



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 12:02 am BST

PDB ID : 3V21  
Title : Crystal structure of Type IIF restriction endonuclease Bse634I with cognate DNA  
Authors : Manakova, E.N.; Grazulis, S.; Golovenko, D.; Tamulaitiene, G.  
Deposited on : 2011-12-11  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

|                                |   |  |
|--------------------------------|---|--|
| MolProbity                     | : | 4.02b-467  |
| Xtriage (Phenix)               | : | 1.13   |
| EDS                            | : | 2.11   |
| Percentile statistics          | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac                         | : | 5.8.0158   |
| CCP4                           | : | 7.0.044 (Gargrove)   |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | 2.11   |

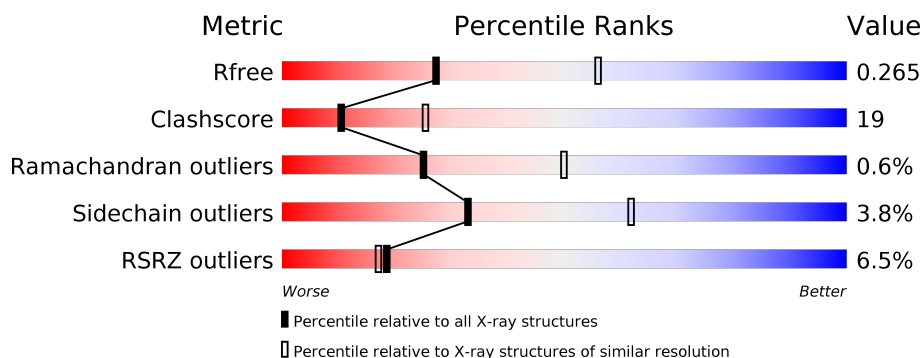
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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





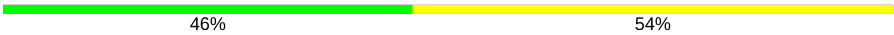


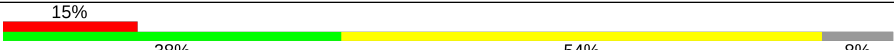
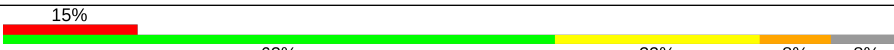
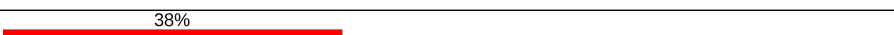
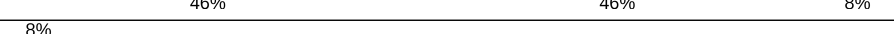

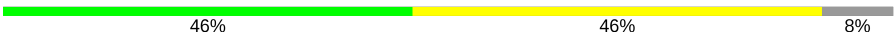
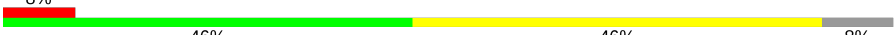
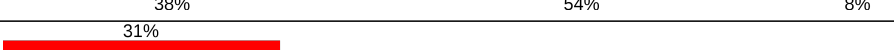
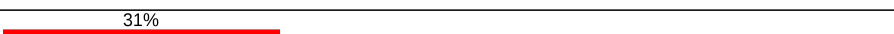


| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 2808 (2.70-2.70)                                      |
| Clashscore            | 141614                      | 3122 (2.70-2.70)                                      |
| Ramachandran outliers | 138981                      | 3069 (2.70-2.70)                                      |
| Sidechain outliers    | 138945                      | 3069 (2.70-2.70)                                      |
| RSRZ outliers         | 127900                      | 2737 (2.70-2.70)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | A     | 293    | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 65%, yellow 65%, yellow 98%, grey 98%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>%</span> <span>65%</span> <span>33%</span> <span>..</span> </div> </div>     |
| 1   | B     | 293    | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, green 2%, green 62%, yellow 62%, yellow 97%, grey 97%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>2%</span> <span>62%</span> <span>35%</span> <span>..</span> </div> </div>    |
| 1   | C     | 293    | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 6%, green 6%, green 64%, yellow 64%, yellow 97%, grey 97%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>6%</span> <span>64%</span> <span>33%</span> <span>..</span> </div> </div>    |
| 1   | D     | 293    | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 13%, green 13%, green 58%, yellow 58%, yellow 97%, grey 97%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>13%</span> <span>58%</span> <span>39%</span> <span>..</span> </div> </div> |
| 1   | E     | 293    | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 8%, green 8%, green 59%, yellow 59%, yellow 97%, grey 97%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>8%</span> <span>59%</span> <span>38%</span> <span>..</span> </div> </div>    |
| 1   | F     | 293    | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 14%, green 14%, green 58%, yellow 58%, yellow 97%, grey 97%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>14%</span> <span>58%</span> <span>38%</span> <span>..</span> </div> </div> |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | G     | 293    |    |
| 1   | H     | 293    |    |
| 2   | I     | 13     |    |
| 2   | J     | 13     |    |
| 2   | K     | 13     |    |
| 2   | L     | 13     |    |
| 2   | M     | 13     |    |
| 2   | N     | 13     |    |
| 2   | O     | 13     |    |
| 2   | P     | 13     |    |
| 2   | R     | 13     |    |
| 2   | S     | 13     |    |
| 2   | V     | 13     |    |
| 2   | X     | 13     |  |
| 2   | Y     | 13     |  |
| 2   | Z     | 13     |  |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22656 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Endonuclease Bse634IR.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 289      | Total | C    | N   | O   | S | 7       | 0       | 0     |
|     |       |          | 2344  | 1495 | 404 | 439 | 6 |         |         |       |
| 1   | B     | 289      | Total | C    | N   | O   | S | 2       | 0       | 0     |
|     |       |          | 2344  | 1495 | 404 | 439 | 6 |         |         |       |
| 1   | C     | 288      | Total | C    | N   | O   | S | 146     | 0       | 0     |
|     |       |          | 2336  | 1491 | 402 | 437 | 6 |         |         |       |
| 1   | D     | 289      | Total | C    | N   | O   | S | 264     | 0       | 0     |
|     |       |          | 2344  | 1495 | 404 | 439 | 6 |         |         |       |
| 1   | E     | 289      | Total | C    | N   | O   | S | 267     | 0       | 0     |
|     |       |          | 2344  | 1495 | 404 | 439 | 6 |         |         |       |
| 1   | F     | 287      | Total | C    | N   | O   | S | 359     | 0       | 0     |
|     |       |          | 2328  | 1485 | 401 | 436 | 6 |         |         |       |
| 1   | G     | 289      | Total | C    | N   | O   | S | 23      | 0       | 0     |
|     |       |          | 2344  | 1495 | 404 | 439 | 6 |         |         |       |
| 1   | H     | 290      | Total | C    | N   | O   | S | 11      | 0       | 0     |
|     |       |          | 2351  | 1499 | 405 | 441 | 6 |         |         |       |

There are 32 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 110     | PHE      | LEU    | SEE REMARK 999      | UNP Q8RT53 |
| A     | 111     | ASP      | HIS    | SEE REMARK 999      | UNP Q8RT53 |
| A     | 130     | SER      | THR    | SEE REMARK 999      | UNP Q8RT53 |
| A     | 226     | ALA      | ARG    | ENGINEERED MUTATION | UNP Q8RT53 |
| B     | 110     | PHE      | LEU    | SEE REMARK 999      | UNP Q8RT53 |
| B     | 111     | ASP      | HIS    | SEE REMARK 999      | UNP Q8RT53 |
| B     | 130     | SER      | THR    | SEE REMARK 999      | UNP Q8RT53 |
| B     | 226     | ALA      | ARG    | ENGINEERED MUTATION | UNP Q8RT53 |
| C     | 110     | PHE      | LEU    | SEE REMARK 999      | UNP Q8RT53 |
| C     | 111     | ASP      | HIS    | SEE REMARK 999      | UNP Q8RT53 |
| C     | 130     | SER      | THR    | SEE REMARK 999      | UNP Q8RT53 |
| C     | 226     | ALA      | ARG    | ENGINEERED MUTATION | UNP Q8RT53 |
| D     | 110     | PHE      | LEU    | SEE REMARK 999      | UNP Q8RT53 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| D     | 111     | ASP      | HIS    | SEE REMARK 999      | UNP Q8RT53 |
| D     | 130     | SER      | THR    | SEE REMARK 999      | UNP Q8RT53 |
| D     | 226     | ALA      | ARG    | ENGINEERED MUTATION | UNP Q8RT53 |
| E     | 110     | PHE      | LEU    | SEE REMARK 999      | UNP Q8RT53 |
| E     | 111     | ASP      | HIS    | SEE REMARK 999      | UNP Q8RT53 |
| E     | 130     | SER      | THR    | SEE REMARK 999      | UNP Q8RT53 |
| E     | 226     | ALA      | ARG    | ENGINEERED MUTATION | UNP Q8RT53 |
| F     | 110     | PHE      | LEU    | SEE REMARK 999      | UNP Q8RT53 |
| F     | 111     | ASP      | HIS    | SEE REMARK 999      | UNP Q8RT53 |
| F     | 130     | SER      | THR    | SEE REMARK 999      | UNP Q8RT53 |
| F     | 226     | ALA      | ARG    | ENGINEERED MUTATION | UNP Q8RT53 |
| G     | 110     | PHE      | LEU    | SEE REMARK 999      | UNP Q8RT53 |
| G     | 111     | ASP      | HIS    | SEE REMARK 999      | UNP Q8RT53 |
| G     | 130     | SER      | THR    | SEE REMARK 999      | UNP Q8RT53 |
| G     | 226     | ALA      | ARG    | ENGINEERED MUTATION | UNP Q8RT53 |
| H     | 110     | PHE      | LEU    | SEE REMARK 999      | UNP Q8RT53 |
| H     | 111     | ASP      | HIS    | SEE REMARK 999      | UNP Q8RT53 |
| H     | 130     | SER      | THR    | SEE REMARK 999      | UNP Q8RT53 |
| H     | 226     | ALA      | ARG    | ENGINEERED MUTATION | UNP Q8RT53 |

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

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 2   | I     | 13       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 263   | 126 | 48 | 77 | 12 |         |         |       |
| 2   | J     | 13       | Total | C   | N  | O  | P  | 9       | 0       | 0     |
|     |       |          | 263   | 126 | 48 | 77 | 12 |         |         |       |
| 2   | K     | 13       | Total | C   | N  | O  | P  | 21      | 0       | 0     |
|     |       |          | 263   | 126 | 48 | 77 | 12 |         |         |       |
| 2   | L     | 12       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 243   | 116 | 46 | 70 | 11 |         |         |       |
| 2   | M     | 12       | Total | C   | N  | O  | P  | 82      | 0       | 0     |
|     |       |          | 243   | 116 | 46 | 70 | 11 |         |         |       |
| 2   | N     | 12       | Total | C   | N  | O  | P  | 17      | 0       | 0     |
|     |       |          | 243   | 116 | 46 | 70 | 11 |         |         |       |
| 2   | O     | 13       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 263   | 126 | 48 | 77 | 12 |         |         |       |
| 2   | P     | 12       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 243   | 116 | 46 | 70 | 11 |         |         |       |
| 2   | R     | 12       | Total | C   | N  | O  | P  | 81      | 0       | 0     |
|     |       |          | 243   | 116 | 46 | 70 | 11 |         |         |       |

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| Mol | Chain | Residues | Atoms        |          |         |         |         | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|---------|---------|---------|-------|
| 2   | S     | 13       | Total<br>263 | C<br>126 | N<br>48 | O<br>77 | P<br>12 | 62      | 0       | 0     |
| 2   | V     | 13       | Total<br>263 | C<br>126 | N<br>48 | O<br>77 | P<br>12 | 0       | 0       | 0     |
| 2   | X     | 13       | Total<br>263 | C<br>126 | N<br>48 | O<br>77 | P<br>12 | 0       | 0       | 0     |
| 2   | Y     | 13       | Total<br>263 | C<br>126 | N<br>48 | O<br>77 | P<br>12 | 0       | 0       | 0     |
| 2   | Z     | 12       | Total<br>243 | C<br>116 | N<br>46 | O<br>70 | P<br>11 | 36      | 0       | 0     |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 3   | A     | 55       | Total<br>55 | O<br>55 | 0       | 0       |
| 3   | B     | 44       | Total<br>44 | O<br>44 | 0       | 0       |
| 3   | C     | 35       | Total<br>35 | O<br>35 | 0       | 0       |
| 3   | D     | 22       | Total<br>22 | O<br>22 | 0       | 0       |
| 3   | E     | 36       | Total<br>36 | O<br>36 | 0       | 0       |
| 3   | F     | 25       | Total<br>25 | O<br>25 | 0       | 0       |
| 3   | G     | 37       | Total<br>37 | O<br>37 | 0       | 0       |
| 3   | H     | 50       | Total<br>50 | O<br>50 | 0       | 0       |
| 3   | I     | 9        | Total<br>9  | O<br>9  | 0       | 0       |
| 3   | J     | 12       | Total<br>12 | O<br>12 | 0       | 0       |
| 3   | K     | 1        | Total<br>1  | O<br>1  | 0       | 0       |
| 3   | L     | 2        | Total<br>2  | O<br>2  | 0       | 0       |
| 3   | M     | 3        | Total<br>3  | O<br>3  | 0       | 0       |
| 3   | N     | 1        | Total<br>1  | O<br>1  | 0       | 0       |

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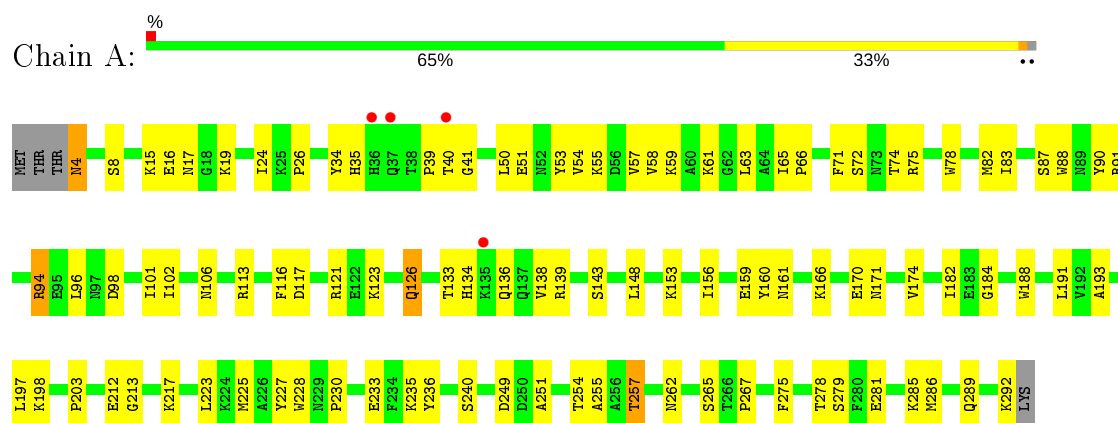
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| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 3   | O     | 6        | Total<br>6 | O<br>6 | 0       | 0       |
| 3   | P     | 3        | Total<br>3 | O<br>3 | 0       | 0       |
| 3   | R     | 2        | Total<br>2 | O<br>2 | 0       | 0       |
| 3   | S     | 5        | Total<br>5 | O<br>5 | 0       | 0       |
| 3   | V     | 2        | Total<br>2 | O<br>2 | 0       | 0       |
| 3   | X     | 4        | Total<br>4 | O<br>4 | 0       | 0       |
| 3   | Y     | 3        | Total<br>3 | O<br>3 | 0       | 0       |
| 3   | Z     | 2        | Total<br>2 | O<br>2 | 0       | 0       |

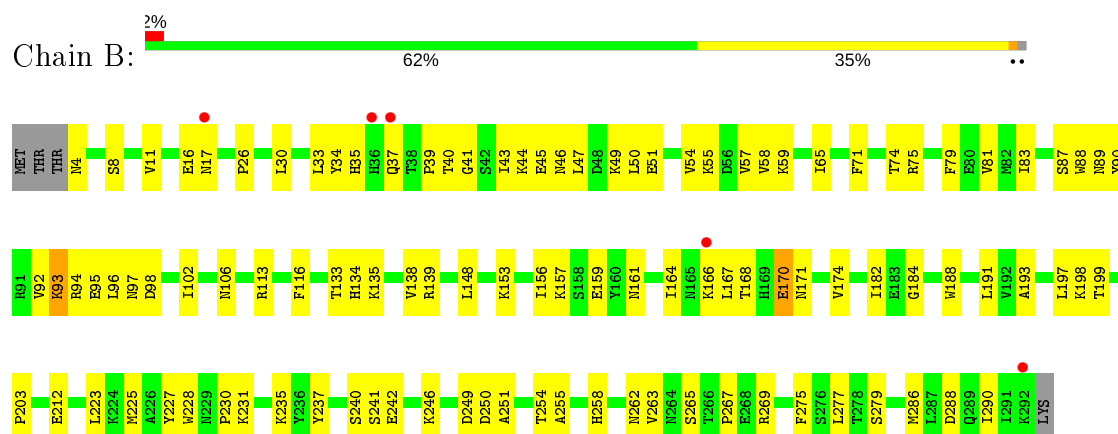
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-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. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

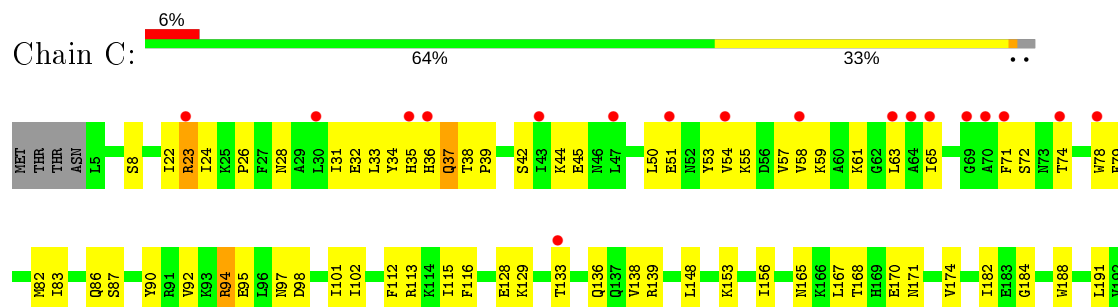
#### • Molecule 1: Endonuclease Bse634IR



#### • Molecule 1: Endonuclease Bse634IR



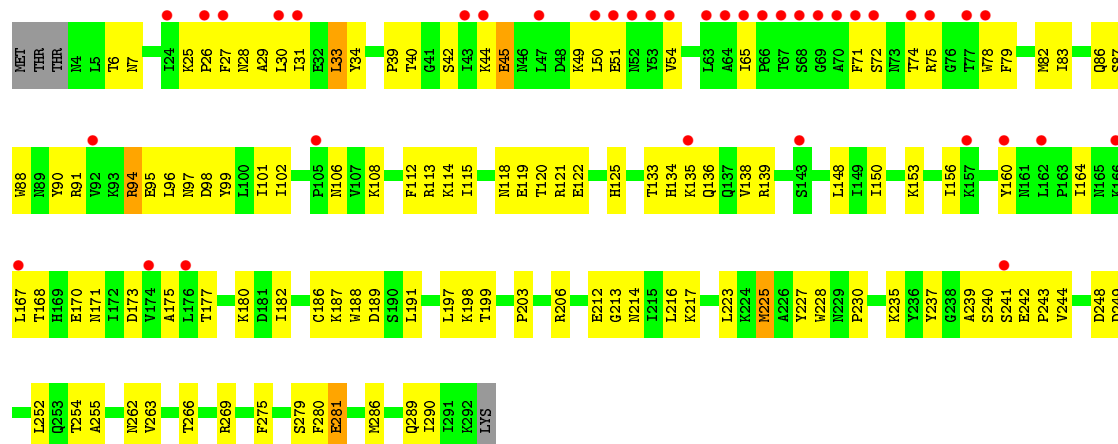
#### • Molecule 1: Endonuclease Bse634IR



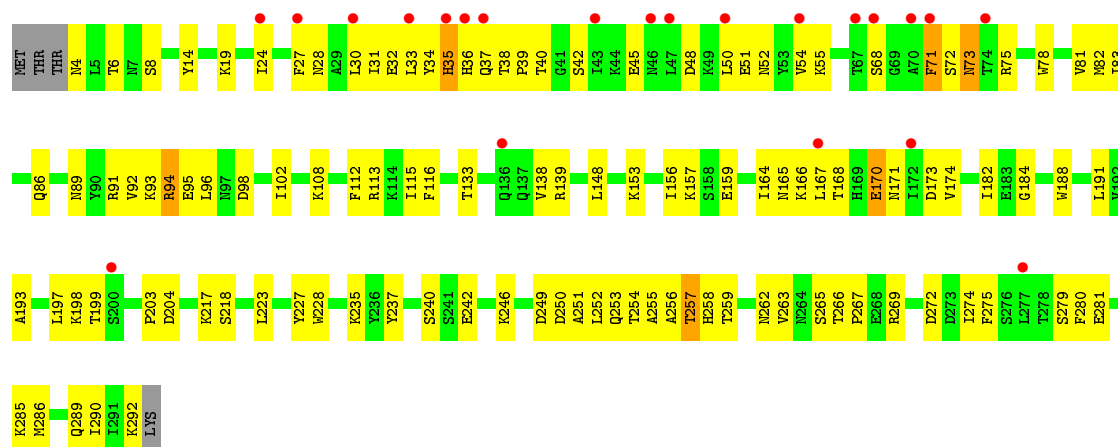




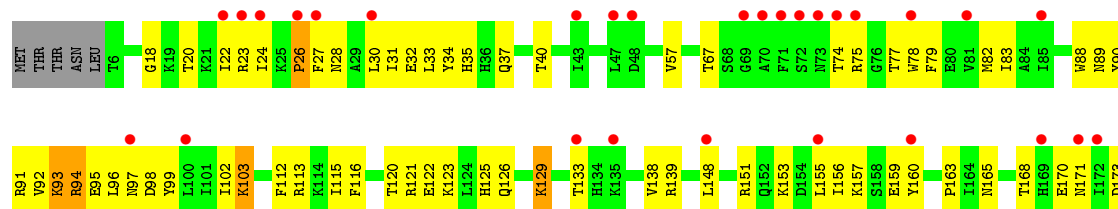
• Molecule 1: Endonuclease Bse634IR



• Molecule 1: Endonuclease Bse634IR



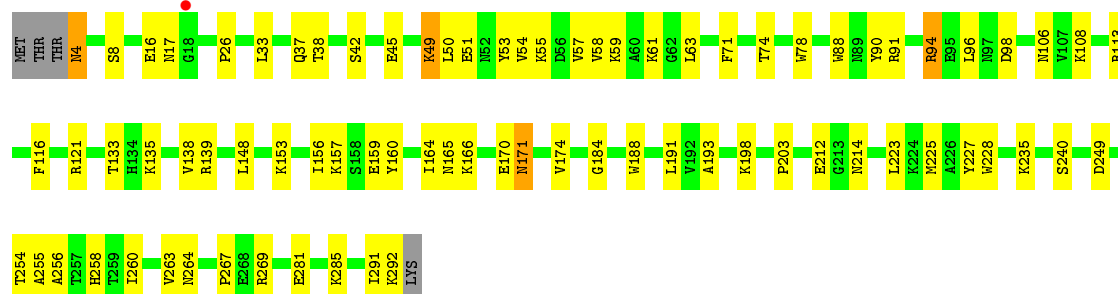
• Molecule 1: Endonuclease Bse634IR





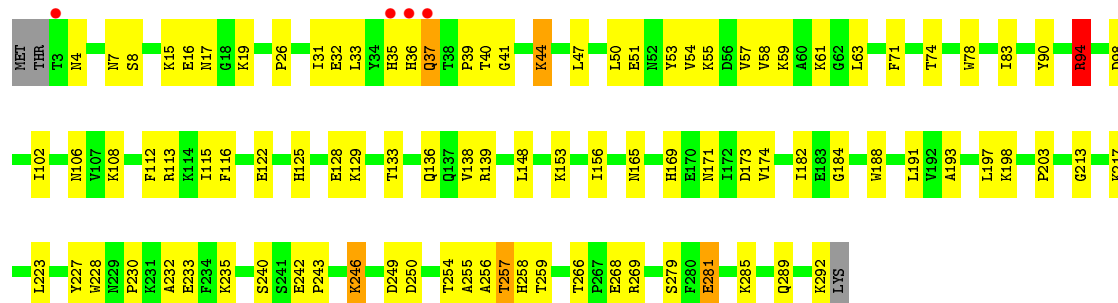
● Molecule 1: Endonuclease Bse634IR

Chain G: 72% 26%



● Molecule 1: Endonuclease Bse634IR

Chain H: 66% 31%



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

Chain I: 46% 54%



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

Chain J: 8% 54% 38% 8%



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

Chain K: 



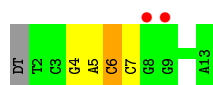
- Molecule 2: DNA (5'-D(\*TP\*TP\*CP\*GP\*AP\*CP\*CP\*GP\*GP\*TP\*CP\*GP\*A)-3')

Chain L: 

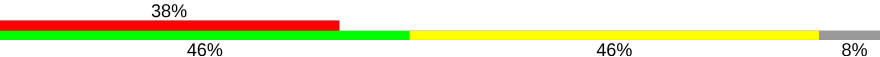


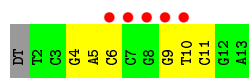
- Molecule 2: DNA (5'-D(\*TP\*TP\*CP\*GP\*AP\*CP\*CP\*GP\*GP\*TP\*CP\*GP\*A)-3')

Chain M: 



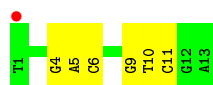
- Molecule 2: DNA (5'-D(\*TP\*TP\*CP\*GP\*AP\*CP\*CP\*GP\*GP\*TP\*CP\*GP\*A)-3')

Chain N: 



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

Chain O: 



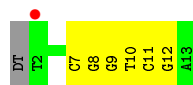
- Molecule 2: DNA (5'-D(\*TP\*TP\*CP\*GP\*AP\*CP\*CP\*GP\*GP\*TP\*CP\*GP\*A)-3')

Chain P: 

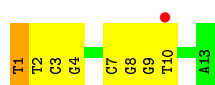


- Molecule 2: DNA (5'-D(\*TP\*TP\*CP\*GP\*AP\*CP\*CP\*GP\*GP\*TP\*CP\*GP\*A)-3')

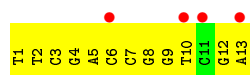
Chain R: 



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



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



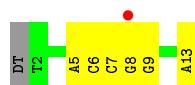
- Molecule 2: DNA (5'-D(\*TP\*TP\*CP\*GP\*AP\*CP\*CP\*GP\*GP\*TP\*CP\*GP\*A)-3')



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



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



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 106.88Å 115.31Å 130.24Å<br>90.00° 112.50° 90.00°            | Depositor        |
| Resolution (Å)  | 65.09 – 2.70<br>65.09 – 2.70                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 100.0 (65.09-2.70)<br>100.0 (65.09-2.70)                    | Depositor<br>EDS |
| $R_{merge}$   | 0.06  | Depositor        |
| $R_{sym}$   | 0.06  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.71 (at 2.69Å)   | Xtriage          |
| Refinement program  | REFMAC  | Depositor        |
| R, $R_{free}$   | 0.230 , 0.267<br>0.227 , 0.265                              | Depositor<br>DCC |
| $R_{free}$ test set   | 7973 reflections (9.93%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 52.8  | Xtriage          |
| Anisotropy  | 0.148   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.36 , 61.1   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction   | 0.033 for h,-k,-h-l   | Xtriage          |
| $F_o, F_c$ correlation  | 0.92  | EDS              |
| Total number of atoms   | 22656   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 54.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 1   | A     | 0.43         | 0/2389  | 0.65        | 0/3228         |
| 1   | B     | 0.43         | 0/2389  | 0.64        | 0/3228         |
| 1   | C     | 0.39         | 0/2381  | 0.63        | 0/3217         |
| 1   | D     | 0.41         | 0/2389  | 0.63        | 0/3228         |
| 1   | E     | 0.39         | 0/2389  | 0.62        | 0/3228         |
| 1   | F     | 0.38         | 0/2373  | 0.62        | 0/3206         |
| 1   | G     | 0.44         | 0/2389  | 0.62        | 0/3228         |
| 1   | H     | 0.43         | 0/2396  | 0.63        | 1/3238 (0.0%)  |
| 2   | I     | 0.49         | 0/294   | 0.72        | 0/452          |
| 2   | J     | 0.47         | 0/294   | 0.70        | 0/452          |
| 2   | K     | 0.43         | 0/294   | 0.72        | 0/452          |
| 2   | L     | 0.35         | 0/272   | 0.70        | 0/418          |
| 2   | M     | 0.41         | 0/272   | 0.75        | 0/418          |
| 2   | N     | 0.37         | 0/272   | 0.71        | 0/418          |
| 2   | O     | 0.53         | 0/294   | 0.72        | 0/452          |
| 2   | P     | 0.49         | 0/272   | 0.76        | 0/418          |
| 2   | R     | 0.41         | 0/272   | 0.72        | 0/418          |
| 2   | S     | 0.49         | 0/294   | 0.75        | 0/452          |
| 2   | V     | 0.43         | 0/294   | 0.70        | 0/452          |
| 2   | X     | 0.41         | 0/294   | 0.68        | 0/452          |
| 2   | Y     | 0.41         | 0/294   | 0.71        | 0/452          |
| 2   | Z     | 0.37         | 0/272   | 0.66        | 0/418          |
| All | All   | 0.42         | 0/23079 | 0.65        | 1/31925 (0.0%) |

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 outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | J     | 0                   | 1                   |
| 2   | M     | 0                   | 1                   |
| 2   | S     | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| All | All   | 0                   | 3                   |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | H     | 94  | ARG  | NE-CZ-NH1 | -5.42 | 117.59      | 120.30   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | J     | 6   | DC   | Sidechain |
| 2   | M     | 6   | DC   | Sidechain |
| 2   | S     | 1   | DT   | Sidechain |

## 5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2344  | 0        | 2385     | 94      | 0            |
| 1   | B     | 2344  | 0        | 2385     | 100     | 0            |
| 1   | C     | 2336  | 0        | 2379     | 86      | 0            |
| 1   | D     | 2344  | 0        | 2385     | 110     | 0            |
| 1   | E     | 2344  | 0        | 2385     | 107     | 0            |
| 1   | F     | 2328  | 0        | 2368     | 136     | 0            |
| 1   | G     | 2344  | 0        | 2385     | 77      | 0            |
| 1   | H     | 2351  | 0        | 2392     | 87      | 0            |
| 2   | I     | 263   | 0        | 148      | 7       | 0            |
| 2   | J     | 263   | 0        | 148      | 6       | 0            |
| 2   | K     | 263   | 0        | 148      | 5       | 0            |
| 2   | L     | 243   | 0        | 136      | 7       | 0            |
| 2   | M     | 243   | 0        | 136      | 3       | 0            |
| 2   | N     | 243   | 0        | 136      | 8       | 0            |
| 2   | O     | 263   | 0        | 148      | 6       | 0            |
| 2   | P     | 243   | 0        | 136      | 6       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | R     | 243   | 0        | 136      | 8       | 0            |
| 2   | S     | 263   | 0        | 148      | 9       | 0            |
| 2   | V     | 263   | 0        | 148      | 16      | 0            |
| 2   | X     | 263   | 0        | 148      | 4       | 0            |
| 2   | Y     | 263   | 0        | 148      | 8       | 0            |
| 2   | Z     | 243   | 0        | 136      | 7       | 0            |
| 3   | A     | 55    | 0        | 0        | 3       | 0            |
| 3   | B     | 44    | 0        | 0        | 1       | 0            |
| 3   | C     | 35    | 0        | 0        | 0       | 0            |
| 3   | D     | 22    | 0        | 0        | 0       | 0            |
| 3   | E     | 36    | 0        | 0        | 1       | 0            |
| 3   | F     | 25    | 0        | 0        | 0       | 0            |
| 3   | G     | 37    | 0        | 0        | 2       | 0            |
| 3   | H     | 50    | 0        | 0        | 0       | 0            |
| 3   | I     | 9     | 0        | 0        | 0       | 0            |
| 3   | J     | 12    | 0        | 0        | 0       | 0            |
| 3   | K     | 1     | 0        | 0        | 0       | 0            |
| 3   | L     | 2     | 0        | 0        | 0       | 0            |
| 3   | M     | 3     | 0        | 0        | 0       | 0            |
| 3   | N     | 1     | 0        | 0        | 0       | 0            |
| 3   | O     | 6     | 0        | 0        | 0       | 0            |
| 3   | P     | 3     | 0        | 0        | 0       | 0            |
| 3   | R     | 2     | 0        | 0        | 0       | 0            |
| 3   | S     | 5     | 0        | 0        | 0       | 0            |
| 3   | V     | 2     | 0        | 0        | 0       | 0            |
| 3   | X     | 4     | 0        | 0        | 0       | 0            |
| 3   | Y     | 3     | 0        | 0        | 0       | 0            |
| 3   | Z     | 2     | 0        | 0        | 1       | 0            |
| All | All   | 22656 | 0        | 21064    | 756     | 0            |

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 19.

All (756) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:G:138:VAL:CG1 | 1:H:255:ALA:HB2 | 1.30                     | 1.55              |
| 1:E:255:ALA:HB2 | 1:F:138:VAL:CG1 | 1.56                     | 1.33              |
| 1:A:138:VAL:CG1 | 1:B:255:ALA:HB2 | 1.60                     | 1.31              |
| 1:E:138:VAL:CG1 | 1:F:255:ALA:HB2 | 1.66                     | 1.25              |
| 1:A:255:ALA:HB2 | 1:B:138:VAL:CG1 | 1.72                     | 1.20              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:138:VAL:HG13 | 1:H:255:ALA:HB2  | 1.25                     | 1.16              |
| 1:G:138:VAL:HG11 | 1:H:255:ALA:CB   | 1.77                     | 1.15              |
| 1:G:138:VAL:CG1  | 1:H:255:ALA:CB   | 2.26                     | 1.13              |
| 1:A:255:ALA:HB2  | 1:B:138:VAL:HG11 | 1.30                     | 1.11              |
| 1:C:255:ALA:HB2  | 1:D:138:VAL:CG1  | 1.80                     | 1.11              |
| 1:F:133:THR:HG23 | 2:R:12:DG:H4'    | 1.30                     | 1.11              |
| 1:A:138:VAL:HG11 | 1:B:255:ALA:HB2  | 1.16                     | 1.10              |
| 1:E:138:VAL:HG11 | 1:F:255:ALA:CB   | 1.80                     | 1.10              |
| 1:E:255:ALA:HB2  | 1:F:138:VAL:HG13 | 1.32                     | 1.09              |
| 1:A:257:THR:HG22 | 1:B:258:HIS:HB3  | 1.09                     | 1.08              |
| 1:E:138:VAL:CG1  | 1:F:255:ALA:CB   | 2.31                     | 1.08              |
| 1:E:255:ALA:HB2  | 1:F:138:VAL:HG11 | 1.22                     | 1.07              |
| 1:F:26:PRO:HB3   | 1:F:74:THR:HG23  | 1.36                     | 1.04              |
| 1:A:225:MET:HE2  | 1:E:263:VAL:H    | 1.23                     | 1.02              |
| 1:A:257:THR:HG21 | 1:B:258:HIS:ND1  | 1.75                     | 1.01              |
| 1:C:26:PRO:HB3   | 1:C:74:THR:HG23  | 1.38                     | 1.01              |
| 1:C:255:ALA:HB2  | 1:D:138:VAL:HG13 | 1.42                     | 1.00              |
| 1:D:31:ILE:HG23  | 1:D:168:THR:HA   | 1.44                     | 0.99              |
| 1:D:263:VAL:H    | 1:G:225:MET:HE2  | 1.27                     | 0.99              |
| 1:A:262:ASN:HB3  | 3:A:308:HOH:O    | 1.64                     | 0.98              |
| 1:E:138:VAL:HG11 | 1:F:255:ALA:HB2  | 1.39                     | 0.97              |
| 1:A:257:THR:HG22 | 1:B:258:HIS:CB   | 1.94                     | 0.96              |
| 1:E:138:VAL:HG13 | 1:F:255:ALA:HB2  | 1.46                     | 0.96              |
| 1:F:31:ILE:HG23  | 1:F:168:THR:HA   | 1.44                     | 0.96              |
| 1:A:262:ASN:HB2  | 1:A:265:SER:HB2  | 1.49                     | 0.95              |
| 1:G:255:ALA:HB2  | 1:H:138:VAL:CG1  | 1.97                     | 0.95              |
| 1:C:65:ILE:H     | 1:C:65:ILE:HD12  | 1.30                     | 0.94              |
| 1:A:26:PRO:HB3   | 1:A:74:THR:HG23  | 1.50                     | 0.93              |
| 1:E:255:ALA:CB   | 1:F:138:VAL:HG11 | 1.98                     | 0.93              |
| 1:E:255:ALA:CB   | 1:F:138:VAL:CG1  | 2.47                     | 0.92              |
| 1:A:138:VAL:HG13 | 1:B:255:ALA:HB2  | 1.50                     | 0.92              |
| 1:G:138:VAL:HG11 | 1:H:255:ALA:HB2  | 0.94                     | 0.92              |
| 1:B:263:VAL:H    | 1:F:225:MET:HE2  | 1.35                     | 0.91              |
| 1:C:255:ALA:HB2  | 1:D:138:VAL:HG11 | 1.52                     | 0.89              |
| 1:E:262:ASN:HB2  | 1:E:265:SER:HB2  | 1.55                     | 0.88              |
| 1:G:26:PRO:HB3   | 1:G:74:THR:HG23  | 1.57                     | 0.86              |
| 1:A:257:THR:CG2  | 1:B:258:HIS:HB3  | 2.02                     | 0.86              |
| 1:D:42:SER:HB3   | 1:D:45:GLU:HB2   | 1.57                     | 0.86              |
| 1:H:26:PRO:HB3   | 1:H:74:THR:HG23  | 1.56                     | 0.85              |
| 1:F:26:PRO:HB3   | 1:F:74:THR:CG2   | 2.05                     | 0.85              |
| 2:S:9:DG:H2''    | 2:S:10:DT:H5''   | 1.56                     | 0.85              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:79:PHE:HA    | 1:F:82:MET:HE2   | 1.58                     | 0.84              |
| 2:Z:5:DA:H2''    | 2:Z:6:DC:H5'     | 1.60                     | 0.83              |
| 1:E:170:GLU:O    | 1:E:174:VAL:HG13 | 1.77                     | 0.83              |
| 1:G:4:ASN:N      | 1:G:4:ASN:HD22   | 1.74                     | 0.83              |
| 1:B:225:MET:HE1  | 1:F:263:VAL:H    | 1.42                     | 0.83              |
| 1:C:42:SER:HB3   | 1:C:45:GLU:HG3   | 1.60                     | 0.82              |
| 1:E:138:VAL:HG11 | 1:F:255:ALA:HB3  | 1.61                     | 0.81              |
| 1:E:138:VAL:HG13 | 1:F:255:ALA:CB   | 2.04                     | 0.79              |
| 1:E:28:ASN:O     | 1:E:32:GLU:HG3   | 1.83                     | 0.79              |
| 1:F:93:LYS:O     | 1:F:94:ARG:HD2   | 1.82                     | 0.79              |
| 1:A:138:VAL:HG11 | 1:B:255:ALA:CB   | 2.05                     | 0.79              |
| 1:F:255:ALA:HB1  | 1:F:268:GLU:O    | 1.83                     | 0.79              |
| 1:A:257:THR:CG2  | 1:B:258:HIS:ND1  | 2.46                     | 0.78              |
| 1:G:138:VAL:HG13 | 1:H:255:ALA:CB   | 2.03                     | 0.78              |
| 1:F:255:ALA:HA   | 1:F:269:ARG:HA   | 1.66                     | 0.78              |
| 1:F:90:TYR:O     | 1:F:94:ARG:HB2   | 1.82                     | 0.78              |
| 1:G:255:ALA:HB2  | 1:H:138:VAL:HG11 | 1.65                     | 0.78              |
| 1:C:138:VAL:CG1  | 1:D:255:ALA:HB2  | 2.14                     | 0.77              |
| 1:C:256:ALA:HB1  | 1:C:258:HIS:CE1  | 2.20                     | 0.76              |
| 1:A:148:LEU:HD22 | 1:A:191:LEU:HD11 | 1.68                     | 0.76              |
| 1:G:170:GLU:O    | 1:G:174:VAL:HG13 | 1.86                     | 0.75              |
| 1:B:26:PRO:HB3   | 1:B:74:THR:HG23  | 1.69                     | 0.74              |
| 1:E:171:ASN:O    | 1:E:174:VAL:HG22 | 1.88                     | 0.74              |
| 1:B:90:TYR:HA    | 1:B:93:LYS:HD3   | 1.68                     | 0.74              |
| 1:D:27:PHE:O     | 1:D:31:ILE:HG13  | 1.86                     | 0.74              |
| 1:C:138:VAL:HG11 | 1:D:255:ALA:HB2  | 1.68                     | 0.73              |
| 1:E:27:PHE:O     | 1:E:31:ILE:HG13  | 1.89                     | 0.73              |
| 1:B:157:LYS:HB3  | 1:B:159:GLU:OE1  | 1.89                     | 0.73              |
| 1:A:4:ASN:HD22   | 1:A:4:ASN:N      | 1.85                     | 0.73              |
| 1:D:133:THR:HG23 | 2:V:2:DT:H72     | 1.70                     | 0.72              |
| 1:F:170:GLU:O    | 1:F:174:VAL:HG13 | 1.89                     | 0.72              |
| 1:F:97:ASN:O     | 1:F:156:ILE:HG12 | 1.89                     | 0.72              |
| 1:C:255:ALA:CB   | 1:D:138:VAL:HG11 | 2.20                     | 0.71              |
| 1:D:164:ILE:HG23 | 1:D:171:ASN:OD1  | 1.89                     | 0.71              |
| 1:B:89:ASN:O     | 1:B:93:LYS:HD2   | 1.90                     | 0.71              |
| 1:E:255:ALA:CB   | 1:F:138:VAL:HG13 | 2.17                     | 0.71              |
| 1:E:68:SER:HA    | 1:E:71:PHE:HB2   | 1.72                     | 0.71              |
| 1:C:170:GLU:O    | 1:C:174:VAL:HG13 | 1.90                     | 0.71              |
| 1:A:34:TYR:CE1   | 1:A:39:PRO:HB3   | 2.26                     | 0.70              |
| 1:E:83:ILE:HD12  | 1:E:197:LEU:HD22 | 1.72                     | 0.70              |
| 2:S:9:DG:H2''    | 2:S:10:DT:C5'    | 2.20                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:255:ALA:CB   | 1:B:138:VAL:HG11 | 2.17                     | 0.70              |
| 2:S:3:DC:H2''    | 2:S:4:DG:C8      | 2.26                     | 0.70              |
| 1:D:133:THR:HG23 | 2:V:2:DT:C7      | 2.21                     | 0.70              |
| 1:C:255:ALA:CB   | 1:D:138:VAL:CG1  | 2.64                     | 0.70              |
| 1:C:34:TYR:CE1   | 1:C:39:PRO:HB3   | 2.27                     | 0.70              |
| 1:C:133:THR:HG22 | 1:C:133:THR:O    | 1.92                     | 0.69              |
| 2:Z:8:DG:H2''    | 2:Z:9:DG:OP2     | 1.90                     | 0.69              |
| 1:A:212:GLU:HG2  | 1:A:236:TYR:OH   | 1.91                     | 0.69              |
| 1:E:86:GLN:OE1   | 1:E:280:PHE:HB3  | 1.92                     | 0.69              |
| 1:D:133:THR:HG22 | 1:D:133:THR:O    | 1.91                     | 0.69              |
| 2:S:9:DG:C2'     | 2:S:10:DT:H5''   | 2.22                     | 0.69              |
| 1:A:16:GLU:O     | 1:A:17:ASN:HB2   | 1.93                     | 0.69              |
| 1:D:198:LYS:O    | 1:D:240:SER:HA   | 1.92                     | 0.69              |
| 1:G:281:GLU:HG2  | 1:G:285:LYS:HE3  | 1.74                     | 0.69              |
| 1:H:4:ASN:HB3    | 1:H:7:ASN:ND2    | 2.07                     | 0.68              |
| 1:E:148:LEU:HD22 | 1:E:191:LEU:HD11 | 1.74                     | 0.68              |
| 1:A:278:THR:HG22 | 3:A:345:HOH:O    | 1.92                     | 0.68              |
| 1:H:4:ASN:HB3    | 1:H:7:ASN:HD22   | 1.58                     | 0.68              |
| 1:F:91:ARG:HG3   | 1:F:92:VAL:N     | 2.08                     | 0.68              |
| 1:B:94:ARG:NH2   | 1:B:288:ASP:OD1  | 2.26                     | 0.68              |
| 1:E:256:ALA:HB1  | 1:E:258:HIS:CE1  | 2.27                     | 0.68              |
| 1:H:148:LEU:HD22 | 1:H:191:LEU:HD11 | 1.75                     | 0.68              |
| 1:F:198:LYS:O    | 1:F:240:SER:HA   | 1.94                     | 0.68              |
| 1:H:16:GLU:O     | 1:H:17:ASN:HB2   | 1.93                     | 0.67              |
| 2:R:8:DG:H2''    | 2:R:9:DG:O5'     | 1.93                     | 0.67              |
| 1:E:78:TRP:HB3   | 1:E:82:MET:CE    | 2.25                     | 0.67              |
| 1:A:255:ALA:HB2  | 1:B:138:VAL:HG13 | 1.73                     | 0.67              |
| 1:B:148:LEU:HD22 | 1:B:191:LEU:HD11 | 1.76                     | 0.67              |
| 1:E:71:PHE:O     | 1:E:75:ARG:HG3   | 1.94                     | 0.67              |
| 1:F:255:ALA:CB   | 1:F:268:GLU:O    | 2.43                     | 0.67              |
| 2:V:9:DG:H2''    | 2:V:10:DT:OP2    | 1.94                     | 0.67              |
| 1:F:148:LEU:HD22 | 1:F:191:LEU:HD11 | 1.75                     | 0.66              |
| 1:H:39:PRO:O     | 1:H:40:THR:HG23  | 1.95                     | 0.66              |
| 2:Y:1:DT:H2''    | 2:Y:2:DT:O5'     | 1.94                     | 0.66              |
| 1:D:197:LEU:O    | 1:D:198:LYS:HG2  | 1.96                     | 0.66              |
| 1:E:289:GLN:HG3  | 3:E:315:HOH:O    | 1.94                     | 0.66              |
| 1:E:281:GLU:HG3  | 1:E:285:LYS:HE3  | 1.77                     | 0.66              |
| 1:B:159:GLU:CD   | 1:B:159:GLU:H    | 1.99                     | 0.66              |
| 1:B:16:GLU:O     | 1:B:17:ASN:HB2   | 1.95                     | 0.66              |
| 1:D:97:ASN:O     | 1:D:156:ILE:HG12 | 1.95                     | 0.66              |
| 1:G:148:LEU:HD22 | 1:G:191:LEU:HD11 | 1.76                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:9:DG:H2'     | 2:R:10:DT:H72    | 1.78                     | 0.66              |
| 1:G:133:THR:HG22 | 1:G:133:THR:O    | 1.95                     | 0.65              |
| 1:H:8:SER:HB3    | 1:H:57:VAL:CG1   | 2.26                     | 0.65              |
| 1:F:199:THR:O    | 1:F:242:GLU:HG3  | 1.96                     | 0.65              |
| 1:G:255:ALA:HB2  | 1:H:138:VAL:HG13 | 1.79                     | 0.65              |
| 1:G:16:GLU:O     | 1:G:17:ASN:HB2   | 1.96                     | 0.65              |
| 1:H:256:ALA:O    | 1:H:258:HIS:N    | 2.30                     | 0.65              |
| 1:D:199:THR:O    | 1:D:242:GLU:HG3  | 1.97                     | 0.64              |
| 1:F:79:PHE:HA    | 1:F:82:MET:CE    | 2.26                     | 0.64              |
| 1:D:34:TYR:CZ    | 1:D:39:PRO:HB3   | 2.32                     | 0.64              |
| 1:F:278:THR:HG23 | 1:H:285:LYS:HZ1  | 1.61                     | 0.64              |
| 1:H:128:GLU:HG3  | 1:H:129:LYS:N    | 2.13                     | 0.64              |
| 1:H:133:THR:O    | 1:H:133:THR:HG22 | 1.96                     | 0.64              |
| 1:E:256:ALA:O    | 1:E:258:HIS:N    | 2.30                     | 0.64              |
| 1:E:133:THR:O    | 1:E:133:THR:HG22 | 1.98                     | 0.64              |
| 1:E:279:SER:OG   | 1:E:281:GLU:HB3  | 1.98                     | 0.64              |
| 1:E:37:GLN:HA    | 1:E:165:ASN:O    | 1.97                     | 0.64              |
| 1:A:138:VAL:CG1  | 1:B:255:ALA:CB   | 2.56                     | 0.63              |
| 1:C:22:ILE:HD13  | 1:C:63:LEU:HD13  | 1.79                     | 0.63              |
| 1:A:225:MET:CE   | 1:E:263:VAL:HG12 | 2.28                     | 0.63              |
| 1:G:214:ASN:ND2  | 1:H:257:THR:HG21 | 2.13                     | 0.63              |
| 1:F:30:LEU:O     | 1:F:34:TYR:HB2   | 1.97                     | 0.63              |
| 1:C:65:ILE:H     | 1:C:65:ILE:CD1   | 2.07                     | 0.63              |
| 1:E:34:TYR:CZ    | 1:E:39:PRO:HB3   | 2.33                     | 0.63              |
| 1:A:8:SER:HB3    | 1:A:57:VAL:CG1   | 2.29                     | 0.62              |
| 1:B:170:GLU:O    | 1:B:174:VAL:HG13 | 1.99                     | 0.62              |
| 1:B:30:LEU:HD13  | 1:B:81:VAL:HG11  | 1.80                     | 0.62              |
| 1:F:197:LEU:O    | 1:F:198:LYS:HG2  | 1.99                     | 0.62              |
| 1:E:35:HIS:ND1   | 1:E:35:HIS:N     | 2.47                     | 0.62              |
| 1:D:177:THR:HB   | 1:D:180:LYS:HE3  | 1.80                     | 0.62              |
| 1:C:34:TYR:CZ    | 1:C:39:PRO:HB3   | 2.34                     | 0.62              |
| 1:C:42:SER:CB    | 1:C:45:GLU:HG3   | 2.30                     | 0.62              |
| 2:S:1:DT:H2''    | 2:S:2:DT:O5'     | 1.97                     | 0.62              |
| 1:E:31:ILE:HG23  | 1:E:168:THR:HA   | 1.81                     | 0.62              |
| 1:B:263:VAL:N    | 1:F:225:MET:HE2  | 2.13                     | 0.62              |
| 1:C:148:LEU:HD22 | 1:C:191:LEU:HD11 | 1.82                     | 0.61              |
| 2:Z:5:DA:H2''    | 2:Z:6:DC:C5'     | 2.29                     | 0.61              |
| 1:C:255:ALA:HA   | 1:C:269:ARG:HA   | 1.82                     | 0.61              |
| 1:E:138:VAL:CG2  | 1:F:255:ALA:HB2  | 2.30                     | 0.61              |
| 2:I:9:DG:H2''    | 2:I:10:DT:O5'    | 2.01                     | 0.61              |
| 1:D:263:VAL:N    | 1:G:225:MET:HE2  | 2.08                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:9:DG:H2''    | 2:J:10:DT:O5'    | 2.01                     | 0.61              |
| 2:P:10:DT:H2'    | 2:P:11:DC:C5     | 2.36                     | 0.61              |
| 1:F:79:PHE:CE1   | 1:F:241:SER:HB3  | 2.36                     | 0.60              |
| 2:N:9:DG:H2''    | 2:N:10:DT:O5'    | 2.01                     | 0.60              |
| 1:F:133:THR:HG22 | 1:F:133:THR:O    | 2.00                     | 0.60              |
| 2:L:9:DG:H2''    | 2:L:10:DT:O5'    | 2.01                     | 0.60              |
| 1:G:33:LEU:HD12  | 1:G:50:LEU:HD23  | 1.83                     | 0.60              |
| 1:D:34:TYR:CD2   | 1:D:167:LEU:HD12 | 2.36                     | 0.60              |
| 1:A:257:THR:CG2  | 1:B:258:HIS:CG   | 2.84                     | 0.60              |
| 1:F:256:ALA:HB3  | 1:F:259:THR:HG23 | 1.83                     | 0.60              |
| 1:E:138:VAL:CG1  | 1:F:255:ALA:HB3  | 2.19                     | 0.60              |
| 1:H:281:GLU:HG3  | 1:H:285:LYS:HE3  | 1.84                     | 0.60              |
| 1:B:133:THR:O    | 1:B:133:THR:HG22 | 2.00                     | 0.60              |
| 1:D:148:LEU:HD22 | 1:D:191:LEU:HD11 | 1.83                     | 0.60              |
| 1:F:103:LYS:O    | 1:F:103:LYS:HG3  | 2.00                     | 0.60              |
| 1:D:135:LYS:HG3  | 2:Z:9:DG:OP2     | 2.02                     | 0.60              |
| 1:A:133:THR:HG22 | 1:A:133:THR:O    | 2.01                     | 0.60              |
| 1:H:44:LYS:HD2   | 1:H:44:LYS:O     | 2.00                     | 0.60              |
| 2:K:9:DG:H2''    | 2:K:10:DT:O5'    | 2.02                     | 0.60              |
| 1:A:170:GLU:O    | 1:A:174:VAL:HG13 | 2.02                     | 0.59              |
| 1:G:4:ASN:ND2    | 1:G:4:ASN:N      | 2.48                     | 0.59              |
| 2:K:10:DT:H2'    | 2:K:11:DC:C5     | 2.37                     | 0.59              |
| 1:D:31:ILE:HG23  | 1:D:168:THR:CA   | 2.28                     | 0.59              |
| 1:E:52:ASN:HA    | 1:E:55:LYS:HB3   | 1.84                     | 0.59              |
| 1:F:88:TRP:HZ3   | 1:F:175:ALA:HA   | 1.66                     | 0.59              |
| 1:H:36:HIS:CG    | 1:H:37:GLN:H     | 2.19                     | 0.59              |
| 2:V:8:DG:H2''    | 2:V:9:DG:OP2     | 2.01                     | 0.59              |
| 1:D:39:PRO:O     | 1:D:40:THR:HG23  | 2.03                     | 0.59              |
| 1:E:139:ARG:O    | 1:F:254:THR:HA   | 2.02                     | 0.59              |
| 1:H:8:SER:HB3    | 1:H:57:VAL:HG11  | 1.84                     | 0.59              |
| 2:Y:6:DC:H1'     | 2:Y:7:DC:H5''    | 1.84                     | 0.59              |
| 1:C:128:GLU:HG2  | 1:C:129:LYS:N    | 2.17                     | 0.59              |
| 2:J:10:DT:H2'    | 2:J:11:DC:C5     | 2.37                     | 0.59              |
| 2:S:7:DC:H2''    | 2:S:8:DG:C8      | 2.37                     | 0.59              |
| 1:C:34:TYR:CD1   | 1:C:39:PRO:HD3   | 2.38                     | 0.59              |
| 1:B:225:MET:HE1  | 1:F:263:VAL:N    | 2.15                     | 0.58              |
| 1:D:34:TYR:CE1   | 1:D:39:PRO:HB3   | 2.38                     | 0.58              |
| 1:E:265:SER:O    | 1:E:267:PRO:HD3  | 2.03                     | 0.58              |
| 1:C:255:ALA:CB   | 1:D:138:VAL:HG13 | 2.26                     | 0.58              |
| 1:F:79:PHE:O     | 1:F:83:ILE:HD12  | 2.02                     | 0.58              |
| 1:F:197:LEU:HD23 | 1:F:239:ALA:HB3  | 1.85                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:136:GLN:HG2  | 1:B:269:ARG:HD3  | 1.85                     | 0.58              |
| 1:B:58:VAL:CG1   | 1:B:65:ILE:HD13  | 2.33                     | 0.58              |
| 1:E:157:LYS:HB3  | 1:E:159:GLU:OE1  | 2.04                     | 0.58              |
| 1:F:278:THR:HG23 | 1:H:285:LYS:NZ   | 2.17                     | 0.58              |
| 1:G:166:LYS:O    | 1:G:171:ASN:OD1  | 2.21                     | 0.58              |
| 1:A:161:ASN:ND2  | 3:A:355:HOH:O    | 2.35                     | 0.58              |
| 1:C:65:ILE:N     | 1:C:65:ILE:HD12  | 2.12                     | 0.58              |
| 2:O:9:DG:H2''    | 2:O:10:DT:O5'    | 2.03                     | 0.58              |
| 1:E:252:LEU:HD13 | 1:E:274:ILE:HB   | 1.85                     | 0.58              |
| 2:P:9:DG:H2''    | 2:P:10:DT:O5'    | 2.03                     | 0.58              |
| 2:N:10:DT:H2'    | 2:N:11:DC:C5     | 2.38                     | 0.58              |
| 2:Y:2:DT:O2      | 2:Z:13:DA:H5''   | 2.03                     | 0.58              |
| 2:V:5:DA:H1'     | 2:V:6:DC:H5'     | 1.84                     | 0.57              |
| 1:C:263:VAL:O    | 1:H:230:PRO:HB3  | 2.05                     | 0.57              |
| 1:D:244:VAL:HG13 | 1:D:248:ASP:HB2  | 1.87                     | 0.57              |
| 2:L:10:DT:H2'    | 2:L:11:DC:C5     | 2.39                     | 0.57              |
| 2:O:10:DT:H2'    | 2:O:11:DC:C5     | 2.39                     | 0.57              |
| 1:B:251:ALA:O    | 1:B:254:THR:OG1  | 2.20                     | 0.57              |
| 1:B:203:PRO:HG2  | 2:I:4:DG:C8      | 2.39                     | 0.57              |
| 1:C:171:ASN:O    | 1:C:174:VAL:HG22 | 2.05                     | 0.57              |
| 2:V:1:DT:H2''    | 2:V:2:DT:H5'     | 1.86                     | 0.57              |
| 1:E:252:LEU:CD1  | 1:E:274:ILE:HB   | 2.34                     | 0.57              |
| 1:A:90:TYR:O     | 1:A:94:ARG:HB2   | 2.05                     | 0.57              |
| 1:H:4:ASN:CB     | 1:H:7:ASN:ND2    | 2.68                     | 0.57              |
| 2:X:1:DT:H2''    | 2:X:2:DT:O5'     | 2.03                     | 0.57              |
| 1:D:34:TYR:HB2   | 1:D:167:LEU:HB2  | 1.87                     | 0.57              |
| 1:F:27:PHE:O     | 1:F:30:LEU:HB2   | 2.05                     | 0.57              |
| 1:D:90:TYR:O     | 1:D:94:ARG:HB2   | 2.05                     | 0.56              |
| 1:G:90:TYR:O     | 1:G:94:ARG:HB2   | 2.04                     | 0.56              |
| 2:I:10:DT:H2'    | 2:I:11:DC:C5     | 2.40                     | 0.56              |
| 1:H:116:PHE:O    | 1:H:184:GLY:HA2  | 2.05                     | 0.56              |
| 2:Y:6:DC:H2''    | 2:Y:7:DC:H5'     | 1.85                     | 0.56              |
| 1:C:168:THR:H    | 1:C:171:ASN:HB2  | 1.70                     | 0.56              |
| 1:H:98:ASP:HB3   | 1:H:153:LYS:HG3  | 1.87                     | 0.56              |
| 1:E:38:THR:HG23  | 1:E:165:ASN:C    | 2.26                     | 0.56              |
| 1:G:291:ILE:HG22 | 1:G:292:LYS:HD2  | 1.88                     | 0.56              |
| 2:R:10:DT:H2''   | 2:R:11:DC:H5'    | 1.87                     | 0.56              |
| 1:C:23:ARG:CZ    | 1:C:23:ARG:HB2   | 2.36                     | 0.56              |
| 1:D:79:PHE:CE1   | 1:D:241:SER:HB3  | 2.41                     | 0.56              |
| 1:A:225:MET:HE2  | 1:E:263:VAL:HG12 | 1.88                     | 0.56              |
| 2:V:3:DC:H5'     | 2:X:13:DA:H5'    | 1.88                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:256:ALA:HB3  | 1:F:259:THR:CG2  | 2.35                     | 0.55              |
| 1:C:98:ASP:HB3   | 1:C:153:LYS:HG3  | 1.87                     | 0.55              |
| 1:E:31:ILE:O     | 1:E:35:HIS:HB3   | 2.07                     | 0.55              |
| 1:F:157:LYS:HE2  | 1:F:159:GLU:OE1  | 2.07                     | 0.55              |
| 1:F:23:ARG:HG2   | 1:F:24:ILE:N     | 2.22                     | 0.55              |
| 1:G:171:ASN:O    | 1:G:174:VAL:HG22 | 2.06                     | 0.55              |
| 1:A:134:HIS:CE1  | 1:B:267:PRO:HG2  | 2.41                     | 0.55              |
| 1:G:88:TRP:CZ2   | 1:G:160:TYR:HA   | 2.42                     | 0.55              |
| 1:B:43:ILE:HD12  | 1:B:277:LEU:O    | 2.06                     | 0.55              |
| 1:B:33:LEU:HD23  | 1:B:33:LEU:O     | 2.06                     | 0.55              |
| 1:D:98:ASP:HB3   | 1:D:153:LYS:HG3  | 1.87                     | 0.55              |
| 1:H:259:THR:HG21 | 1:H:268:GLU:HB3  | 1.89                     | 0.55              |
| 1:G:98:ASP:HB3   | 1:G:153:LYS:HG3  | 1.88                     | 0.55              |
| 1:A:8:SER:HB3    | 1:A:57:VAL:HG11  | 1.88                     | 0.55              |
| 1:D:34:TYR:CD1   | 1:D:39:PRO:HD3   | 2.42                     | 0.55              |
| 1:E:262:ASN:O    | 1:E:265:SER:HB3  | 2.06                     | 0.55              |
| 2:R:7:DC:H42     | 2:S:8:DG:H1      | 1.54                     | 0.55              |
| 1:E:102:ILE:CD1  | 1:E:182:ILE:HD13 | 2.37                     | 0.55              |
| 1:F:244:VAL:HG13 | 1:F:248:ASP:HB2  | 1.88                     | 0.55              |
| 1:F:278:THR:CG2  | 1:H:285:LYS:NZ   | 2.70                     | 0.54              |
| 1:E:36:HIS:O     | 1:E:166:LYS:HB3  | 2.07                     | 0.54              |
| 1:F:291:ILE:O    | 1:F:292:LYS:HB2  | 2.08                     | 0.54              |
| 1:A:102:ILE:CD1  | 1:A:182:ILE:HD13 | 2.38                     | 0.54              |
| 1:D:29:ALA:O     | 1:D:33:LEU:HB2   | 2.08                     | 0.54              |
| 1:F:31:ILE:CG2   | 1:F:168:THR:HA   | 2.29                     | 0.54              |
| 2:L:5:DA:H2"     | 2:L:6:DC:OP2     | 2.07                     | 0.54              |
| 1:D:120:THR:OG1  | 1:D:188:TRP:HB3  | 2.08                     | 0.54              |
| 1:H:90:TYR:O     | 1:H:94:ARG:HB2   | 2.07                     | 0.54              |
| 1:D:197:LEU:HD23 | 1:D:239:ALA:HB3  | 1.89                     | 0.54              |
| 1:D:31:ILE:CG2   | 1:D:168:THR:HA   | 2.30                     | 0.54              |
| 1:E:38:THR:HG21  | 1:E:164:ILE:O    | 2.07                     | 0.54              |
| 1:F:156:ILE:HD12 | 1:F:156:ILE:N    | 2.23                     | 0.54              |
| 1:C:97:ASN:ND2   | 1:C:153:LYS:HE2  | 2.23                     | 0.54              |
| 1:F:122:GLU:OE1  | 1:F:122:GLU:HA   | 2.07                     | 0.54              |
| 1:H:128:GLU:HG3  | 1:H:129:LYS:H    | 1.72                     | 0.54              |
| 1:H:232:ALA:O    | 1:H:233:GLU:HG3  | 2.07                     | 0.54              |
| 1:F:96:LEU:HB3   | 1:F:99:TYR:HB2   | 1.90                     | 0.54              |
| 1:H:83:ILE:HD13  | 1:H:197:LEU:HD22 | 1.90                     | 0.54              |
| 1:H:4:ASN:CB     | 1:H:7:ASN:HD22   | 2.20                     | 0.54              |
| 1:H:171:ASN:O    | 1:H:174:VAL:HG22 | 2.08                     | 0.54              |
| 1:A:257:THR:HG22 | 1:B:258:HIS:CG   | 2.43                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:31:ILE:HG23  | 1:F:168:THR:CA   | 2.29                     | 0.53              |
| 1:H:217:LYS:HD3  | 1:H:268:GLU:OE2  | 2.08                     | 0.53              |
| 1:B:166:LYS:O    | 1:B:171:ASN:OD1  | 2.27                     | 0.53              |
| 1:C:139:ARG:O    | 1:D:254:THR:HA   | 2.08                     | 0.53              |
| 1:H:246:LYS:HE2  | 1:H:250:ASP:OD1  | 2.08                     | 0.53              |
| 2:K:5:DA:H2''    | 2:K:6:DC:OP2     | 2.06                     | 0.53              |
| 1:B:164:ILE:HG23 | 1:B:171:ASN:CG   | 2.29                     | 0.53              |
| 1:C:74:THR:HG22  | 1:C:78:TRP:CE2   | 2.44                     | 0.53              |
| 1:E:257:THR:HG21 | 1:F:214:ASN:ND2  | 2.23                     | 0.53              |
| 1:A:225:MET:CE   | 1:E:263:VAL:H    | 2.08                     | 0.53              |
| 1:F:78:TRP:O     | 1:F:82:MET:HG3   | 2.07                     | 0.53              |
| 1:E:255:ALA:HA   | 1:E:269:ARG:HA   | 1.90                     | 0.53              |
| 1:F:83:ILE:HD12  | 1:F:83:ILE:H     | 1.73                     | 0.53              |
| 1:B:79:PHE:CE1   | 1:B:241:SER:HB3  | 2.44                     | 0.53              |
| 1:F:75:ARG:CZ    | 1:F:75:ARG:HB3   | 2.38                     | 0.53              |
| 2:N:5:DA:H2''    | 2:N:6:DC:OP2     | 2.08                     | 0.53              |
| 1:D:114:LYS:HA   | 1:D:121:ARG:HH21 | 1.74                     | 0.53              |
| 1:D:134:HIS:HD2  | 3:Z:286:HOH:O    | 1.90                     | 0.53              |
| 1:G:269:ARG:HD3  | 1:H:136:GLN:HG3  | 1.91                     | 0.53              |
| 1:D:225:MET:HG2  | 1:G:263:VAL:HG12 | 1.91                     | 0.53              |
| 1:A:35:HIS:O     | 1:A:166:LYS:HB2  | 2.07                     | 0.52              |
| 1:B:50:LEU:O     | 1:B:54:VAL:HG23  | 2.09                     | 0.52              |
| 1:D:96:LEU:HB3   | 1:D:99:TYR:HB2   | 1.90                     | 0.52              |
| 1:G:91:ARG:HA    | 1:G:96:LEU:HD12  | 1.90                     | 0.52              |
| 2:M:5:DA:H2''    | 2:M:6:DC:OP2     | 2.07                     | 0.52              |
| 1:D:50:LEU:O     | 1:D:54:VAL:HG23  | 2.09                     | 0.52              |
| 1:H:256:ALA:N    | 1:H:268:GLU:O    | 2.41                     | 0.52              |
| 1:C:92:VAL:O     | 1:C:95:GLU:HG3   | 2.09                     | 0.52              |
| 1:G:8:SER:HB3    | 1:G:57:VAL:CG1   | 2.40                     | 0.52              |
| 1:D:44:LYS:HE2   | 1:D:75:ARG:NH2   | 2.25                     | 0.52              |
| 1:H:106:ASN:HB2  | 2:P:4:DG:O3'     | 2.10                     | 0.52              |
| 1:C:265:SER:O    | 1:C:267:PRO:HD3  | 2.10                     | 0.52              |
| 1:H:106:ASN:OD1  | 1:H:108:LYS:HB3  | 2.10                     | 0.52              |
| 1:H:156:ILE:N    | 1:H:156:ILE:HD12 | 2.24                     | 0.52              |
| 1:A:171:ASN:O    | 1:A:174:VAL:HG22 | 2.10                     | 0.52              |
| 1:F:278:THR:CG2  | 1:H:285:LYS:HZ2  | 2.23                     | 0.52              |
| 1:D:122:GLU:O    | 1:D:125:HIS:N    | 2.43                     | 0.51              |
| 1:E:164:ILE:HG23 | 1:E:171:ASN:OD1  | 2.10                     | 0.51              |
| 1:F:98:ASP:HB3   | 1:F:153:LYS:HG3  | 1.91                     | 0.51              |
| 1:G:106:ASN:HB2  | 2:O:4:DG:O3'     | 2.10                     | 0.51              |
| 1:G:164:ILE:HG23 | 1:G:171:ASN:CG   | 2.31                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:156:ILE:HD12 | 1:E:156:ILE:N    | 2.25                     | 0.51              |
| 1:E:94:ARG:O     | 1:E:95:GLU:HB2   | 2.10                     | 0.51              |
| 1:A:225:MET:HE3  | 1:E:263:VAL:HG12 | 1.93                     | 0.51              |
| 1:B:92:VAL:HG22  | 1:B:161:ASN:HA   | 1.93                     | 0.51              |
| 1:B:106:ASN:HB2  | 2:J:4:DG:O3'     | 2.11                     | 0.51              |
| 1:D:262:ASN:HA   | 1:G:225:MET:CE   | 2.41                     | 0.51              |
| 1:E:198:LYS:O    | 1:E:240:SER:HA   | 2.11                     | 0.51              |
| 1:H:8:SER:HB3    | 1:H:57:VAL:HG13  | 1.92                     | 0.51              |
| 1:B:113:ARG:HH11 | 1:B:113:ARG:HG3  | 1.76                     | 0.51              |
| 1:E:138:VAL:HG13 | 1:F:255:ALA:H    | 1.75                     | 0.51              |
| 1:G:198:LYS:O    | 1:G:240:SER:HA   | 2.10                     | 0.51              |
| 2:X:1:DT:C6      | 2:X:2:DT:H72     | 2.46                     | 0.51              |
| 1:A:58:VAL:CG2   | 1:A:63:LEU:HB2   | 2.41                     | 0.51              |
| 1:B:33:LEU:HD11  | 1:B:49:LYS:HG2   | 1.93                     | 0.51              |
| 1:F:28:ASN:C     | 1:F:30:LEU:H     | 2.15                     | 0.51              |
| 2:J:5:DA:H2''    | 2:J:6:DC:OP2     | 2.11                     | 0.51              |
| 1:G:156:ILE:N    | 1:G:156:ILE:HD12 | 2.26                     | 0.51              |
| 1:G:203:PRO:HG2  | 2:P:4:DG:C8      | 2.46                     | 0.51              |
| 2:X:7:DC:H2''    | 2:X:8:DG:C8      | 2.46                     | 0.51              |
| 1:E:89:ASN:O     | 1:E:92:VAL:HB    | 2.12                     | 0.50              |
| 1:G:256:ALA:O    | 1:G:258:HIS:N    | 2.44                     | 0.50              |
| 2:R:9:DG:H2'     | 2:R:10:DT:C7     | 2.40                     | 0.50              |
| 2:V:3:DC:H2''    | 2:V:4:DG:C8      | 2.45                     | 0.50              |
| 1:A:98:ASP:HB3   | 1:A:153:LYS:HG3  | 1.93                     | 0.50              |
| 1:F:168:THR:HG23 | 1:F:171:ASN:OD1  | 2.11                     | 0.50              |
| 1:B:58:VAL:HG11  | 1:B:65:ILE:HA    | 1.94                     | 0.50              |
| 1:E:218:SER:HB2  | 1:F:257:THR:CG2  | 2.42                     | 0.50              |
| 1:C:198:LYS:O    | 1:C:240:SER:HA   | 2.11                     | 0.50              |
| 1:D:74:THR:HG22  | 1:D:78:TRP:CE2   | 2.46                     | 0.50              |
| 1:F:188:TRP:HB2  | 1:F:223:LEU:HD13 | 1.92                     | 0.50              |
| 1:C:188:TRP:HB2  | 1:C:223:LEU:HD13 | 1.93                     | 0.50              |
| 1:B:263:VAL:HB   | 1:F:225:MET:HG3  | 1.93                     | 0.50              |
| 1:G:55:LYS:O     | 1:G:59:LYS:HB2   | 2.12                     | 0.50              |
| 1:H:256:ALA:HB3  | 1:H:259:THR:HG23 | 1.93                     | 0.50              |
| 2:P:5:DA:H2''    | 2:P:6:DC:OP2     | 2.12                     | 0.50              |
| 2:R:7:DC:N3      | 2:S:8:DG:N2      | 2.52                     | 0.50              |
| 1:A:8:SER:HB3    | 1:A:57:VAL:HG13  | 1.93                     | 0.50              |
| 1:B:33:LEU:HD21  | 1:B:49:LYS:HE3   | 1.93                     | 0.50              |
| 1:G:260:ILE:HG22 | 1:G:267:PRO:HB3  | 1.92                     | 0.50              |
| 1:C:90:TYR:O     | 1:C:94:ARG:HB2   | 2.11                     | 0.50              |
| 1:H:256:ALA:O    | 1:H:259:THR:N    | 2.24                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:41:GLY:O     | 1:B:279:SER:HA   | 2.12                     | 0.49              |
| 1:C:156:ILE:N    | 1:C:156:ILE:HD12 | 2.26                     | 0.49              |
| 1:D:156:ILE:HD12 | 1:D:156:ILE:N    | 2.27                     | 0.49              |
| 1:A:230:PRO:HB3  | 1:E:263:VAL:O    | 2.12                     | 0.49              |
| 1:B:156:ILE:HD12 | 1:B:156:ILE:N    | 2.27                     | 0.49              |
| 1:F:102:ILE:CD1  | 1:F:182:ILE:HD13 | 2.42                     | 0.49              |
| 1:D:188:TRP:HB2  | 1:D:223:LEU:HD13 | 1.93                     | 0.49              |
| 1:E:113:ARG:HG3  | 1:E:113:ARG:HH11 | 1.77                     | 0.49              |
| 1:H:125:HIS:HA   | 1:H:128:GLU:HG2  | 1.95                     | 0.49              |
| 1:A:138:VAL:HG13 | 1:B:255:ALA:CB   | 2.32                     | 0.49              |
| 1:A:83:ILE:HD13  | 1:A:197:LEU:HD22 | 1.94                     | 0.49              |
| 1:C:255:ALA:HB1  | 1:C:268:GLU:O    | 2.10                     | 0.49              |
| 1:E:116:PHE:O    | 1:E:184:GLY:HA2  | 2.12                     | 0.49              |
| 1:H:198:LYS:O    | 1:H:240:SER:HA   | 2.13                     | 0.49              |
| 2:I:5:DA:H2"     | 2:I:6:DC:OP2     | 2.12                     | 0.49              |
| 1:B:59:LYS:HG2   | 1:B:65:ILE:HD11  | 1.95                     | 0.49              |
| 1:G:42:SER:HB3   | 1:G:45:GLU:HG3   | 1.93                     | 0.49              |
| 2:V:12:DG:H2"    | 2:V:13:DA:O5'    | 2.11                     | 0.49              |
| 1:C:37:GLN:HG2   | 1:C:38:THR:N     | 2.28                     | 0.49              |
| 1:C:116:PHE:O    | 1:C:184:GLY:HA2  | 2.13                     | 0.49              |
| 1:G:108:LYS:HE3  | 3:G:308:HOH:O    | 2.12                     | 0.49              |
| 1:H:55:LYS:O     | 1:H:58:VAL:HG12  | 2.13                     | 0.49              |
| 2:O:5:DA:H2"     | 2:O:6:DC:OP2     | 2.13                     | 0.49              |
| 1:B:33:LEU:HD21  | 1:B:49:LYS:CE    | 2.43                     | 0.49              |
| 1:C:57:VAL:O     | 1:C:61:LYS:HG3   | 2.11                     | 0.49              |
| 1:D:87:SER:HB3   | 1:D:101:ILE:HG21 | 1.95                     | 0.49              |
| 1:G:74:THR:HG22  | 1:G:78:TRP:CE2   | 2.47                     | 0.49              |
| 1:E:98:ASP:HB3   | 1:E:153:LYS:HG3  | 1.94                     | 0.48              |
| 1:B:102:ILE:CD1  | 1:B:182:ILE:HD13 | 2.43                     | 0.48              |
| 1:B:44:LYS:O     | 1:B:47:LEU:N     | 2.46                     | 0.48              |
| 1:C:50:LEU:O     | 1:C:54:VAL:HG23  | 2.12                     | 0.48              |
| 1:E:24:ILE:HB    | 2:N:11:DC:H5"    | 1.94                     | 0.48              |
| 1:F:255:ALA:CA   | 1:F:268:GLU:O    | 2.61                     | 0.48              |
| 1:H:113:ARG:HG3  | 1:H:113:ARG:HH11 | 1.77                     | 0.48              |
| 1:H:102:ILE:CD1  | 1:H:182:ILE:HD13 | 2.43                     | 0.48              |
| 1:F:155:LEU:HD21 | 1:F:185:LYS:HB3  | 1.94                     | 0.48              |
| 1:B:159:GLU:N    | 1:B:159:GLU:CD   | 2.64                     | 0.48              |
| 1:C:53:TYR:O     | 1:C:57:VAL:HG23  | 2.14                     | 0.48              |
| 1:G:8:SER:HB3    | 1:G:57:VAL:HG11  | 1.95                     | 0.48              |
| 1:A:148:LEU:HD22 | 1:A:191:LEU:CD1  | 2.40                     | 0.48              |
| 1:A:255:ALA:CB   | 1:B:138:VAL:CG1  | 2.67                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:119:GLU:O    | 1:D:122:GLU:HB3  | 2.13                     | 0.48              |
| 1:D:97:ASN:O     | 1:D:156:ILE:CG1  | 2.62                     | 0.48              |
| 1:D:235:LYS:HD3  | 1:D:237:TYR:OH   | 2.13                     | 0.48              |
| 2:S:1:DT:H2'     | 2:S:2:DT:H72     | 1.95                     | 0.48              |
| 1:C:55:LYS:O     | 1:C:59:LYS:HB2   | 2.13                     | 0.48              |
| 1:E:188:TRP:HB2  | 1:E:223:LEU:HD13 | 1.94                     | 0.48              |
| 1:F:203:PRO:HG2  | 2:M:4:DG:C8      | 2.48                     | 0.48              |
| 1:H:203:PRO:HG2  | 2:O:4:DG:C8      | 2.48                     | 0.48              |
| 1:D:91:ARG:HA    | 1:D:96:LEU:HD12  | 1.96                     | 0.48              |
| 1:G:116:PHE:O    | 1:G:184:GLY:HA2  | 2.13                     | 0.48              |
| 1:B:188:TRP:HB2  | 1:B:223:LEU:HD13 | 1.96                     | 0.48              |
| 1:D:279:SER:OG   | 1:D:281:GLU:HG3  | 2.14                     | 0.48              |
| 1:G:113:ARG:HH11 | 1:G:113:ARG:HG3  | 1.79                     | 0.48              |
| 2:I:10:DT:H4'    | 2:I:10:DT:OP1    | 2.14                     | 0.48              |
| 1:A:74:THR:HG22  | 1:A:78:TRP:CE2   | 2.49                     | 0.48              |
| 1:A:156:ILE:N    | 1:A:156:ILE:HD12 | 2.29                     | 0.47              |
| 1:A:72:SER:HB3   | 2:I:7:DC:O4'     | 2.13                     | 0.47              |
| 1:H:94:ARG:HG3   | 1:H:292:LYS:NZ   | 2.29                     | 0.47              |
| 1:A:50:LEU:O     | 1:A:54:VAL:HG23  | 2.13                     | 0.47              |
| 1:D:106:ASN:HB2  | 2:L:4:DG:O3'     | 2.14                     | 0.47              |
| 1:E:251:ALA:O    | 1:E:254:THR:OG1  | 2.28                     | 0.47              |
| 1:B:98:ASP:HB3   | 1:B:153:LYS:HG3  | 1.94                     | 0.47              |
| 1:C:113:ARG:HH11 | 1:C:113:ARG:HG3  | 1.79                     | 0.47              |
| 1:C:35:HIS:NE2   | 1:C:36:HIS:CE1   | 2.82                     | 0.47              |
| 1:C:58:VAL:CG2   | 1:C:63:LEU:HB2   | 2.45                     | 0.47              |
| 1:E:250:ASP:O    | 1:E:253:GLN:HB2  | 2.14                     | 0.47              |
| 1:C:257:THR:HG21 | 1:D:214:ASN:ND2  | 2.30                     | 0.47              |
| 1:G:188:TRP:HB2  | 1:G:223:LEU:HD13 | 1.96                     | 0.47              |
| 1:G:58:VAL:CG2   | 1:G:63:LEU:HB2   | 2.45                     | 0.47              |
| 1:A:113:ARG:HH11 | 1:A:113:ARG:HG3  | 1.78                     | 0.47              |
| 1:H:255:ALA:HA   | 1:H:269:ARG:HA   | 1.97                     | 0.47              |
| 1:A:257:THR:O    | 1:A:257:THR:HG22 | 2.15                     | 0.47              |
| 1:B:55:LYS:O     | 1:B:59:LYS:HG3   | 2.15                     | 0.47              |
| 1:A:58:VAL:HG23  | 1:A:63:LEU:HB2   | 1.96                     | 0.47              |
| 1:C:87:SER:HB3   | 1:C:101:ILE:HG21 | 1.96                     | 0.47              |
| 1:D:213:GLY:O    | 1:D:217:LYS:HG3  | 2.15                     | 0.47              |
| 1:E:50:LEU:O     | 1:E:54:VAL:HG12  | 2.14                     | 0.47              |
| 1:E:30:LEU:HD23  | 1:E:50:LEU:HD11  | 1.97                     | 0.47              |
| 1:B:51:GLU:HG3   | 1:B:71:PHE:CE1   | 2.50                     | 0.47              |
| 1:B:58:VAL:HG12  | 1:B:65:ILE:HD13  | 1.97                     | 0.47              |
| 1:F:278:THR:HG21 | 1:H:285:LYS:HZ2  | 1.80                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:138:VAL:HG13 | 1:H:255:ALA:CA   | 2.45                     | 0.47              |
| 1:D:34:TYR:HD2   | 1:D:167:LEU:HD12 | 1.80                     | 0.46              |
| 1:E:51:GLU:O     | 1:E:55:LYS:HB2   | 2.15                     | 0.46              |
| 1:H:55:LYS:O     | 1:H:59:LYS:HB2   | 2.16                     | 0.46              |
| 1:B:33:LEU:CD2   | 1:B:49:LYS:HE3   | 2.45                     | 0.46              |
| 1:C:83:ILE:HD13  | 1:C:197:LEU:HD22 | 1.96                     | 0.46              |
| 1:F:74:THR:HG22  | 1:F:78:TRP:CZ2   | 2.50                     | 0.46              |
| 1:D:230:PRO:HG3  | 1:G:263:VAL:HG22 | 1.97                     | 0.46              |
| 1:H:50:LEU:O     | 1:H:54:VAL:HG23  | 2.15                     | 0.46              |
| 1:B:230:PRO:HB3  | 1:F:263:VAL:O    | 2.15                     | 0.46              |
| 1:D:173:ASP:O    | 1:D:177:THR:OG1  | 2.28                     | 0.46              |
| 1:D:72:SER:HB3   | 2:L:7:DC:O4'     | 2.15                     | 0.46              |
| 1:H:58:VAL:CG2   | 1:H:63:LEU:HB2   | 2.45                     | 0.46              |
| 1:A:83:ILE:CD1   | 1:A:197:LEU:HD22 | 2.46                     | 0.46              |
| 1:E:33:LEU:CD1   | 1:E:50:LEU:HA    | 2.44                     | 0.46              |
| 1:E:24:ILE:O     | 2:N:11:DC:H3'    | 2.15                     | 0.46              |
| 2:V:5:DA:H2''    | 2:V:6:DC:O5'     | 2.14                     | 0.46              |
| 1:A:143:SER:O    | 1:A:212:GLU:OE2  | 2.33                     | 0.46              |
| 1:A:55:LYS:O     | 1:A:59:LYS:HB2   | 2.15                     | 0.46              |
| 1:D:115:ILE:O    | 1:D:186:CYS:HB2  | 2.15                     | 0.46              |
| 1:D:91:ARG:HB2   | 1:D:96:LEU:HB2   | 1.97                     | 0.46              |
| 1:B:94:ARG:O     | 1:B:95:GLU:HB2   | 2.15                     | 0.46              |
| 1:C:275:PHE:CD2  | 1:C:286:MET:HG3  | 2.51                     | 0.46              |
| 1:F:235:LYS:HD3  | 1:F:237:TYR:OH   | 2.16                     | 0.46              |
| 1:F:242:GLU:HB3  | 1:F:243:PRO:CD   | 2.45                     | 0.46              |
| 1:F:97:ASN:O     | 1:F:156:ILE:CG1  | 2.60                     | 0.46              |
| 1:A:188:TRP:HB2  | 1:A:223:LEU:HD13 | 1.97                     | 0.46              |
| 1:A:203:PRO:HG2  | 2:J:4:DG:C8      | 2.50                     | 0.46              |
| 1:A:94:ARG:HA    | 1:A:94:ARG:HD3   | 1.68                     | 0.46              |
| 1:B:71:PHE:O     | 1:B:75:ARG:HG3   | 2.16                     | 0.46              |
| 1:A:78:TRP:O     | 1:A:82:MET:HG3   | 2.16                     | 0.46              |
| 1:B:44:LYS:O     | 1:B:46:ASN:N     | 2.49                     | 0.46              |
| 1:D:97:ASN:HD21  | 1:D:153:LYS:HE2  | 1.81                     | 0.46              |
| 1:E:237:TYR:CE2  | 1:E:290:ILE:HG23 | 2.51                     | 0.46              |
| 1:F:151:ARG:CG   | 1:F:151:ARG:O    | 2.63                     | 0.46              |
| 1:C:231:LYS:HD3  | 2:V:10:DT:OP1    | 2.16                     | 0.46              |
| 1:C:44:LYS:HD3   | 1:C:242:GLU:HG2  | 1.97                     | 0.46              |
| 1:D:34:TYR:O     | 1:D:167:LEU:N    | 2.46                     | 0.46              |
| 1:F:74:THR:HG22  | 1:F:78:TRP:CE2   | 2.51                     | 0.46              |
| 1:G:159:GLU:CD   | 1:G:159:GLU:H    | 2.20                     | 0.46              |
| 1:G:38:THR:HG23  | 1:G:165:ASN:C    | 2.37                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:90:TYR:HA    | 1:B:93:LYS:CD    | 2.42                     | 0.46              |
| 1:F:88:TRP:O     | 1:F:92:VAL:HG23  | 2.16                     | 0.46              |
| 1:G:157:LYS:HD3  | 1:G:160:TYR:OH   | 2.16                     | 0.46              |
| 1:A:4:ASN:ND2    | 1:A:4:ASN:N      | 2.56                     | 0.45              |
| 1:C:24:ILE:HG22  | 1:C:26:PRO:HD3   | 1.98                     | 0.45              |
| 1:C:33:LEU:HD21  | 1:C:53:TYR:CZ    | 2.51                     | 0.45              |
| 1:D:113:ARG:HG3  | 1:D:113:ARG:HH11 | 1.79                     | 0.45              |
| 1:H:58:VAL:HG23  | 1:H:63:LEU:HB2   | 1.98                     | 0.45              |
| 1:B:116:PHE:O    | 1:B:184:GLY:HA2  | 2.16                     | 0.45              |
| 1:C:237:TYR:CE2  | 1:C:290:ILE:HG23 | 2.51                     | 0.45              |
| 1:D:45:GLU:O     | 1:D:49:LYS:HB2   | 2.17                     | 0.45              |
| 1:D:79:PHE:HA    | 1:D:82:MET:HE3   | 1.97                     | 0.45              |
| 1:E:91:ARG:HA    | 1:E:96:LEU:HD12  | 1.99                     | 0.45              |
| 1:E:93:LYS:HG3   | 1:E:94:ARG:N     | 2.30                     | 0.45              |
| 1:F:113:ARG:HG3  | 1:F:113:ARG:HH11 | 1.81                     | 0.45              |
| 1:D:225:MET:HG2  | 1:G:263:VAL:CG1  | 2.46                     | 0.45              |
| 1:E:48:ASP:O     | 1:E:51:GLU:HB3   | 2.16                     | 0.45              |
| 1:B:44:LYS:C     | 1:B:46:ASN:N     | 2.68                     | 0.45              |
| 1:D:34:TYR:HH    | 1:D:39:PRO:HB3   | 1.81                     | 0.45              |
| 1:F:92:VAL:HG11  | 1:F:163:PRO:HD3  | 1.97                     | 0.45              |
| 1:E:138:VAL:CB   | 1:F:255:ALA:HB2  | 2.40                     | 0.45              |
| 1:D:170:GLU:O    | 1:D:173:ASP:HB2  | 2.17                     | 0.45              |
| 1:A:136:GLN:CG   | 1:B:269:ARG:HD3  | 2.45                     | 0.45              |
| 1:C:37:GLN:HA    | 1:C:165:ASN:O    | 2.16                     | 0.45              |
| 1:F:263:VAL:HG22 | 1:F:263:VAL:O    | 2.15                     | 0.45              |
| 2:Y:2:DT:H6      | 2:Y:2:DT:H2'     | 1.64                     | 0.45              |
| 1:B:198:LYS:O    | 1:B:240:SER:HA   | 2.16                     | 0.45              |
| 1:D:96:LEU:HD22  | 1:D:99:TYR:CD2   | 2.52                     | 0.45              |
| 1:E:73:ASN:OD1   | 1:E:73:ASN:C     | 2.54                     | 0.45              |
| 1:F:255:ALA:HA   | 1:F:268:GLU:O    | 2.17                     | 0.45              |
| 1:F:275:PHE:CD2  | 1:F:286:MET:HG3  | 2.52                     | 0.45              |
| 1:F:213:GLY:O    | 1:F:217:LYS:HG3  | 2.17                     | 0.45              |
| 1:G:193:ALA:HA   | 1:G:235:LYS:O    | 2.16                     | 0.45              |
| 1:H:36:HIS:CG    | 1:H:37:GLN:N     | 2.85                     | 0.45              |
| 2:N:10:DT:OP1    | 2:N:10:DT:H4'    | 2.17                     | 0.45              |
| 1:C:203:PRO:HG2  | 2:L:4:DG:C8      | 2.52                     | 0.45              |
| 1:F:91:ARG:HH11  | 1:F:160:TYR:HB3  | 1.81                     | 0.45              |
| 2:Y:2:DT:H2''    | 2:Y:3:DC:OP2     | 2.16                     | 0.45              |
| 1:A:138:VAL:HG22 | 1:B:269:ARG:HG3  | 1.99                     | 0.45              |
| 1:D:203:PRO:HA   | 1:D:206:ARG:CZ   | 2.47                     | 0.45              |
| 1:C:138:VAL:HG13 | 1:D:255:ALA:HB2  | 1.97                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:275:PHE:CD2  | 1:E:286:MET:HG3  | 2.52                     | 0.45              |
| 1:H:41:GLY:O     | 1:H:279:SER:HA   | 2.17                     | 0.45              |
| 1:D:212:GLU:O    | 1:D:216:LEU:HG   | 2.16                     | 0.44              |
| 1:E:199:THR:O    | 1:E:242:GLU:HG3  | 2.17                     | 0.44              |
| 1:C:102:ILE:CD1  | 1:C:182:ILE:HD13 | 2.47                     | 0.44              |
| 1:E:254:THR:HA   | 1:F:139:ARG:O    | 2.17                     | 0.44              |
| 1:F:23:ARG:HG2   | 1:F:24:ILE:H     | 1.82                     | 0.44              |
| 2:Y:6:DC:H1'     | 2:Y:7:DC:C5'     | 2.47                     | 0.44              |
| 1:B:168:THR:H    | 1:B:171:ASN:HB2  | 1.82                     | 0.44              |
| 1:D:94:ARG:O     | 1:D:95:GLU:HB2   | 2.18                     | 0.44              |
| 1:B:193:ALA:HA   | 1:B:235:LYS:O    | 2.17                     | 0.44              |
| 1:G:269:ARG:HG3  | 1:H:138:VAL:HG22 | 2.00                     | 0.44              |
| 1:G:37:GLN:HB2   | 3:G:305:HOH:O    | 2.18                     | 0.44              |
| 1:A:275:PHE:CD2  | 1:A:286:MET:HG3  | 2.53                     | 0.44              |
| 1:A:55:LYS:O     | 1:A:58:VAL:HG12  | 2.16                     | 0.44              |
| 1:D:242:GLU:HB3  | 1:D:243:PRO:CD   | 2.48                     | 0.44              |
| 1:D:25:LYS:HA    | 1:D:26:PRO:HD2   | 1.82                     | 0.44              |
| 1:E:138:VAL:HG13 | 1:F:255:ALA:N    | 2.32                     | 0.44              |
| 1:F:90:TYR:CZ    | 1:F:94:ARG:HG2   | 2.52                     | 0.44              |
| 1:H:112:PHE:O    | 1:H:115:ILE:HG12 | 2.18                     | 0.44              |
| 1:E:24:ILE:HG13  | 2:N:11:DC:OP1    | 2.18                     | 0.44              |
| 1:E:68:SER:O     | 1:E:72:SER:N     | 2.41                     | 0.44              |
| 1:H:57:VAL:O     | 1:H:61:LYS:HG3   | 2.16                     | 0.44              |
| 2:O:10:DT:H4'    | 2:O:10:DT:OP1    | 2.18                     | 0.44              |
| 1:B:237:TYR:CE2  | 1:B:290:ILE:HG23 | 2.53                     | 0.44              |
| 1:B:44:LYS:O     | 1:B:45:GLU:C     | 2.55                     | 0.44              |
| 1:C:42:SER:HB3   | 1:C:45:GLU:CG    | 2.39                     | 0.44              |
| 1:E:256:ALA:C    | 1:E:258:HIS:N    | 2.71                     | 0.44              |
| 1:E:42:SER:HB3   | 1:E:45:GLU:HB2   | 2.00                     | 0.44              |
| 2:Z:5:DA:H1'     | 2:Z:6:DC:H5''    | 1.98                     | 0.44              |
| 1:E:227:TYR:O    | 1:E:228:TRP:C    | 2.55                     | 0.44              |
| 1:F:120:THR:OG1  | 1:F:188:TRP:HB3  | 2.18                     | 0.44              |
| 1:F:77:THR:O     | 1:F:78:TRP:C     | 2.56                     | 0.44              |
| 2:Y:1:DT:H2'     | 2:Y:2:DT:H71     | 1.99                     | 0.44              |
| 1:A:116:PHE:O    | 1:A:184:GLY:HA2  | 2.18                     | 0.44              |
| 1:F:123:LYS:O    | 1:F:126:GLN:HB2  | 2.18                     | 0.44              |
| 1:G:55:LYS:O     | 1:G:58:VAL:HG12  | 2.17                     | 0.44              |
| 1:H:256:ALA:O    | 1:H:257:THR:C    | 2.55                     | 0.44              |
| 1:A:123:LYS:O    | 1:A:126:GLN:HB2  | 2.18                     | 0.43              |
| 1:A:251:ALA:O    | 1:A:254:THR:OG1  | 2.25                     | 0.43              |
| 1:B:83:ILE:HD13  | 1:B:197:LEU:HD22 | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:34:TYR:HB2   | 1:B:167:LEU:HD12 | 1.98                     | 0.43              |
| 1:B:4:ASN:HA     | 3:B:341:HOH:O    | 2.17                     | 0.43              |
| 1:B:88:TRP:C     | 1:B:88:TRP:CD1   | 2.91                     | 0.43              |
| 1:D:44:LYS:HD3   | 1:D:44:LYS:HA    | 1.86                     | 0.43              |
| 1:F:103:LYS:CG   | 1:F:103:LYS:O    | 2.66                     | 0.43              |
| 1:G:164:ILE:HG23 | 1:G:171:ASN:OD1  | 2.18                     | 0.43              |
| 1:H:227:TYR:O    | 1:H:228:TRP:C    | 2.56                     | 0.43              |
| 2:J:10:DT:OP1    | 2:J:10:DT:H4'    | 2.18                     | 0.43              |
| 2:V:13:DA:OP1    | 2:V:13:DA:H4'    | 2.18                     | 0.43              |
| 1:C:31:ILE:O     | 1:C:32:GLU:C     | 2.54                     | 0.43              |
| 1:D:237:TYR:CE2  | 1:D:290:ILE:HG23 | 2.53                     | 0.43              |
| 1:E:112:PHE:O    | 1:E:115:ILE:HG12 | 2.18                     | 0.43              |
| 1:F:91:ARG:NH1   | 1:F:160:TYR:HB2  | 2.33                     | 0.43              |
| 1:G:50:LEU:O     | 1:G:54:VAL:HG23  | 2.19                     | 0.43              |
| 2:P:10:DT:H4'    | 2:P:10:DT:OP1    | 2.17                     | 0.43              |
| 1:A:41:GLY:O     | 1:A:279:SER:HA   | 2.18                     | 0.43              |
| 1:A:51:GLU:HG3   | 1:A:71:PHE:CD1   | 2.53                     | 0.43              |
| 1:C:136:GLN:CG   | 1:D:269:ARG:HD3  | 2.48                     | 0.43              |
| 1:C:51:GLU:HG3   | 1:C:71:PHE:CD1   | 2.54                     | 0.43              |
| 1:D:88:TRP:CZ2   | 1:D:160:TYR:HA   | 2.53                     | 0.43              |
| 1:F:168:THR:OG1  | 1:F:171:ASN:OD1  | 2.36                     | 0.43              |
| 1:H:188:TRP:HB2  | 1:H:223:LEU:HD13 | 1.99                     | 0.43              |
| 1:H:51:GLU:HG3   | 1:H:71:PHE:CD1   | 2.53                     | 0.43              |
| 1:A:91:ARG:HA    | 1:A:96:LEU:HD12  | 2.00                     | 0.43              |
| 1:E:34:TYR:HB2   | 1:E:167:LEU:HD12 | 2.00                     | 0.43              |
| 1:F:78:TRP:O     | 1:F:79:PHE:C     | 2.56                     | 0.43              |
| 2:V:1:DT:H2''    | 2:V:2:DT:C5'     | 2.48                     | 0.43              |
| 1:B:227:TYR:O    | 1:B:228:TRP:C    | 2.56                     | 0.43              |
| 1:B:58:VAL:HG11  | 1:B:65:ILE:HD13  | 1.99                     | 0.43              |
| 1:C:79:PHE:HA    | 1:C:82:MET:HE3   | 2.00                     | 0.43              |
| 1:E:72:SER:HB3   | 2:M:7:DC:O4'     | 2.19                     | 0.43              |
| 1:B:246:LYS:NZ   | 1:B:250:ASP:OD1  | 2.45                     | 0.43              |
| 1:F:187:LYS:HE2  | 1:F:187:LYS:HB3  | 1.81                     | 0.43              |
| 1:A:15:LYS:HA    | 1:A:19:LYS:O     | 2.19                     | 0.43              |
| 1:B:8:SER:HB3    | 1:B:57:VAL:HG11  | 1.99                     | 0.43              |
| 1:C:193:ALA:HA   | 1:C:235:LYS:O    | 2.17                     | 0.43              |
| 1:H:32:GLU:OE1   | 1:H:53:TYR:OH    | 2.34                     | 0.43              |
| 1:A:24:ILE:HD11  | 1:A:66:PRO:CB    | 2.49                     | 0.43              |
| 1:B:8:SER:HB3    | 1:B:57:VAL:CG1   | 2.48                     | 0.43              |
| 1:C:58:VAL:HG23  | 1:C:63:LEU:HB2   | 2.01                     | 0.43              |
| 1:D:83:ILE:CD1   | 1:D:197:LEU:HD22 | 2.49                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:256:ALA:C    | 1:H:258:HIS:N    | 2.72                     | 0.43              |
| 1:A:198:LYS:O    | 1:A:240:SER:HA   | 2.19                     | 0.43              |
| 1:C:254:THR:HA   | 1:D:139:ARG:O    | 2.19                     | 0.43              |
| 1:C:55:LYS:O     | 1:C:58:VAL:HG12  | 2.19                     | 0.43              |
| 1:A:267:PRO:HG2  | 1:B:134:HIS:CE1  | 2.53                     | 0.42              |
| 1:F:291:ILE:O    | 1:F:292:LYS:CB   | 2.67                     | 0.42              |
| 1:F:75:ARG:HH11  | 1:F:75:ARG:HG2   | 1.84                     | 0.42              |
| 1:F:91:ARG:HG3   | 1:F:92:VAL:H     | 1.81                     | 0.42              |
| 1:A:88:TRP:CZ2   | 1:A:160:TYR:HA   | 2.54                     | 0.42              |
| 1:A:193:ALA:HA   | 1:A:235:LYS:O    | 2.18                     | 0.42              |
| 1:B:39:PRO:O     | 1:B:40:THR:HG23  | 2.18                     | 0.42              |
| 1:E:218:SER:HB2  | 1:F:257:THR:HG21 | 2.00                     | 0.42              |
| 1:G:58:VAL:HG23  | 1:G:63:LEU:HB2   | 2.00                     | 0.42              |
| 1:H:74:THR:HG22  | 1:H:78:TRP:CE2   | 2.54                     | 0.42              |
| 1:C:112:PHE:O    | 1:C:115:ILE:HG12 | 2.19                     | 0.42              |
| 1:C:74:THR:CG2   | 1:C:78:TRP:CZ2   | 3.02                     | 0.42              |
| 1:E:55:LYS:O     | 1:E:55:LYS:HG2   | 2.19                     | 0.42              |
| 1:A:213:GLY:O    | 1:A:217:LYS:HG3  | 2.19                     | 0.42              |
| 1:D:188:TRP:CG   | 1:D:189:ASP:N    | 2.87                     | 0.42              |
| 1:D:51:GLU:HG3   | 1:D:71:PHE:CD1   | 2.55                     | 0.42              |
| 1:F:188:TRP:CG   | 1:F:189:ASP:N    | 2.87                     | 0.42              |
| 1:G:135:LYS:HB2  | 2:V:8:DG:H5"     | 2.01                     | 0.42              |
| 1:G:214:ASN:ND2  | 1:H:257:THR:CG2  | 2.80                     | 0.42              |
| 1:H:242:GLU:HB3  | 1:H:243:PRO:CD   | 2.49                     | 0.42              |
| 1:D:86:GLN:OE1   | 1:D:280:PHE:HD2  | 2.03                     | 0.42              |
| 1:E:218:SER:CB   | 1:F:257:THR:HG22 | 2.50                     | 0.42              |
| 1:F:74:THR:CG2   | 1:F:78:TRP:CZ2   | 3.02                     | 0.42              |
| 1:G:53:TYR:O     | 1:G:57:VAL:HG23  | 2.19                     | 0.42              |
| 1:H:169:HIS:O    | 1:H:173:ASP:OD2  | 2.37                     | 0.42              |
| 1:B:98:ASP:N     | 1:B:98:ASP:OD1   | 2.50                     | 0.42              |
| 1:C:44:LYS:HB3   | 1:C:44:LYS:HE3   | 1.86                     | 0.42              |
| 1:D:281:GLU:HG3  | 1:D:281:GLU:H    | 1.50                     | 0.42              |
| 1:F:223:LEU:O    | 1:F:227:TYR:HD2  | 2.03                     | 0.42              |
| 1:G:57:VAL:O     | 1:G:61:LYS:HG3   | 2.19                     | 0.42              |
| 1:G:139:ARG:O    | 1:H:254:THR:HA   | 2.19                     | 0.42              |
| 2:K:10:DT:OP1    | 2:K:10:DT:H4'    | 2.20                     | 0.42              |
| 1:A:281:GLU:HG3  | 1:A:285:LYS:HE3  | 2.02                     | 0.42              |
| 1:A:51:GLU:OE1   | 1:A:75:ARG:HD2   | 2.20                     | 0.42              |
| 1:B:54:VAL:O     | 1:B:58:VAL:HG23  | 2.19                     | 0.42              |
| 1:C:263:VAL:HG22 | 1:H:230:PRO:HB3  | 2.01                     | 0.42              |
| 1:D:28:ASN:C     | 1:D:30:LEU:N     | 2.72                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:193:ALA:HA   | 1:E:235:LYS:O    | 2.19                     | 0.42              |
| 2:L:10:DT:H4'    | 2:L:10:DT:OP1    | 2.20                     | 0.42              |
| 1:G:171:ASN:HD22 | 1:G:171:ASN:HA   | 1.52                     | 0.42              |
| 1:E:256:ALA:HB3  | 1:E:259:THR:HG23 | 2.01                     | 0.42              |
| 1:F:88:TRP:CZ3   | 1:F:175:ALA:HA   | 2.52                     | 0.42              |
| 1:G:45:GLU:O     | 1:G:49:LYS:HB2   | 2.20                     | 0.42              |
| 1:B:262:ASN:HB2  | 1:B:265:SER:HB2  | 2.02                     | 0.42              |
| 1:B:87:SER:O     | 1:B:90:TYR:HB3   | 2.20                     | 0.42              |
| 1:D:275:PHE:CD2  | 1:D:286:MET:HG3  | 2.55                     | 0.42              |
| 1:F:203:PRO:HA   | 1:F:206:ARG:CZ   | 2.50                     | 0.42              |
| 1:F:217:LYS:NZ   | 1:F:268:GLU:OE2  | 2.36                     | 0.42              |
| 1:A:223:LEU:HA   | 1:A:223:LEU:HD23 | 1.91                     | 0.41              |
| 1:A:227:TYR:O    | 1:A:228:TRP:C    | 2.57                     | 0.41              |
| 1:B:11:VAL:HG11  | 1:B:58:VAL:CG2   | 2.50                     | 0.41              |
| 1:C:214:ASN:OD1  | 1:C:256:ALA:HA   | 2.20                     | 0.41              |
| 1:C:86:GLN:HG2   | 1:C:283:ILE:HD12 | 2.02                     | 0.41              |
| 1:D:227:TYR:O    | 1:D:228:TRP:C    | 2.58                     | 0.41              |
| 1:F:197:LEU:C    | 1:F:198:LYS:HG2  | 2.41                     | 0.41              |
| 1:G:42:SER:CB    | 1:G:45:GLU:HG3   | 2.50                     | 0.41              |
| 1:A:87:SER:HB3   | 1:A:101:ILE:HG21 | 2.02                     | 0.41              |
| 1:A:139:ARG:O    | 1:B:254:THR:HA   | 2.21                     | 0.41              |
| 1:A:57:VAL:O     | 1:A:61:LYS:HG3   | 2.18                     | 0.41              |
| 1:B:90:TYR:OH    | 1:B:288:ASP:OD1  | 2.28                     | 0.41              |
| 1:D:197:LEU:C    | 1:D:198:LYS:HG2  | 2.40                     | 0.41              |
| 1:H:44:LYS:HA    | 1:H:47:LEU:HD12  | 2.02                     | 0.41              |
| 1:E:30:LEU:CD1   | 1:E:81:VAL:HG11  | 2.51                     | 0.41              |
| 1:F:94:ARG:O     | 1:F:95:GLU:HB2   | 2.21                     | 0.41              |
| 1:A:136:GLN:HG2  | 1:B:269:ARG:CD   | 2.50                     | 0.41              |
| 1:B:275:PHE:CD2  | 1:B:286:MET:HG3  | 2.55                     | 0.41              |
| 1:C:269:ARG:HD3  | 1:D:136:GLN:CG   | 2.51                     | 0.41              |
| 1:C:86:GLN:OE1   | 1:C:280:PHE:HD2  | 2.03                     | 0.41              |
| 1:D:133:THR:HG23 | 2:V:2:DT:H71     | 1.99                     | 0.41              |
| 1:D:65:ILE:HG23  | 1:D:65:ILE:O     | 2.20                     | 0.41              |
| 1:E:217:LYS:HZ1  | 1:E:272:ASP:CG   | 2.24                     | 0.41              |
| 1:E:257:THR:CG2  | 1:F:214:ASN:ND2  | 2.84                     | 0.41              |
| 1:F:79:PHE:CE1   | 1:F:83:ILE:HD11  | 2.55                     | 0.41              |
| 1:G:51:GLU:HG2   | 1:G:55:LYS:HE3   | 2.02                     | 0.41              |
| 1:A:106:ASN:HB2  | 2:I:4:DG:O3'     | 2.20                     | 0.41              |
| 1:A:53:TYR:O     | 1:A:57:VAL:HG23  | 2.21                     | 0.41              |
| 1:D:112:PHE:O    | 1:D:115:ILE:HG12 | 2.21                     | 0.41              |
| 1:D:150:ILE:CD1  | 1:D:191:LEU:HD13 | 2.51                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:175:ALA:C    | 1:F:177:THR:H    | 2.24                     | 0.41              |
| 1:F:89:ASN:O     | 1:F:93:LYS:HB2   | 2.21                     | 0.41              |
| 1:H:213:GLY:O    | 1:H:217:LYS:HG3  | 2.21                     | 0.41              |
| 2:Z:6:DC:H2"     | 2:Z:7:DC:O5'     | 2.20                     | 0.41              |
| 1:F:125:HIS:O    | 1:F:129:LYS:HB2  | 2.20                     | 0.41              |
| 1:F:28:ASN:C     | 1:F:30:LEU:N     | 2.73                     | 0.41              |
| 1:F:91:ARG:NH2   | 1:F:97:ASN:HA    | 2.35                     | 0.41              |
| 1:A:65:ILE:HA    | 1:A:66:PRO:HD3   | 1.91                     | 0.41              |
| 1:E:203:PRO:HG2  | 2:N:4:DG:C8      | 2.54                     | 0.41              |
| 1:H:53:TYR:O     | 1:H:57:VAL:HG23  | 2.20                     | 0.41              |
| 2:R:9:DG:H2"     | 2:R:10:DT:O5'    | 2.20                     | 0.41              |
| 1:C:23:ARG:HB2   | 1:C:23:ARG:NH1   | 2.35                     | 0.41              |
| 1:C:42:SER:O     | 1:C:45:GLU:HB2   | 2.21                     | 0.41              |
| 1:D:262:ASN:HA   | 1:G:225:MET:HE2  | 2.02                     | 0.41              |
| 1:F:112:PHE:O    | 1:F:115:ILE:HG12 | 2.21                     | 0.41              |
| 1:F:240:SER:C    | 1:F:242:GLU:H    | 2.23                     | 0.41              |
| 1:F:266:THR:HA   | 1:F:267:PRO:HD3  | 1.95                     | 0.41              |
| 1:G:38:THR:HG23  | 1:G:166:LYS:N    | 2.35                     | 0.41              |
| 1:G:227:TYR:O    | 1:G:228:TRP:C    | 2.58                     | 0.41              |
| 1:C:138:VAL:HG22 | 1:D:269:ARG:HG3  | 2.03                     | 0.41              |
| 1:E:148:LEU:HD22 | 1:E:191:LEU:CD1  | 2.48                     | 0.41              |
| 1:E:30:LEU:HD13  | 1:E:81:VAL:HG11  | 2.03                     | 0.41              |
| 1:D:263:VAL:HG12 | 1:G:225:MET:CE   | 2.50                     | 0.41              |
| 2:V:6:DC:H2"     | 2:V:7:DC:OP2     | 2.20                     | 0.41              |
| 1:C:213:GLY:O    | 1:C:217:LYS:HG3  | 2.21                     | 0.41              |
| 1:G:51:GLU:HG3   | 1:G:71:PHE:CD1   | 2.55                     | 0.41              |
| 1:H:15:LYS:HA    | 1:H:19:LYS:O     | 2.21                     | 0.41              |
| 1:H:193:ALA:HA   | 1:H:235:LYS:O    | 2.20                     | 0.41              |
| 1:C:199:THR:O    | 1:C:242:GLU:HG3  | 2.21                     | 0.40              |
| 1:C:28:ASN:O     | 1:C:32:GLU:HG3   | 2.20                     | 0.40              |
| 1:F:116:PHE:HB2  | 1:F:121:ARG:HG2  | 2.04                     | 0.40              |
| 1:F:227:TYR:O    | 1:F:228:TRP:C    | 2.59                     | 0.40              |
| 1:F:79:PHE:O     | 1:F:83:ILE:CD1   | 2.67                     | 0.40              |
| 1:A:254:THR:HA   | 1:B:139:ARG:O    | 2.21                     | 0.40              |
| 1:D:175:ALA:C    | 1:D:177:THR:H    | 2.23                     | 0.40              |
| 1:D:102:ILE:CD1  | 1:D:182:ILE:HD13 | 2.51                     | 0.40              |
| 1:D:230:PRO:HG3  | 1:G:263:VAL:CG2  | 2.51                     | 0.40              |
| 1:E:204:ASP:HB2  | 1:F:208:GLN:OE1  | 2.21                     | 0.40              |
| 1:F:212:GLU:O    | 1:F:216:LEU:HG   | 2.20                     | 0.40              |
| 1:F:91:ARG:HB2   | 1:F:91:ARG:HE    | 1.68                     | 0.40              |
| 1:A:117:ASP:O    | 1:A:121:ARG:HG3  | 2.21                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:D:106:ASN:OD1  | 1:D:108:LYS:HB2 | 2.21                     | 0.40              |
| 1:D:252:LEU:HD23 | 1:D:252:LEU:HA  | 1.88                     | 0.40              |
| 1:D:44:LYS:HE2   | 1:D:75:ARG:HH22 | 1.86                     | 0.40              |
| 1:E:108:LYS:HD3  | 1:E:108:LYS:HA  | 1.88                     | 0.40              |
| 1:E:52:ASN:O     | 1:E:55:LYS:N    | 2.54                     | 0.40              |
| 1:C:72:SER:HB3   | 2:K:7:DC:O4'    | 2.21                     | 0.40              |
| 1:C:34:TYR:HB2   | 1:C:167:LEU:HB2 | 2.02                     | 0.40              |
| 1:F:168:THR:HG1  | 1:F:171:ASN:CG  | 2.25                     | 0.40              |
| 1:H:31:ILE:O     | 1:H:35:HIS:HB3  | 2.22                     | 0.40              |
| 1:B:199:THR:O    | 1:B:242:GLU:HG3 | 2.22                     | 0.40              |
| 1:D:187:LYS:HG3  | 1:D:189:ASP:OD1 | 2.21                     | 0.40              |
| 1:F:91:ARG:NH1   | 1:F:160:TYR:CB  | 2.84                     | 0.40              |
| 1:G:254:THR:HA   | 1:H:139:ARG:O   | 2.20                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 287/293 (98%)   | 278 (97%)  | 8 (3%)   | 1 (0%)   | 41          | 66  |
| 1   | B     | 287/293 (98%)   | 268 (93%)  | 18 (6%)  | 1 (0%)   | 41          | 66  |
| 1   | C     | 286/293 (98%)   | 267 (93%)  | 18 (6%)  | 1 (0%)   | 41          | 66  |
| 1   | D     | 287/293 (98%)   | 267 (93%)  | 20 (7%)  | 0        | 100         | 100 |
| 1   | E     | 287/293 (98%)   | 260 (91%)  | 24 (8%)  | 3 (1%)   | 15          | 37  |
| 1   | F     | 285/293 (97%)   | 246 (86%)  | 33 (12%) | 6 (2%)   | 7           | 18  |
| 1   | G     | 287/293 (98%)   | 275 (96%)  | 12 (4%)  | 0        | 100         | 100 |
| 1   | H     | 288/293 (98%)   | 278 (96%)  | 9 (3%)   | 1 (0%)   | 41          | 66  |
| All | All   | 2294/2344 (98%) | 2139 (93%) | 142 (6%) | 13 (1%)  | 25          | 50  |

All (13) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 257 | THR  |
| 1   | H     | 257 | THR  |
| 1   | A     | 257 | THR  |
| 1   | F     | 57  | VAL  |
| 1   | B     | 97  | ASN  |
| 1   | E     | 6   | THR  |
| 1   | F     | 18  | GLY  |
| 1   | F     | 32  | GLU  |
| 1   | C     | 8   | SER  |
| 1   | E     | 19  | LYS  |
| 1   | F     | 20  | THR  |
| 1   | F     | 67  | THR  |
| 1   | F     | 26  | PRO  |

### 5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 263/267 (98%)   | 254 (97%)  | 9 (3%)   | 37          | 66 |
| 1   | B     | 263/267 (98%)   | 254 (97%)  | 9 (3%)   | 37          | 66 |
| 1   | C     | 262/267 (98%)   | 257 (98%)  | 5 (2%)   | 57          | 82 |
| 1   | D     | 263/267 (98%)   | 252 (96%)  | 11 (4%)  | 30          | 58 |
| 1   | E     | 263/267 (98%)   | 249 (95%)  | 14 (5%)  | 22          | 48 |
| 1   | F     | 261/267 (98%)   | 248 (95%)  | 13 (5%)  | 24          | 51 |
| 1   | G     | 263/267 (98%)   | 255 (97%)  | 8 (3%)   | 41          | 70 |
| 1   | H     | 264/267 (99%)   | 253 (96%)  | 11 (4%)  | 30          | 58 |
| All | All   | 2102/2136 (98%) | 2022 (96%) | 80 (4%)  | 33          | 62 |

All (80) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 4   | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 40  | THR  |
| 1   | A     | 94  | ARG  |
| 1   | A     | 126 | GLN  |
| 1   | A     | 159 | GLU  |
| 1   | A     | 233 | GLU  |
| 1   | A     | 249 | ASP  |
| 1   | A     | 289 | GLN  |
| 1   | A     | 292 | LYS  |
| 1   | B     | 35  | HIS  |
| 1   | B     | 37  | GLN  |
| 1   | B     | 93  | LYS  |
| 1   | B     | 96  | LEU  |
| 1   | B     | 135 | LYS  |
| 1   | B     | 170 | GLU  |
| 1   | B     | 212 | GLU  |
| 1   | B     | 231 | LYS  |
| 1   | B     | 249 | ASP  |
| 1   | C     | 23  | ARG  |
| 1   | C     | 37  | GLN  |
| 1   | C     | 94  | ARG  |
| 1   | C     | 249 | ASP  |
| 1   | C     | 292 | LYS  |
| 1   | D     | 6   | THR  |
| 1   | D     | 7   | ASN  |
| 1   | D     | 33  | LEU  |
| 1   | D     | 45  | GLU  |
| 1   | D     | 94  | ARG  |
| 1   | D     | 118 | ASN  |
| 1   | D     | 225 | MET  |
| 1   | D     | 249 | ASP  |
| 1   | D     | 266 | THR  |
| 1   | D     | 281 | GLU  |
| 1   | D     | 289 | GLN  |
| 1   | E     | 4   | ASN  |
| 1   | E     | 8   | SER  |
| 1   | E     | 14  | TYR  |
| 1   | E     | 35  | HIS  |
| 1   | E     | 40  | THR  |
| 1   | E     | 71  | PHE  |
| 1   | E     | 73  | ASN  |
| 1   | E     | 94  | ARG  |
| 1   | E     | 170 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 173 | ASP  |
| 1   | E     | 246 | LYS  |
| 1   | E     | 249 | ASP  |
| 1   | E     | 266 | THR  |
| 1   | E     | 292 | LYS  |
| 1   | F     | 22  | ILE  |
| 1   | F     | 33  | LEU  |
| 1   | F     | 35  | HIS  |
| 1   | F     | 37  | GLN  |
| 1   | F     | 40  | THR  |
| 1   | F     | 93  | LYS  |
| 1   | F     | 94  | ARG  |
| 1   | F     | 103 | LYS  |
| 1   | F     | 129 | LYS  |
| 1   | F     | 165 | ASN  |
| 1   | F     | 173 | ASP  |
| 1   | F     | 266 | THR  |
| 1   | F     | 289 | GLN  |
| 1   | G     | 4   | ASN  |
| 1   | G     | 49  | LYS  |
| 1   | G     | 94  | ARG  |
| 1   | G     | 121 | ARG  |
| 1   | G     | 171 | ASN  |
| 1   | G     | 212 | GLU  |
| 1   | G     | 249 | ASP  |
| 1   | G     | 264 | ASN  |
| 1   | H     | 33  | LEU  |
| 1   | H     | 37  | GLN  |
| 1   | H     | 44  | LYS  |
| 1   | H     | 94  | ARG  |
| 1   | H     | 122 | GLU  |
| 1   | H     | 165 | ASN  |
| 1   | H     | 246 | LYS  |
| 1   | H     | 249 | ASP  |
| 1   | H     | 266 | THR  |
| 1   | H     | 281 | GLU  |
| 1   | H     | 289 | GLN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 134 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 161 | ASN  |
| 1   | A     | 214 | ASN  |
| 1   | B     | 134 | HIS  |
| 1   | B     | 171 | ASN  |
| 1   | B     | 208 | GLN  |
| 1   | B     | 214 | ASN  |
| 1   | C     | 258 | HIS  |
| 1   | D     | 28  | ASN  |
| 1   | D     | 134 | HIS  |
| 1   | D     | 214 | ASN  |
| 1   | E     | 171 | ASN  |
| 1   | E     | 214 | ASN  |
| 1   | E     | 258 | HIS  |
| 1   | F     | 165 | ASN  |
| 1   | F     | 214 | ASN  |
| 1   | G     | 126 | GLN  |
| 1   | G     | 171 | ASN  |
| 1   | G     | 208 | GLN  |
| 1   | H     | 7   | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9   |
|-----|-------|-----------------|--------|----------------|-----------------------|---------|
| 1   | A     | 289/293 (98%)   | 0.21   | 4 (1%) 75 77   | 23, 40, 60, 76        | 2 (0%)  |
| 1   | B     | 289/293 (98%)   | 0.12   | 5 (1%) 70 72   | 23, 45, 63, 79        | 1 (0%)  |
| 1   | C     | 272/293 (92%)   | 0.41   | 19 (6%) 16 14  | 27, 47, 81, 89        | 5 (1%)  |
| 1   | D     | 257/293 (87%)   | 0.78   | 39 (15%) 2 1   | 26, 56, 87, 98        | 3 (1%)  |
| 1   | E     | 258/293 (88%)   | 0.42   | 22 (8%) 10 9   | 27, 53, 84, 90        | 8 (3%)  |
| 1   | F     | 245/293 (83%)   | 0.83   | 40 (16%) 1 1   | 32, 63, 90, 94        | 9 (3%)  |
| 1   | G     | 289/293 (98%)   | 0.11   | 1 (0%) 94 95   | 20, 41, 59, 68        | 7 (2%)  |
| 1   | H     | 290/293 (98%)   | 0.15   | 4 (1%) 75 77   | 20, 39, 58, 82        | 4 (1%)  |
| 2   | I     | 13/13 (100%)    | 0.26   | 0 100 100      | 28, 37, 61, 81        | 0       |
| 2   | J     | 13/13 (100%)    | 0.52   | 1 (7%) 13 11   | 30, 41, 66, 93        | 1 (7%)  |
| 2   | K     | 12/13 (92%)     | 1.02   | 0 100 100      | 47, 66, 87, 87        | 1 (8%)  |
| 2   | L     | 12/13 (92%)     | 1.30   | 2 (16%) 1 1    | 52, 69, 78, 84        | 0       |
| 2   | M     | 8/13 (61%)      | 1.43   | 2 (25%) 0 0    | 55, 61, 73, 88        | 0       |
| 2   | N     | 11/13 (84%)     | 1.89   | 5 (45%) 0 0    | 60, 81, 88, 89        | 0       |
| 2   | O     | 13/13 (100%)    | 0.33   | 1 (7%) 13 11   | 27, 37, 79, 99        | 0       |
| 2   | P     | 12/13 (92%)     | 0.19   | 0 100 100      | 26, 39, 50, 51        | 0       |
| 2   | R     | 8/13 (61%)      | 0.74   | 1 (12%) 3 3    | 54, 58, 82, 99        | 0       |
| 2   | S     | 10/13 (76%)     | 0.63   | 1 (10%) 7 5    | 45, 53, 86, 97        | 0       |
| 2   | V     | 13/13 (100%)    | 1.51   | 4 (30%) 0 0    | 80, 95, 100, 100      | 0       |
| 2   | X     | 13/13 (100%)    | 0.27   | 0 100 100      | 55, 67, 86, 87        | 0       |
| 2   | Y     | 13/13 (100%)    | 0.50   | 0 100 100      | 41, 69, 82, 84        | 0       |
| 2   | Z     | 10/13 (76%)     | 0.85   | 1 (10%) 7 5    | 68, 88, 98, 100       | 0       |
| All | All   | 2350/2526 (93%) | 0.39   | 152 (6%) 18 17 | 20, 48, 84, 100       | 41 (1%) |

All (152) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 69  | GLY  | 8.4  |
| 1   | D     | 65  | ILE  | 7.6  |
| 1   | D     | 66  | PRO  | 6.6  |
| 1   | F     | 47  | LEU  | 6.0  |
| 1   | F     | 70  | ALA  | 5.9  |
| 1   | F     | 71  | PHE  | 5.8  |
| 1   | F     | 43  | ILE  | 5.4  |
| 1   | C     | 63  | LEU  | 5.3  |
| 1   | D     | 167 | LEU  | 5.2  |
| 1   | D     | 27  | PHE  | 4.8  |
| 1   | D     | 30  | LEU  | 4.7  |
| 2   | N     | 8   | DG   | 4.5  |
| 1   | D     | 71  | PHE  | 4.4  |
| 1   | D     | 174 | VAL  | 4.3  |
| 1   | D     | 74  | THR  | 4.3  |
| 1   | F     | 27  | PHE  | 4.2  |
| 2   | J     | 1   | DT   | 4.2  |
| 1   | D     | 68  | SER  | 4.1  |
| 1   | C     | 64  | ALA  | 4.1  |
| 1   | D     | 63  | LEU  | 4.0  |
| 1   | E     | 167 | LEU  | 4.0  |
| 1   | G     | 18  | GLY  | 3.9  |
| 1   | D     | 24  | ILE  | 3.9  |
| 1   | F     | 22  | ILE  | 3.8  |
| 1   | A     | 36  | HIS  | 3.8  |
| 1   | F     | 85  | ILE  | 3.7  |
| 1   | D     | 78  | TRP  | 3.7  |
| 2   | M     | 9   | DG   | 3.7  |
| 1   | C     | 70  | ALA  | 3.6  |
| 1   | E     | 136 | GLN  | 3.6  |
| 1   | F     | 73  | ASN  | 3.6  |
| 1   | F     | 169 | HIS  | 3.5  |
| 1   | D     | 166 | LYS  | 3.5  |
| 1   | A     | 37  | GLN  | 3.5  |
| 1   | D     | 64  | ALA  | 3.5  |
| 1   | C     | 78  | TRP  | 3.5  |
| 1   | F     | 78  | TRP  | 3.5  |
| 1   | H     | 35  | HIS  | 3.5  |
| 1   | D     | 157 | LYS  | 3.5  |
| 1   | F     | 160 | TYR  | 3.4  |
| 1   | F     | 133 | THR  | 3.4  |
| 1   | D     | 75  | ARG  | 3.4  |
| 1   | D     | 51  | GLU  | 3.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 135 | LYS  | 3.3  |
| 1   | F     | 100 | LEU  | 3.2  |
| 1   | C     | 36  | HIS  | 3.2  |
| 1   | D     | 176 | LEU  | 3.2  |
| 1   | D     | 50  | LEU  | 3.2  |
| 1   | F     | 69  | GLY  | 3.2  |
| 1   | F     | 30  | LEU  | 3.1  |
| 2   | N     | 7   | DC   | 3.1  |
| 1   | C     | 58  | VAL  | 3.1  |
| 1   | E     | 70  | ALA  | 3.1  |
| 1   | E     | 200 | SER  | 3.1  |
| 1   | D     | 67  | THR  | 3.0  |
| 1   | C     | 71  | PHE  | 3.0  |
| 1   | D     | 54  | VAL  | 3.0  |
| 1   | F     | 75  | ARG  | 3.0  |
| 1   | E     | 37  | GLN  | 3.0  |
| 2   | M     | 8   | DG   | 3.0  |
| 1   | D     | 43  | ILE  | 3.0  |
| 1   | F     | 26  | PRO  | 3.0  |
| 1   | E     | 50  | LEU  | 2.9  |
| 1   | F     | 148 | LEU  | 2.9  |
| 1   | F     | 171 | ASN  | 2.9  |
| 1   | C     | 30  | LEU  | 2.8  |
| 1   | E     | 68  | SER  | 2.8  |
| 1   | H     | 36  | HIS  | 2.8  |
| 1   | C     | 51  | GLU  | 2.8  |
| 1   | E     | 71  | PHE  | 2.8  |
| 1   | E     | 47  | LEU  | 2.7  |
| 1   | D     | 47  | LEU  | 2.7  |
| 1   | B     | 36  | HIS  | 2.7  |
| 1   | C     | 23  | ARG  | 2.7  |
| 1   | F     | 255 | ALA  | 2.7  |
| 1   | E     | 172 | ILE  | 2.6  |
| 2   | N     | 9   | DG   | 2.6  |
| 2   | N     | 6   | DC   | 2.6  |
| 1   | D     | 77  | THR  | 2.6  |
| 1   | E     | 43  | ILE  | 2.6  |
| 1   | B     | 17  | ASN  | 2.6  |
| 1   | D     | 53  | TYR  | 2.5  |
| 1   | F     | 172 | ILE  | 2.5  |
| 1   | D     | 92  | VAL  | 2.5  |
| 1   | E     | 46  | ASN  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 160 | TYR  | 2.5  |
| 1   | F     | 184 | GLY  | 2.5  |
| 1   | F     | 241 | SER  | 2.5  |
| 1   | F     | 74  | THR  | 2.5  |
| 1   | E     | 27  | PHE  | 2.5  |
| 1   | C     | 43  | ILE  | 2.4  |
| 1   | F     | 155 | LEU  | 2.4  |
| 1   | D     | 241 | SER  | 2.4  |
| 2   | S     | 10  | DT   | 2.4  |
| 2   | O     | 1   | DT   | 2.4  |
| 1   | F     | 97  | ASN  | 2.4  |
| 2   | V     | 11  | DC   | 2.4  |
| 1   | F     | 280 | PHE  | 2.4  |
| 2   | R     | 2   | DT   | 2.4  |
| 1   | C     | 54  | VAL  | 2.4  |
| 1   | E     | 36  | HIS  | 2.3  |
| 1   | C     | 133 | THR  | 2.3  |
| 1   | D     | 72  | SER  | 2.3  |
| 1   | E     | 277 | LEU  | 2.3  |
| 1   | C     | 65  | ILE  | 2.3  |
| 1   | C     | 255 | ALA  | 2.3  |
| 2   | V     | 6   | DC   | 2.3  |
| 1   | D     | 70  | ALA  | 2.3  |
| 1   | H     | 37  | GLN  | 2.3  |
| 2   | N     | 10  | DT   | 2.2  |
| 1   | F     | 81  | VAL  | 2.2  |
| 1   | B     | 166 | LYS  | 2.2  |
| 1   | E     | 54  | VAL  | 2.2  |
| 1   | F     | 174 | VAL  | 2.2  |
| 1   | C     | 47  | LEU  | 2.2  |
| 1   | F     | 277 | LEU  | 2.2  |
| 2   | L     | 8   | DG   | 2.2  |
| 1   | D     | 26  | PRO  | 2.2  |
| 1   | F     | 48  | ASP  | 2.2  |
| 1   | D     | 69  | GLY  | 2.2  |
| 1   | D     | 52  | ASN  | 2.2  |
| 2   | V     | 10  | DT   | 2.2  |
| 1   | E     | 24  | ILE  | 2.1  |
| 2   | Z     | 8   | DG   | 2.1  |
| 1   | F     | 72  | SER  | 2.1  |
| 1   | F     | 204 | ASP  | 2.1  |
| 1   | F     | 256 | ALA  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 40  | THR  | 2.1  |
| 1   | F     | 244 | VAL  | 2.1  |
| 1   | C     | 35  | HIS  | 2.1  |
| 1   | D     | 135 | LYS  | 2.1  |
| 1   | F     | 23  | ARG  | 2.1  |
| 1   | D     | 31  | ILE  | 2.1  |
| 1   | E     | 35  | HIS  | 2.1  |
| 2   | V     | 13  | DA   | 2.1  |
| 1   | A     | 135 | LYS  | 2.1  |
| 1   | F     | 24  | ILE  | 2.1  |
| 1   | F     | 182 | ILE  | 2.1  |
| 1   | B     | 37  | GLN  | 2.1  |
| 1   | E     | 74  | THR  | 2.1  |
| 1   | D     | 105 | PRO  | 2.1  |
| 2   | L     | 5   | DA   | 2.1  |
| 1   | C     | 74  | THR  | 2.1  |
| 1   | E     | 67  | THR  | 2.1  |
| 1   | D     | 143 | SER  | 2.0  |
| 1   | H     | 3   | THR  | 2.0  |
| 1   | D     | 44  | LYS  | 2.0  |
| 1   | D     | 162 | LEU  | 2.0  |
| 1   | E     | 30  | LEU  | 2.0  |
| 1   | E     | 33  | LEU  | 2.0  |
| 1   | F     | 178 | LEU  | 2.0  |
| 1   | B     | 292 | LYS  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.