2:A:81:LYS:HB2 | 0.42 | 2.45 | 3 | 1 |
| 2:A:182:PHE:O | 2:A:183:GLU:C | 0.42 | 2.57 | 3 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:A:120:ILE:O | 2:A:121:VAL:HB | 0.42 | 2.14 | 3 | 2 |
| 2:A:39:PHE:O | 2:A:40:ASP:C | 0.42 | 2.57 | 3 | 2 |
| 2:A:48:VAL:HA | 2:A:80:PHE:O | 0.42 | 2.14 | 6 | 1 |
| 2:A:22:THR:HA | 2:A:130:MET:HG3 | 0.42 | 1.91 | 7 | 1 |
| 1:B:2:DT:C6 | 1:B:3:DG:C5 | 0.42 | 3.07 | 7 | 1 |
| 2:A:91:THR:O | 2:A:95:LYS:HG3 | 0.42 | 2.13 | 7 | 1 |
| 2:A:122:CYS:HB2 | 2:A:143:GLU:O | 0.42 | 2.14 | 2 | 1 |
| 2:A:154:ALA:O | 2:A:155:SER:O | 0.42 | 2.36 | 8 | 1 |
| 2:A:68:ILE:CD1 | 2:A:177:ALA:HB1 | 0.42 | 2.44 | 9 | 1 |
| 2:A:27:TYR:C | 2:A:28:ILE:CG2 | 0.42 | 2.87 | 5 | 1 |
| 2:A:67:LEU:CD1 | 2:A:74:LEU:HG | 0.42 | 2.45 | 5 | 2 |
| 2:A:168:ARG:NH1 | 2:A:172:ARG:NH1 | 0.42 | 2.67 | 5 | 1 |
| 1:B:3:DG:O3' | 1:B:4:DT:H3' | 0.42 | 2.13 | 1 | 1 |
| 2:A:44:PHE:CG | 2:A:83:ILE:HB | 0.42 | 2.49 | 3 | 1 |
| 1:B:8:DT:H4' | 2:A:61:TYR:CE2 | 0.42 | 2.50 | 6 | 1 |
| 2:A:180:ARG:N | 2:A:180:ARG:CD | 0.42 | 2.79 | 6 | 1 |
| 2:A:74:LEU:HD13 | 2:A:78:GLU:CB | 0.42 | 2.43 | 8 | 1 |
| 2:A:71:GLU:C | 2:A:71:GLU:OE1 | 0.42 | 2.58 | 8 | 1 |
| 1:B:8:DT:C2' | 2:A:61:TYR:CE1 | 0.42 | 3.02 | 5 | 1 |
| 1:B:8:DT:C7 | 1:B:8:DT:P | 0.42 | 3.07 | 5 | 1 |
| 2:A:180:ARG:HD3 | 2:A:180:ARG:N | 0.42 | 2.29 | 6 | 2 |
| 2:A:101:ASN:O | 2:A:101:ASN:CG | 0.42 | 2.57 | 2 | 3 |
| 2:A:80:PHE:CZ | 2:A:126:ILE:CD1 | 0.42 | 3.03 | 2 | 1 |
| 2:A:13:ILE:HB | 2:A:17:GLN:HB3 | 0.42 | 1.90 | 2 | 1 |
| 2:A:84:MET:O | 2:A:84:MET:CG | 0.42 | 2.67 | 9 | 1 |
| 2:A:13:ILE:HG12 | 2:A:28:ILE:CG2 | 0.42 | 2.45 | 4 | 1 |
| 2:A:129:LYS:HG3 | 2:A:136:ASN:CB | 0.42 | 2.44 | 5 | 1 |
| 1:B:1:DG:H2' | 2:A:25:THR:CG2 | 0.42 | 2.45 | 1 | 1 |
| 2:A:126:ILE:HG22 | 2:A:128:VAL:HG13 | 0.42 | 1.91 | 3 | 1 |
| 2:A:156:PRO:O | 2:A:157:SER:HB2 | 0.42 | 2.14 | 3 | 1 |
| 2:A:21:ASP:N | 2:A:24:GLU:HB2 | 0.42 | 2.30 | 3 | 1 |
| 2:A:75:GLU:OE1 | 2:A:78:GLU:CD | 0.42 | 2.57 | 6 | 1 |
| 1:B:4:DT:C3' | 2:A:83:ILE:HD12 | 0.42 | 2.44 | 6 | 1 |
| 2:A:16:CYS:HB2 | 2:A:53:THR:HG22 | 0.42 | 1.91 | 7 | 1 |
| 1:B:9:DG:H1' | 1:B:10:DT:H3' | 0.42 | 1.91 | 2 | 1 |
| 2:A:92:PHE:HE2 | 2:A:104:LEU:HD21 | 0.42 | 1.74 | 2 | 1 |
| 2:A:143:GLU:OE2 | 2:A:153:ILE:HG23 | 0.42 | 2.14 | 2 | 1 |
| 2:A:124:MET:HA | 2:A:141:GLU:CG | 0.42 | 2.44 | 8 | 1 |
| 1:B:5:DG:O4' | 1:B:6:DG:C5' | 0.42 | 2.67 | 9 | 1 |
| 2:A:18:LEU:HD12 | 2:A:57:ILE:HG13 | 0.42 | 1.91 | 4 | 1 |
| 2:A:166:TYR:O | 2:A:170:PHE:CD2 | 0.42 | 2.73 | 4 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:A:123:LYS:NZ | 2:A:153:ILE:O | 0.42 | 2.42 | 5 | 1 |
| 2:A:35:VAL:HG11 | 2:A:65:ARG:O | 0.42 | 2.15 | 3 | 1 |
| 2:A:62:LEU:HD13 | 2:A:79:GLY:O | 0.42 | 2.15 | 6 | 1 |
| 2:A:50:SER:HB2 | 2:A:74:LEU:CD1 | 0.42 | 2.45 | 10 | 1 |
| 1:B:2:DT:C2' | 1:B:3:DG:C5' | 0.42 | 2.97 | 9 | 1 |
| 2:A:93:ASP:HA | 2:A:96:LEU:HB2 | 0.42 | 1.91 | 9 | 1 |
| 1:B:10:DT:C2' | 1:B:11:DG:O4' | 0.42 | 2.56 | 4 | 1 |
| 1:B:3:DG:OP2 | 2:A:138:ILE:HD13 | 0.42 | 2.15 | 4 | 1 |
| 2:A:155:SER:OG | 2:A:156:PRO:HD2 | 0.42 | 2.15 | 4 | 1 |
| 2:A:57:ILE:CG2 | 2:A:135:LEU:HB2 | 0.42 | 2.45 | 5 | 1 |
| 2:A:35:VAL:HB | 2:A:48:VAL:O | 0.42 | 2.14 | 2 | 3 |
| 1:B:5:DG:O4' | 2:A:136:ASN:OD1 | 0.42 | 2.37 | 3 | 1 |
| 2:A:186:ARG:O | 2:A:189:PHE:HB2 | 0.42 | 2.14 | 3 | 1 |
| 2:A:61:TYR:C | 2:A:63:TYR:N | 0.42 | 2.73 | 6 | 1 |
| 2:A:127:LYS:HB3 | 2:A:138:ILE:HG13 | 0.42 | 1.91 | 7 | 1 |
| 2:A:181:TYR:O | 2:A:185:TYR:N | 0.42 | 2.49 | 8 | 2 |
| 2:A:118:TYR:CD1 | 2:A:118:TYR:O | 0.42 | 2.73 | 7 | 1 |
| 2:A:75:GLU:HG3 | 2:A:77:ASN:CB | 0.42 | 2.45 | 8 | 1 |
| 1:B:8:DT:OP2 | 1:B:9:DG:N7 | 0.42 | 2.53 | 9 | 1 |
| 2:A:35:VAL:HG11 | 2:A:74:LEU:CD1 | 0.42 | 2.45 | 9 | 1 |
| 2:A:36:SER:OG | 2:A:64:ASP:HB2 | 0.42 | 2.15 | 4 | 1 |
| 1:B:4:DT:C4' | 1:B:5:DG:O5' | 0.42 | 2.68 | 5 | 1 |
| 2:A:183:GLU:HA | 2:A:186:ARG:CG | 0.42 | 2.44 | 5 | 1 |
| 1:B:3:DG:OP2 | 2:A:138:ILE:CD1 | 0.42 | 2.68 | 3 | 1 |
| 2:A:14:GLU:HA | 2:A:30:MET:SD | 0.42 | 2.55 | 3 | 1 |
| 2:A:189:PHE:O | 2:A:189:PHE:CD1 | 0.42 | 2.72 | 7 | 1 |
| 1:B:5:DG:H3' | 2:A:131:TYR:OH | 0.42 | 2.15 | 4 | 1 |
| 1:B:10:DT:C4' | 2:A:66:TYR:CD2 | 0.42 | 3.03 | 1 | 1 |
| 2:A:94:SER:O | 2:A:98:LYS:HG2 | 0.42 | 2.15 | 1 | 2 |
| 2:A:13:ILE:HA | 2:A:17:GLN:HB3 | 0.41 | 1.91 | 10 | 1 |
| 2:A:101:ASN:CG | 2:A:101:ASN:O | 0.41 | 2.58 | 5 | 1 |
| 2:A:59:GLN:O | 2:A:134:LYS:HG2 | 0.41 | 2.15 | 1 | 1 |
| 2:A:14:GLU:C | 2:A:16:CYS:N | 0.41 | 2.72 | 3 | 1 |
| 2:A:36:SER:OG | 2:A:64:ASP:C | 0.41 | 2.59 | 6 | 1 |
| 2:A:64:ASP:N | 2:A:64:ASP:OD1 | 0.41 | 2.53 | 6 | 1 |
| 1:B:10:DT:OP2 | 2:A:66:TYR:CD1 | 0.41 | 2.73 | 6 | 1 |
| 2:A:45:ILE:HG13 | 2:A:89:PHE:HB2 | 0.41 | 1.92 | 7 | 1 |
| 2:A:141:GLU:O | 2:A:142:CYS:HB3 | 0.41 | 2.15 | 8 | 1 |
| 2:A:18:LEU:HD12 | 2:A:57:ILE:CG2 | 0.41 | 2.45 | 10 | 1 |
| 2:A:97:ARG:HG2 | 2:A:102:ASN:C | 0.41 | 2.35 | 10 | 1 |
| 1:B:7:DG:O3' | 1:B:8:DT:C5 | 0.41 | 2.74 | 9 | 4 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:B:8:DT:OP2 | 1:B:9:DG:C5 | 0.41 | 2.73 | 9 | 1 |
| 2:A:15:PHE:CE1 | 2:A:55:ASN:ND2 | 0.41 | 2.89 | 5 | 1 |
| 1:B:1:DG:C4' | 2:A:27:TYR:CE2 | 0.41 | 3.03 | 6 | 1 |
| 2:A:28:ILE:HD12 | 2:A:30:MET:CG | 0.41 | 2.45 | 6 | 1 |
| 1:B:7:DG:N9 | 2:A:63:TYR:HD2 | 0.41 | 2.13 | 6 | 1 |
| 2:A:74:LEU:HD12 | 2:A:75:GLU:N | 0.41 | 2.30 | 7 | 1 |
| 2:A:94:SER:HA | 2:A:97:ARG:CD | 0.41 | 2.45 | 10 | 1 |
| 2:A:52:PHE:CE1 | 2:A:172:ARG:HG3 | 0.41 | 2.49 | 4 | 1 |
| 2:A:64:ASP:C | 2:A:65:ARG:HG2 | 0.41 | 2.36 | 1 | 1 |
| 2:A:100:PHE:O | 2:A:102:ASN:CG | 0.41 | 2.58 | 1 | 1 |
| 2:A:34:LEU:N | 2:A:49:PHE:CE1 | 0.41 | 2.88 | 3 | 1 |
| 2:A:12:THR:CB | 2:A:29:THR:HB | 0.41 | 2.45 | 3 | 1 |
| 1:B:1:DG:H5' | 1:B:2:DT:OP2 | 0.41 | 2.15 | 7 | 1 |
| 1:B:2:DT:C4 | 1:B:3:DG:C2 | 0.41 | 3.09 | 7 | 1 |
| 2:A:115:LEU:O | 2:A:116:SER:C | 0.41 | 2.56 | 8 | 1 |
| 1:B:6:DG:H2' | 1:B:7:DG:C2 | 0.41 | 2.51 | 10 | 1 |
| 2:A:166:TYR:O | 2:A:170:PHE:CD1 | 0.41 | 2.73 | 10 | 1 |
| 2:A:123:LYS:HG3 | 2:A:123:LYS:O | 0.41 | 2.14 | 4 | 1 |
| 2:A:31:PHE:CE1 | 2:A:123:LYS:HB3 | 0.41 | 2.50 | 4 | 1 |
| 2:A:135:LEU:HG | 2:A:136:ASN:N | 0.41 | 2.30 | 3 | 1 |
| 1:B:5:DG:O5' | 2:A:83:ILE:HD11 | 0.41 | 2.15 | 8 | 1 |
| 1:B:4:DT:O2 | 2:A:43:ALA:HA | 0.41 | 2.15 | 7 | 2 |
| 2:A:63:TYR:C | 2:A:65:ARG:N | 0.41 | 2.73 | 9 | 1 |
| 1:B:3:DG:H2' | 1:B:4:DT:H72 | 0.41 | 1.91 | 9 | 1 |
| 2:A:92:PHE:CD1 | 2:A:92:PHE:O | 0.41 | 2.73 | 5 | 1 |
| 2:A:189:PHE:CG | 2:A:190:PRO:CD | 0.41 | 3.03 | 6 | 1 |
| 1:B:5:DG:C2' | 2:A:131:TYR:HD2 | 0.41 | 2.28 | 2 | 1 |
| 2:A:118:TYR:CD1 | 2:A:184:GLU:O | 0.41 | 2.73 | 2 | 1 |
| 2:A:83:ILE:HG12 | 2:A:137:ALA:O | 0.41 | 2.16 | 8 | 1 |
| 2:A:25:THR:O | 2:A:26:LYS:HG3 | 0.41 | 2.16 | 4 | 1 |
| 1:B:1:DG:O4' | 2:A:27:TYR:HE1 | 0.41 | 1.98 | 1 | 1 |
| 2:A:11:PRO:C | 2:A:12:THR:OG1 | 0.41 | 2.59 | 1 | 1 |
| 1:B:1:DG:H4' | 2:A:27:TYR:CZ | 0.41 | 2.50 | 3 | 1 |
| 1:B:3:DG:H1' | 1:B:4:DT:OP1 | 0.41 | 2.16 | 6 | 2 |
| 2:A:104:LEU:HD12 | 2:A:107:LEU:CD1 | 0.41 | 2.45 | 7 | 1 |
| 1:B:4:DT:C5' | 1:B:5:DG:H3' | 0.41 | 2.45 | 9 | 1 |
| 2:A:133:GLY:C | 2:A:134:LYS:HD2 | 0.41 | 2.36 | 4 | 1 |
| 1:B:7:DG:H21 | 2:A:41:LYS:NZ | 0.41 | 2.11 | 5 | 1 |
| 2:A:50:SER:OG | 2:A:65:ARG:HD2 | 0.41 | 2.15 | 1 | 1 |
| 1:B:11:DG:C2' | 2:A:70:TYR:HE2 | 0.41 | 2.23 | 1 | 1 |
| 2:A:37:CYS:CB | 2:A:104:LEU:HD23 | 0.41 | 2.46 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:A:33:MET:O | 2:A:34:LEU:C | 0.41 | 2.57 | 6 | 2 |
| 2:A:66:TYR:O | 2:A:67:LEU:HB2 | 0.41 | 2.16 | 4 | 1 |
| 1:B:10:DT:OP1 | 2:A:73:LYS:HG2 | 0.41 | 2.15 | 1 | 1 |
| 2:A:62:LEU:CD2 | 2:A:80:PHE:CA | 0.41 | 2.99 | 1 | 1 |
| 2:A:14:GLU:CD | 2:A:30:MET:HE2 | 0.41 | 2.36 | 7 | 1 |
| 1:B:2:DT:N3 | 1:B:3:DG:C2 | 0.41 | 2.89 | 7 | 1 |
| 2:A:176:SER:O | 2:A:179:SER:OG | 0.41 | 2.34 | 7 | 1 |
| 1:B:2:DT:O4' | 1:B:3:DG:N7 | 0.41 | 2.54 | 2 | 1 |
| 2:A:38:SER:OG | 2:A:46:SER:OG | 0.41 | 2.35 | 2 | 1 |
| 1:B:7:DG:N2 | 2:A:41:LYS:HE2 | 0.41 | 2.31 | 10 | 1 |
| 2:A:20:LEU:HD23 | 2:A:26:LYS:HE2 | 0.41 | 1.91 | 5 | 1 |
| 2:A:65:ARG:HG3 | 2:A:65:ARG:O | 0.41 | 2.16 | 1 | 1 |
| 2:A:35:VAL:CG2 | 2:A:50:SER:HB3 | 0.41 | 2.45 | 3 | 1 |
| 1:B:8:DT:H4' | 2:A:63:TYR:CD1 | 0.41 | 2.49 | 3 | 1 |
| 2:A:12:THR:OG1 | 2:A:29:THR:O | 0.41 | 2.32 | 3 | 1 |
| 2:A:25:THR:HG23 | 2:A:127:LYS:CE | 0.41 | 2.46 | 7 | 1 |
| 2:A:49:PHE:O | 2:A:79:GLY:HA3 | 0.41 | 2.16 | 7 | 1 |
| 2:A:63:TYR:O | 2:A:65:ARG:HG2 | 0.41 | 2.15 | 2 | 1 |
| 2:A:143:GLU:O | 2:A:143:GLU:HG2 | 0.41 | 2.15 | 2 | 1 |
| 2:A:169:ALA:O | 2:A:173:ILE:HD12 | 0.41 | 2.16 | 8 | 1 |
| 2:A:86:LYS:HA | 2:A:89:PHE:HB3 | 0.41 | 1.93 | 8 | 1 |
| 2:A:178:ILE:HG22 | 2:A:182:PHE:CD1 | 0.41 | 2.50 | 8 | 1 |
| 2:A:47:PHE:HB2 | 2:A:82:ALA:O | 0.41 | 2.16 | 8 | 1 |
| 2:A:82:ALA:HB1 | 2:A:139:VAL:CG1 | 0.41 | 2.45 | 9 | 1 |
| 2:A:168:ARG:NH1 | 2:A:169:ALA:CA | 0.41 | 2.84 | 9 | 1 |
| 1:B:3:DG:OP1 | 2:A:129:LYS:HD3 | 0.41 | 2.16 | 4 | 1 |
| 2:A:18:LEU:HD12 | 2:A:57:ILE:CG1 | 0.41 | 2.46 | 4 | 1 |
| 2:A:67:LEU:CD1 | 2:A:74:LEU:CG | 0.41 | 2.99 | 5 | 1 |
| 1:B:2:DT:O2 | 1:B:3:DG:C6 | 0.41 | 2.74 | 5 | 1 |
| 2:A:57:ILE:HG22 | 2:A:59:GLN:N | 0.41 | 2.31 | 8 | 2 |
| 2:A:127:LYS:CG | 2:A:138:ILE:HD11 | 0.41 | 2.45 | 7 | 1 |
| 1:B:2:DT:N3 | 1:B:3:DG:N2 | 0.41 | 2.69 | 7 | 1 |
| 2:A:169:ALA:O | 2:A:173:ILE:HG13 | 0.41 | 2.16 | 7 | 1 |
| 2:A:125:ASN:O | 2:A:140:ARG:CB | 0.41 | 2.70 | 2 | 1 |
| 2:A:155:SER:OG | 2:A:156:PRO:CD | 0.40 | 2.69 | 10 | 1 |
| 1:B:2:DT:C1' | 1:B:3:DG:N7 | 0.40 | 2.82 | 4 | 1 |
| 2:A:10:ASP:OD1 | 2:A:27:TYR:O | 0.40 | 2.39 | 4 | 1 |
| 2:A:118:TYR:OH | 2:A:184:GLU:OE2 | 0.40 | 2.38 | 4 | 1 |
| 2:A:128:VAL:HA | 2:A:136:ASN:O | 0.40 | 2.15 | 5 | 1 |
| 2:A:48:VAL:HG23 | 2:A:64:ASP:HB2 | 0.40 | 1.92 | 5 | 1 |
| 2:A:180:ARG:C | 2:A:181:TYR:CD1 | 0.40 | 2.94 | 5 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:A:141:GLU:O | 2:A:142:CYS:CB | 0.40 | 2.68 | 1 | 2 |
| 2:A:83:ILE:HG13 | 2:A:137:ALA:O | 0.40 | 2.16 | 3 | 1 |
| 2:A:14:GLU:CD | 2:A:53:THR:CG2 | 0.40 | 2.88 | 3 | 1 |
| 2:A:21:ASP:CA | 2:A:24:GLU:HB2 | 0.40 | 2.46 | 6 | 1 |
| 2:A:127:LYS:O | 2:A:127:LYS:HG3 | 0.40 | 2.16 | 7 | 1 |
| 2:A:160:GLU:HG2 | 2:A:161:HIS:N | 0.40 | 2.32 | 7 | 1 |
| 2:A:55:ASN:O | 2:A:77:ASN:OD1 | 0.40 | 2.39 | 8 | 1 |
| 2:A:149:GLN:O | 2:A:150:ILE:C | 0.40 | 2.57 | 4 | 1 |
| 2:A:85:TYR:O | 2:A:86:LYS:C | 0.40 | 2.60 | 2 | 2 |
| 1:B:9:DG:OP2 | 2:A:61:TYR:CE1 | 0.40 | 2.74 | 3 | 2 |
| 1:B:10:DT:H5' | 1:B:10:DT:C6 | 0.40 | 2.51 | 7 | 1 |
| 2:A:104:LEU:O | 2:A:107:LEU:HB2 | 0.40 | 2.16 | 2 | 1 |
| 1:B:4:DT:C3' | 2:A:83:ILE:HD13 | 0.40 | 2.45 | 9 | 1 |
| 2:A:55:ASN:HB2 | 2:A:77:ASN:HA | 0.40 | 1.92 | 4 | 1 |
| 2:A:37:CYS:SG | 2:A:104:LEU:HD23 | 0.40 | 2.55 | 4 | 1 |
| 1:B:1:DG:C4' | 2:A:27:TYR:HE1 | 0.40 | 2.28 | 3 | 1 |
| 2:A:93:ASP:O | 2:A:97:ARG:HG3 | 0.40 | 2.16 | 3 | 1 |
| 2:A:103:GLY:O | 2:A:107:LEU:HG | 0.40 | 2.17 | 6 | 1 |
| 2:A:69:ASP:OD1 | 2:A:69:ASP:N | 0.40 | 2.55 | 7 | 1 |
| 2:A:13:ILE:CA | 2:A:17:GLN:HB3 | 0.40 | 2.47 | 10 | 1 |
| 1:B:10:DT:OP1 | 1:B:10:DT:H72 | 0.40 | 2.17 | 10 | 1 |
| 2:A:88:GLN:NE2 | 2:A:140:ARG:O | 0.40 | 2.53 | 10 | 1 |
| 2:A:134:LYS:HD3 | 2:A:134:LYS:N | 0.40 | 2.31 | 4 | 1 |
| 2:A:13:ILE:HA | 2:A:17:GLN:CB | 0.40 | 2.46 | 4 | 1 |
| 2:A:17:GLN:HA | 2:A:17:GLN:OE1 | 0.40 | 2.16 | 4 | 1 |
| 2:A:32:GLY:HA3 | 2:A:50:SER:O | 0.40 | 2.16 | 4 | 1 |
| 1:B:5:DG:C2' | 2:A:131:TYR:HE1 | 0.40 | 2.30 | 5 | 1 |
| 2:A:62:LEU:CD1 | 2:A:80:PHE:HA | 0.40 | 2.46 | 5 | 1 |
| 2:A:58:VAL:O | 2:A:59:GLN:HG3 | 0.40 | 2.15 | 1 | 1 |
| 1:B:10:DT:H4' | 2:A:66:TYR:CB | 0.40 | 2.46 | 1 | 1 |
| 2:A:121:VAL:CG1 | 2:A:162:LEU:HD21 | 0.40 | 2.47 | 2 | 1 |
| 1:B:5:DG:O5' | 2:A:83:ILE:CD1 | 0.40 | 2.69 | 2 | 1 |
| 1:B:6:DG:OP2 | 2:A:60:ASN:CG | 0.40 | 2.60 | 8 | 1 |
| 2:A:178:ILE:O | 2:A:182:PHE:HB3 | 0.40 | 2.16 | 5 | 1 |
| 2:A:92:PHE:HB2 | 2:A:142:CYS:CB | 0.40 | 2.47 | 1 | 1 |
| 2:A:53:THR:O | 2:A:78:GLU:OE1 | 0.40 | 2.40 | 3 | 1 |
| 2:A:15:PHE:HB2 | 2:A:53:THR:HB | 0.40 | 1.93 | 7 | 1 |
| 1:B:2:DT:H1' | 1:B:3:DG:C1' | 0.40 | 2.46 | 7 | 1 |
| 2:A:59:GLN:O | 2:A:134:LYS:HB2 | 0.40 | 2.17 | 2 | 1 |
| 2:A:74:LEU:HD21 | 2:A:78:GLU:CD | 0.40 | 2.37 | 2 | 1 |
| 2:A:155:SER:N | 2:A:158:GLN:NE2 | 0.40 | 2.69 | 2 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|----------------|---------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 2:A:87:ASN:HA | 2:A:90:GLU:CG | 0.40 | 2.46 | 8 | 1 |
| 2:A:180:ARG:CD | 2:A:180:ARG:N | 0.40 | 2.83 | 8 | 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 | |
|-----|-------|-----------------|---------------|--------------|--------------|-------------|-----------|
| 2 | A | 175/199 (88%) | 131±4 (75±2%) | 27±4 (15±2%) | 17±3 (10±2%) | 2 | 11 |
| All | All | 1750/1990 (88%) | 1308 (75%) | 270 (15%) | 172 (10%) | 2 | 11 |

All 43 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2 | A | 44 | PHE | 10 |
| 2 | A | 18 | LEU | 10 |
| 2 | A | 20 | LEU | 10 |
| 2 | A | 59 | GLN | 9 |
| 2 | A | 25 | THR | 9 |
| 2 | A | 155 | SER | 8 |
| 2 | A | 146 | PRO | 8 |
| 2 | A | 15 | PHE | 8 |
| 2 | A | 67 | LEU | 8 |
| 2 | A | 187 | ARG | 7 |
| 2 | A | 24 | GLU | 7 |
| 2 | A | 142 | CYS | 6 |
| 2 | A | 22 | THR | 5 |
| 2 | A | 68 | ILE | 5 |
| 2 | A | 13 | ILE | 4 |
| 2 | A | 66 | TYR | 4 |
| 2 | A | 63 | TYR | 4 |
| 2 | A | 14 | GLU | 3 |
| 2 | A | 73 | LYS | 3 |
| 2 | A | 74 | LEU | 3 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2 | A | 19 | GLY | 3 |
| 2 | A | 51 | ASP | 3 |
| 2 | A | 64 | ASP | 3 |
| 2 | A | 101 | ASN | 3 |
| 2 | A | 53 | THR | 3 |
| 2 | A | 147 | HIS | 2 |
| 2 | A | 189 | PHE | 2 |
| 2 | A | 57 | ILE | 2 |
| 2 | A | 121 | VAL | 2 |
| 2 | A | 119 | GLY | 2 |
| 2 | A | 133 | GLY | 2 |
| 2 | A | 65 | ARG | 2 |
| 2 | A | 108 | GLN | 2 |
| 2 | A | 152 | SER | 1 |
| 2 | A | 58 | VAL | 1 |
| 2 | A | 10 | ASP | 1 |
| 2 | A | 61 | TYR | 1 |
| 2 | A | 52 | PHE | 1 |
| 2 | A | 188 | PHE | 1 |
| 2 | A | 11 | PRO | 1 |
| 2 | A | 34 | LEU | 1 |
| 2 | A | 150 | ILE | 1 |
| 2 | A | 46 | SER | 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 | |
|-----|-------|-----------------|---------------|--------------|-------------|----|
| 2 | A | 163/182 (90%) | 113±5 (69±3%) | 50±5 (31±3%) | 2 | 16 |
| All | All | 1630/1820 (90%) | 1127 (69%) | 503 (31%) | 2 | 16 |

All 122 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) |
|-----|-------|-----|------|----------------|
| 2 | A | 150 | ILE | 10 |
| 2 | A | 18 | LEU | 10 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2 | A | 185 | TYR | 10 |
| 2 | A | 20 | LEU | 10 |
| 2 | A | 155 | SER | 9 |
| 2 | A | 162 | LEU | 9 |
| 2 | A | 105 | ARG | 9 |
| 2 | A | 100 | PHE | 9 |
| 2 | A | 134 | LYS | 9 |
| 2 | A | 24 | GLU | 8 |
| 2 | A | 71 | GLU | 8 |
| 2 | A | 93 | ASP | 8 |
| 2 | A | 21 | ASP | 8 |
| 2 | A | 131 | TYR | 8 |
| 2 | A | 168 | ARG | 8 |
| 2 | A | 140 | ARG | 7 |
| 2 | A | 66 | TYR | 7 |
| 2 | A | 75 | GLU | 7 |
| 2 | A | 88 | GLN | 7 |
| 2 | A | 67 | LEU | 7 |
| 2 | A | 148 | SER | 7 |
| 2 | A | 12 | THR | 7 |
| 2 | A | 38 | SER | 7 |
| 2 | A | 53 | THR | 7 |
| 2 | A | 130 | MET | 7 |
| 2 | A | 34 | LEU | 7 |
| 2 | A | 54 | LYS | 7 |
| 2 | A | 94 | SER | 7 |
| 2 | A | 46 | SER | 7 |
| 2 | A | 152 | SER | 6 |
| 2 | A | 56 | ASP | 6 |
| 2 | A | 44 | PHE | 6 |
| 2 | A | 39 | PHE | 6 |
| 2 | A | 172 | ARG | 6 |
| 2 | A | 59 | GLN | 6 |
| 2 | A | 23 | PHE | 6 |
| 2 | A | 16 | CYS | 6 |
| 2 | A | 188 | PHE | 6 |
| 2 | A | 106 | ASP | 6 |
| 2 | A | 129 | LYS | 6 |
| 2 | A | 165 | PHE | 6 |
| 2 | A | 127 | LYS | 6 |
| 2 | A | 179 | SER | 6 |
| 2 | A | 170 | PHE | 6 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2 | A | 73 | LYS | 5 |
| 2 | A | 92 | PHE | 5 |
| 2 | A | 136 | ASN | 5 |
| 2 | A | 157 | SER | 5 |
| 2 | A | 64 | ASP | 5 |
| 2 | A | 63 | TYR | 5 |
| 2 | A | 90 | GLU | 5 |
| 2 | A | 151 | SER | 5 |
| 2 | A | 116 | SER | 4 |
| 2 | A | 74 | LEU | 4 |
| 2 | A | 143 | GLU | 4 |
| 2 | A | 95 | LYS | 4 |
| 2 | A | 14 | GLU | 4 |
| 2 | A | 26 | LYS | 4 |
| 2 | A | 189 | PHE | 4 |
| 2 | A | 78 | GLU | 4 |
| 2 | A | 147 | HIS | 3 |
| 2 | A | 31 | PHE | 3 |
| 2 | A | 65 | ARG | 3 |
| 2 | A | 158 | GLN | 3 |
| 2 | A | 36 | SER | 3 |
| 2 | A | 50 | SER | 3 |
| 2 | A | 81 | LYS | 3 |
| 2 | A | 124 | MET | 3 |
| 2 | A | 161 | HIS | 3 |
| 2 | A | 115 | LEU | 3 |
| 2 | A | 123 | LYS | 3 |
| 2 | A | 97 | ARG | 3 |
| 2 | A | 85 | TYR | 3 |
| 2 | A | 60 | ASN | 2 |
| 2 | A | 76 | LEU | 2 |
| 2 | A | 15 | PHE | 2 |
| 2 | A | 89 | PHE | 2 |
| 2 | A | 102 | ASN | 2 |
| 2 | A | 47 | PHE | 2 |
| 2 | A | 55 | ASN | 2 |
| 2 | A | 176 | SER | 2 |
| 2 | A | 182 | PHE | 2 |
| 2 | A | 10 | ASP | 2 |
| 2 | A | 62 | LEU | 2 |
| 2 | A | 141 | GLU | 2 |
| 2 | A | 52 | PHE | 2 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2 | A | 183 | GLU | 2 |
| 2 | A | 135 | LEU | 2 |
| 2 | A | 187 | ARG | 2 |
| 2 | A | 159 | CYS | 2 |
| 2 | A | 41 | LYS | 2 |
| 2 | A | 61 | TYR | 2 |
| 2 | A | 57 | ILE | 2 |
| 2 | A | 104 | LEU | 2 |
| 2 | A | 175 | GLU | 2 |
| 2 | A | 86 | LYS | 1 |
| 2 | A | 149 | GLN | 1 |
| 2 | A | 171 | LYS | 1 |
| 2 | A | 186 | ARG | 1 |
| 2 | A | 132 | ASN | 1 |
| 2 | A | 40 | ASP | 1 |
| 2 | A | 125 | ASN | 1 |
| 2 | A | 164 | LEU | 1 |
| 2 | A | 167 | GLN | 1 |
| 2 | A | 138 | ILE | 1 |
| 2 | A | 173 | ILE | 1 |
| 2 | A | 180 | ARG | 1 |
| 2 | A | 139 | VAL | 1 |
| 2 | A | 118 | TYR | 1 |
| 2 | A | 91 | THR | 1 |
| 2 | A | 142 | CYS | 1 |
| 2 | A | 160 | GLU | 1 |
| 2 | A | 84 | MET | 1 |
| 2 | A | 101 | ASN | 1 |
| 2 | A | 30 | MET | 1 |
| 2 | A | 68 | ILE | 1 |
| 2 | A | 17 | GLN | 1 |
| 2 | A | 27 | TYR | 1 |
| 2 | A | 51 | ASP | 1 |
| 2 | A | 122 | CYS | 1 |
| 2 | A | 87 | ASN | 1 |
| 2 | A | 184 | GLU | 1 |

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided