



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:20 PM GMT

PDB ID : 1BHN  
Title : NUCLEOSIDE DIPHOSPHATE KINASE ISOFORM A FROM BOVINE RETINA  
Authors : Ladner, J.E.; Abdulaev, N.G.; Kakuev, D.L.; Karaschuk, G.N.; Tordova, M.; Eisenstein, E.; Fujiwara, J.H.; Ridge, K.D.; Gilliland, G.L.  
Deposited on : 1998-06-10  
Resolution : 2.40 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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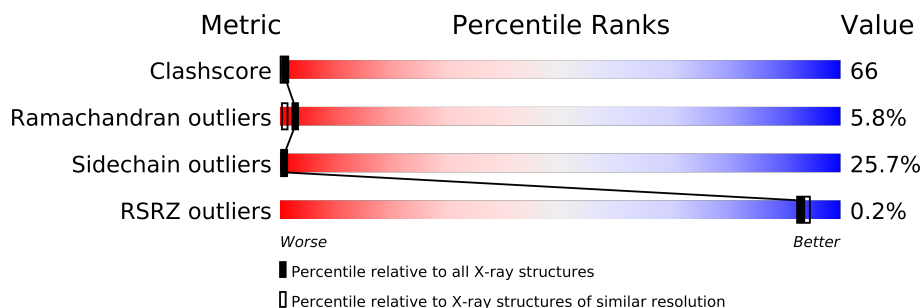
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.40 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)) |
|-----------------------|-----------------------------|---|
| Clashscore            | 79885                       | 2789 (2.40-2.40)                                      |
| Ramachandran outliers | 78287                       | 2736 (2.40-2.40)                                      |
| Sidechain outliers    | 78261                       | 2737 (2.40-2.40)                                      |
| RSRZ outliers         | 66119                       | 2210 (2.40-2.40)                                      |

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 152    |                  |
| 1   | B     | 152    |                  |
| 1   | C     | 152    |                  |
| 1   | D     | 152    |                  |
| 1   | E     | 152    |                  |
| 1   | F     | 152    |                  |

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Geometry | Electron density |
|-----|------|-------|-----|----------|------------------|
| 2   | GDP  | F     | 161 | -        | X                |

## 2 Entry composition i

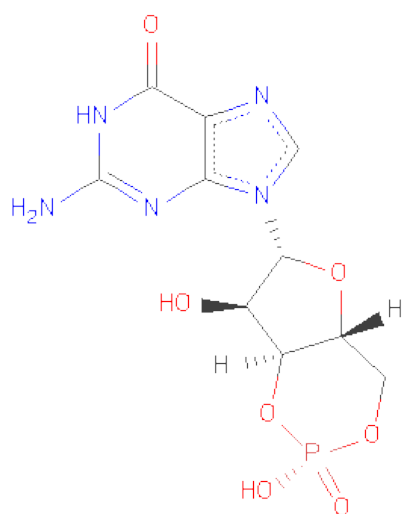
There are 3 unique types of molecules in this entry. The entry contains 7848 atoms, of which 0 are hydrogen and 0 are deuterium.

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 NUCLEOSIDE DIPHOSPHATE TRANSFERASE.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 151      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1206  | 771 | 210 | 218 | 7 |         |         |       |
| 1   | B     | 151      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1206  | 771 | 210 | 218 | 7 |         |         |       |
| 1   | C     | 151      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1206  | 771 | 210 | 218 | 7 |         |         |       |
| 1   | D     | 151      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1206  | 771 | 210 | 218 | 7 |         |         |       |
| 1   | E     | 151      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1206  | 771 | 210 | 218 | 7 |         |         |       |
| 1   | F     | 151      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1206  | 771 | 210 | 218 | 7 |         |         |       |

- Molecule 2 is GUANOSINE-3',5'-MONOPHOSPHATE (three-letter code: 35G, GDP) (formula:  $C_{10}H_{12}N_5O_7P$ ,  $C_{10}H_{15}N_5O_{11}P_2$ ).



| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|----|---|---------|---------|
| 2   | A     | 2        | Total | C  | N  | O  | P | 0       | 0       |
|     |       |          | 51    | 20 | 10 | 18 | 3 |         |         |
| 2   | B     | 2        | Total | C  | N  | O  | P | 0       | 0       |
|     |       |          | 51    | 20 | 10 | 18 | 3 |         |         |
| 2   | C     | 2        | Total | C  | N  | O  | P | 0       | 0       |
|     |       |          | 51    | 20 | 10 | 18 | 3 |         |         |
| 2   | D     | 2        | Total | C  | N  | O  | P | 0       | 0       |
|     |       |          | 51    | 20 | 10 | 18 | 3 |         |         |
| 2   | E     | 2        | Total | C  | N  | O  | P | 0       | 0       |
|     |       |          | 51    | 20 | 10 | 18 | 3 |         |         |
| 2   | F     | 2        | Total | C  | N  | O  | P | 0       | 0       |
|     |       |          | 51    | 20 | 10 | 18 | 3 |         |         |

- Molecule 3 is water.

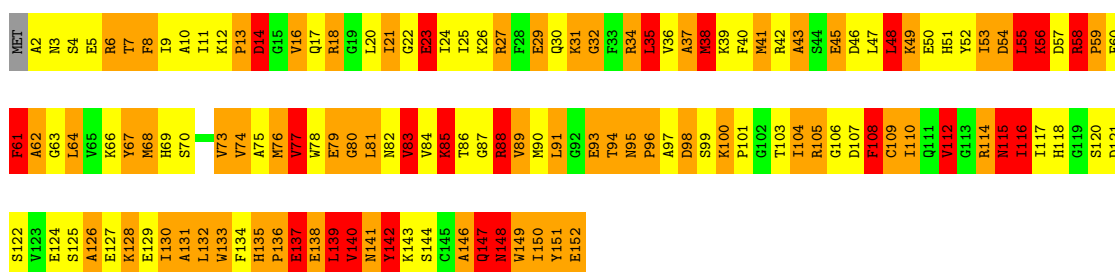
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 49       | Total | O  | 0       | 0       |
|     |       |          | 49    | 49 |         |         |
| 3   | B     | 49       | Total | O  | 0       | 0       |
|     |       |          | 49    | 49 |         |         |
| 3   | C     | 50       | Total | O  | 0       | 0       |
|     |       |          | 50    | 50 |         |         |
| 3   | D     | 40       | Total | O  | 0       | 0       |
|     |       |          | 40    | 40 |         |         |
| 3   | E     | 62       | Total | O  | 0       | 0       |
|     |       |          | 62    | 62 |         |         |
| 3   | F     | 56       | Total | O  | 0       | 0       |
|     |       |          | 56    | 56 |         |         |

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $RSRZ > 2$ ). 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.

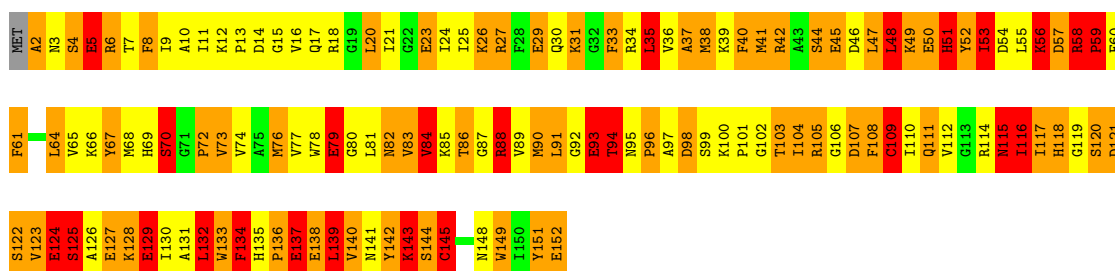
#### • Molecule 1: NUCLEOSIDE DIPHOSPHATE TRANSFERASE

Chain A:



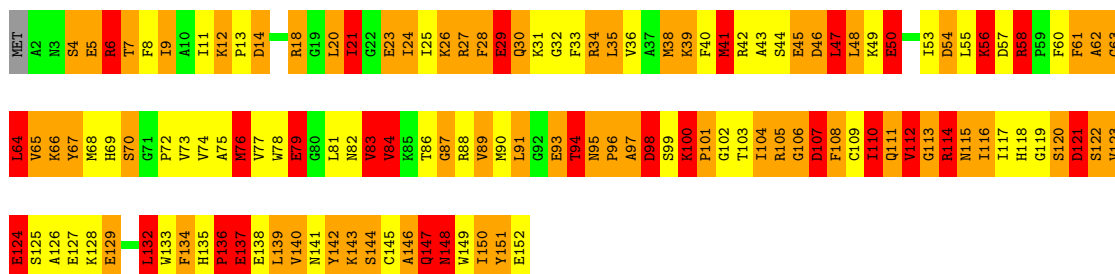
#### • Molecule 1: NUCLEOSIDE DIPHOSPHATE TRANSFERASE

Chain B:



#### • Molecule 1: NUCLEOSIDE DIPHOSPHATE TRANSFERASE

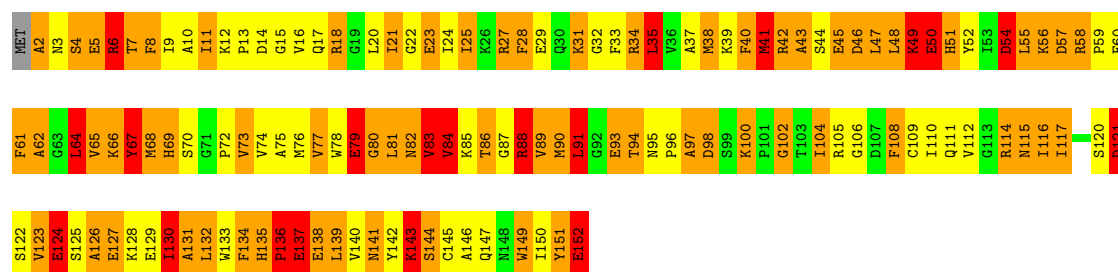
Chain C:



#### • Molecule 1: NUCLEOSIDE DIPHOSPHATE TRANSFERASE

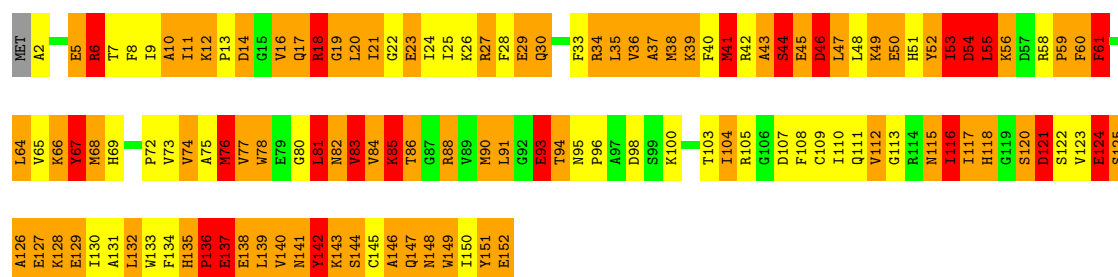
Chain D:





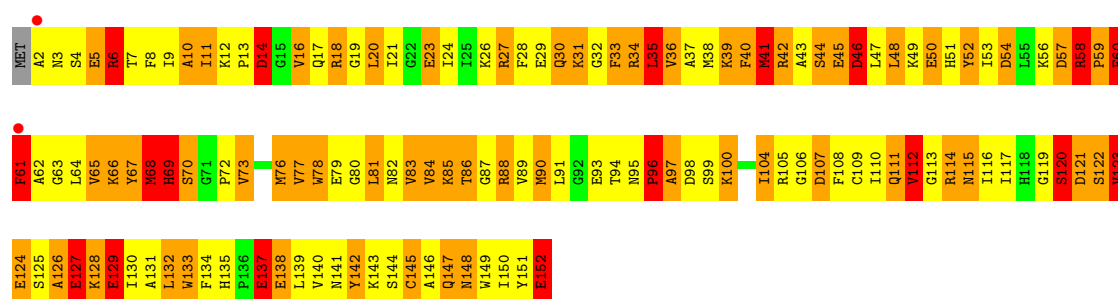
### • Molecule 1: NUCLEOSIDE DIPHOSPHATE TRANSFERASE

Chain E:



### • Molecule 1: NUCLEOSIDE DIPHOSPHATE TRANSFERASE

Chain F:



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 89.88Å 92.11Å 131.63Å<br>90.00° 90.00° 90.00°               | Depositor        |
| Resolution (Å)  | 20.00 – 2.40<br>29.95 – 2.26                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 79.0 (20.00-2.40)<br>72.2 (29.95-2.26)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | 0.12  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.10 (at 2.26Å)   | Xtriage          |
| Refinement program  | TNT V. 5-E  | Depositor        |
| R, $R_{free}$   | 0.200 , (Not available)<br>0.201 , (Not available)          | Depositor<br>DCC |
| $R_{free}$ test set   | No test flags present.                                      | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 24.4  | Xtriage          |
| Anisotropy  | 0.909   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 99.5   | EDS              |
| Estimated twinning fraction   | 0.027 for k,h,-l  | Xtriage          |
| L-test for twinning   | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Outliers  | 0 of 37331 reflections                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.94  | EDS              |
| Total number of atoms   | 7848  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 32.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 35G, GDP

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     | 1.50         | 15/1233 (1.2%) | 2.95        | 143/1659 (8.6%) |
| 1   | B     | 1.40         | 14/1233 (1.1%) | 3.03        | 131/1659 (7.9%) |
| 1   | C     | 1.42         | 11/1233 (0.9%) | 3.00        | 128/1659 (7.7%) |
| 1   | D     | 1.46         | 11/1233 (0.9%) | 3.00        | 126/1659 (7.6%) |
| 1   | E     | 1.50         | 14/1233 (1.1%) | 2.90        | 116/1659 (7.0%) |
| 1   | F     | 1.44         | 12/1233 (1.0%) | 3.12        | 145/1659 (8.7%) |
| All | All   | 1.45         | 77/7398 (1.0%) | 3.00        | 789/9954 (7.9%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | B     | 3                   | 0                   |
| 1   | C     | 0                   | 2                   |
| 1   | D     | 2                   | 0                   |
| 1   | E     | 0                   | 1                   |
| All | All   | 5                   | 3                   |

All (77) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 45  | GLU  | CD-OE2 | 11.47 | 1.38        | 1.25     |
| 1   | F     | 29  | GLU  | CD-OE1 | 10.86 | 1.37        | 1.25     |
| 1   | D     | 79  | GLU  | CD-OE2 | 10.70 | 1.37        | 1.25     |
| 1   | B     | 5   | GLU  | CD-OE2 | 9.09  | 1.35        | 1.25     |
| 1   | A     | 29  | GLU  | CD-OE1 | 8.83  | 1.35        | 1.25     |
| 1   | D     | 129 | GLU  | CD-OE2 | 8.60  | 1.35        | 1.25     |
| 1   | F     | 45  | GLU  | CD-OE2 | 8.44  | 1.34        | 1.25     |
| 1   | A     | 79  | GLU  | CD-OE2 | 8.43  | 1.34        | 1.25     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 124 | GLU  | CD-OE2 | 8.33  | 1.34        | 1.25     |
| 1   | D     | 152 | GLU  | CD-OE2 | 8.31  | 1.34        | 1.25     |
| 1   | A     | 45  | GLU  | CD-OE1 | 8.25  | 1.34        | 1.25     |
| 1   | F     | 138 | GLU  | CD-OE1 | 8.21  | 1.34        | 1.25     |
| 1   | E     | 45  | GLU  | CD-OE1 | 8.11  | 1.34        | 1.25     |
| 1   | C     | 5   | GLU  | CD-OE2 | 8.08  | 1.34        | 1.25     |
| 1   | E     | 124 | GLU  | CD-OE1 | 7.87  | 1.34        | 1.25     |
| 1   | C     | 129 | GLU  | CD-OE2 | 7.82  | 1.34        | 1.25     |
| 1   | E     | 127 | GLU  | CD-OE2 | 7.61  | 1.34        | 1.25     |
| 1   | A     | 5   | GLU  | CD-OE2 | 7.52  | 1.33        | 1.25     |
| 1   | C     | 79  | GLU  | CD-OE2 | 7.49  | 1.33        | 1.25     |
| 1   | F     | 5   | GLU  | CD-OE2 | 7.46  | 1.33        | 1.25     |
| 1   | A     | 152 | GLU  | CD-OE1 | 7.45  | 1.33        | 1.25     |
| 1   | A     | 23  | GLU  | CD-OE2 | 7.30  | 1.33        | 1.25     |
| 1   | D     | 124 | GLU  | CD-OE1 | 7.30  | 1.33        | 1.25     |
| 1   | C     | 93  | GLU  | CD-OE2 | 7.25  | 1.33        | 1.25     |
| 1   | D     | 23  | GLU  | CD-OE1 | 7.21  | 1.33        | 1.25     |
| 1   | C     | 124 | GLU  | CD-OE1 | 7.16  | 1.33        | 1.25     |
| 1   | E     | 152 | GLU  | CD-OE2 | 7.03  | 1.33        | 1.25     |
| 1   | E     | 138 | GLU  | CD-OE1 | 6.98  | 1.33        | 1.25     |
| 1   | A     | 32  | GLY  | CA-C   | 6.97  | 1.63        | 1.51     |
| 1   | C     | 152 | GLU  | CD-OE1 | 6.87  | 1.33        | 1.25     |
| 1   | E     | 93  | GLU  | CD-OE1 | 6.87  | 1.33        | 1.25     |
| 1   | C     | 50  | GLU  | CD-OE1 | 6.85  | 1.33        | 1.25     |
| 1   | E     | 137 | GLU  | CD-OE2 | 6.78  | 1.33        | 1.25     |
| 1   | F     | 79  | GLU  | CD-OE1 | 6.78  | 1.33        | 1.25     |
| 1   | B     | 129 | GLU  | CD-OE2 | 6.76  | 1.33        | 1.25     |
| 1   | D     | 45  | GLU  | CD-OE2 | 6.73  | 1.33        | 1.25     |
| 1   | A     | 93  | GLU  | CD-OE1 | 6.63  | 1.32        | 1.25     |
| 1   | D     | 137 | GLU  | CD-OE2 | 6.59  | 1.32        | 1.25     |
| 1   | F     | 50  | GLU  | CD-OE1 | 6.56  | 1.32        | 1.25     |
| 1   | A     | 138 | GLU  | CD-OE2 | 6.55  | 1.32        | 1.25     |
| 1   | F     | 61  | PHE  | CB-CG  | 6.36  | 1.62        | 1.51     |
| 1   | A     | 79  | GLU  | CD-OE1 | -6.31 | 1.18        | 1.25     |
| 1   | C     | 23  | GLU  | CD-OE2 | 6.30  | 1.32        | 1.25     |
| 1   | B     | 124 | GLU  | CD-OE1 | 6.21  | 1.32        | 1.25     |
| 1   | D     | 29  | GLU  | CD-OE1 | -6.21 | 1.18        | 1.25     |
| 1   | D     | 50  | GLU  | CD-OE1 | 6.17  | 1.32        | 1.25     |
| 1   | F     | 152 | GLU  | CD-OE1 | 6.17  | 1.32        | 1.25     |
| 1   | F     | 127 | GLU  | CD-OE2 | 6.15  | 1.32        | 1.25     |
| 1   | B     | 23  | GLU  | CD-OE2 | 6.08  | 1.32        | 1.25     |
| 1   | B     | 127 | GLU  | CD-OE2 | 6.06  | 1.32        | 1.25     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 34  | ARG  | NE-CZ  | 5.98  | 1.40        | 1.33     |
| 1   | B     | 50  | GLU  | CD-OE1 | 5.93  | 1.32        | 1.25     |
| 1   | A     | 50  | GLU  | CD-OE1 | 5.88  | 1.32        | 1.25     |
| 1   | B     | 138 | GLU  | CD-OE2 | 5.88  | 1.32        | 1.25     |
| 1   | A     | 127 | GLU  | CD-OE2 | 5.86  | 1.32        | 1.25     |
| 1   | D     | 138 | GLU  | CD-OE1 | 5.85  | 1.32        | 1.25     |
| 1   | E     | 129 | GLU  | CD-OE2 | 5.83  | 1.32        | 1.25     |
| 1   | E     | 5   | GLU  | CD-OE2 | 5.56  | 1.31        | 1.25     |
| 1   | E     | 50  | GLU  | CD-OE2 | 5.53  | 1.31        | 1.25     |
| 1   | B     | 29  | GLU  | CD-OE1 | 5.52  | 1.31        | 1.25     |
| 1   | C     | 137 | GLU  | CD-OE2 | 5.47  | 1.31        | 1.25     |
| 1   | E     | 14  | ASP  | CG-OD2 | 5.46  | 1.38        | 1.25     |
| 1   | C     | 127 | GLU  | CD-OE2 | 5.45  | 1.31        | 1.25     |
| 1   | D     | 127 | GLU  | CD-OE2 | 5.43  | 1.31        | 1.25     |
| 1   | B     | 56  | LYS  | C-N    | -5.39 | 1.21        | 1.34     |
| 1   | A     | 137 | GLU  | CD-OE2 | 5.26  | 1.31        | 1.25     |
| 1   | F     | 124 | GLU  | CD-OE1 | 5.22  | 1.31        | 1.25     |
| 1   | F     | 137 | GLU  | CD-OE2 | 5.21  | 1.31        | 1.25     |
| 1   | F     | 23  | GLU  | CD-OE2 | 5.20  | 1.31        | 1.25     |
| 1   | B     | 137 | GLU  | CD-OE2 | 5.20  | 1.31        | 1.25     |
| 1   | B     | 93  | GLU  | CD-OE1 | 5.16  | 1.31        | 1.25     |
| 1   | C     | 45  | GLU  | CD-OE1 | 5.15  | 1.31        | 1.25     |
| 1   | E     | 29  | GLU  | CD-OE1 | -5.15 | 1.20        | 1.25     |
| 1   | E     | 42  | ARG  | NE-CZ  | 5.12  | 1.39        | 1.33     |
| 1   | B     | 79  | GLU  | CD-OE2 | 5.09  | 1.31        | 1.25     |
| 1   | B     | 55  | LEU  | CA-C   | 5.03  | 1.66        | 1.52     |
| 1   | E     | 135 | HIS  | C-N    | -5.01 | 1.24        | 1.34     |

All (789) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | B     | 98  | ASP  | CB-CG-OD2 | -25.48 | 95.37       | 118.30   |
| 1   | D     | 18  | ARG  | NE-CZ-NH2 | 22.93  | 131.76      | 120.30   |
| 1   | F     | 67  | TYR  | CB-CG-CD2 | -22.41 | 107.55      | 121.00   |
| 1   | D     | 114 | ARG  | NE-CZ-NH1 | 20.97  | 130.78      | 120.30   |
| 1   | A     | 88  | ARG  | NE-CZ-NH2 | -20.26 | 110.17      | 120.30   |
| 1   | E     | 27  | ARG  | NE-CZ-NH2 | -19.90 | 110.35      | 120.30   |
| 1   | C     | 88  | ARG  | CD-NE-CZ  | -18.23 | 98.08       | 123.60   |
| 1   | D     | 98  | ASP  | CB-CG-OD2 | -17.74 | 102.33      | 118.30   |
| 1   | F     | 61  | PHE  | CB-CG-CD2 | 17.61  | 133.13      | 120.80   |
| 1   | B     | 98  | ASP  | CB-CG-OD1 | 17.43  | 133.99      | 118.30   |
| 1   | F     | 58  | ARG  | NE-CZ-NH2 | -17.01 | 111.80      | 120.30   |

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| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | F     | 58  | ARG  | NE-CZ-NH1 | 16.83  | 128.72      | 120.30   |
| 1   | D     | 88  | ARG  | NE-CZ-NH2 | -16.61 | 111.99      | 120.30   |
| 1   | C     | 34  | ARG  | NE-CZ-NH1 | 16.21  | 128.41      | 120.30   |
| 1   | F     | 114 | ARG  | NE-CZ-NH2 | -15.42 | 112.59      | 120.30   |
| 1   | C     | 58  | ARG  | NE-CZ-NH1 | 15.30  | 127.95      | 120.30   |
| 1   | E     | 105 | ARG  | NE-CZ-NH1 | 14.80  | 127.70      | 120.30   |
| 1   | D     | 27  | ARG  | NE-CZ-NH1 | 14.47  | 127.53      | 120.30   |
| 1   | C     | 146 | ALA  | CB-CA-C   | -14.24 | 88.74       | 110.10   |
| 1   | A     | 27  | ARG  | NE-CZ-NH1 | 14.19  | 127.39      | 120.30   |
| 1   | F     | 18  | ARG  | NE-CZ-NH2 | -14.06 | 113.27      | 120.30   |
| 1   | C     | 6   | ARG  | NE-CZ-NH2 | -14.01 | 113.29      | 120.30   |
| 1   | B     | 108 | PHE  | CB-CG-CD2 | -13.90 | 111.07      | 120.80   |
| 1   | B     | 8   | PHE  | CB-CG-CD1 | -13.86 | 111.10      | 120.80   |
| 1   | C     | 88  | ARG  | NE-CZ-NH1 | -13.77 | 113.41      | 120.30   |
| 1   | D     | 88  | ARG  | NE-CZ-NH1 | 13.62  | 127.11      | 120.30   |
| 1   | A     | 88  | ARG  | NE-CZ-NH1 | 13.56  | 127.08      | 120.30   |
| 1   | B     | 121 | ASP  | CB-CG-OD1 | 13.49  | 130.44      | 118.30   |
| 1   | B     | 121 | ASP  | CB-CG-OD2 | -13.48 | 106.17      | 118.30   |
| 1   | C     | 14  | ASP  | CB-CG-OD1 | 13.37  | 130.33      | 118.30   |
| 1   | A     | 114 | ARG  | NE-CZ-NH2 | -13.31 | 113.64      | 120.30   |
| 1   | F     | 41  | MET  | CG-SD-CE  | 13.27  | 121.42      | 100.20   |
| 1   | B     | 151 | TYR  | CB-CG-CD1 | 13.21  | 128.93      | 121.00   |
| 1   | C     | 58  | ARG  | NE-CZ-NH2 | -13.20 | 113.70      | 120.30   |
| 1   | F     | 38  | MET  | CG-SD-CE  | -13.11 | 79.23       | 100.20   |
| 1   | E     | 90  | MET  | CG-SD-CE  | 12.92  | 120.88      | 100.20   |
| 1   | B     | 74  | VAL  | CA-CB-CG1 | -12.87 | 91.59       | 110.90   |
| 1   | F     | 67  | TYR  | CB-CG-CD1 | 12.77  | 128.66      | 121.00   |
| 1   | D     | 114 | ARG  | NE-CZ-NH2 | -12.66 | 113.97      | 120.30   |
| 1   | A     | 112 | VAL  | CB-CA-C   | -12.65 | 87.36       | 111.40   |
| 1   | F     | 36  | VAL  | CA-CB-CG1 | -12.63 | 91.96       | 110.90   |
| 1   | E     | 42  | ARG  | NE-CZ-NH2 | 12.51  | 126.55      | 120.30   |
| 1   | B     | 76  | MET  | CG-SD-CE  | -12.50 | 80.20       | 100.20   |
| 1   | D     | 41  | MET  | CG-SD-CE  | -12.49 | 80.22       | 100.20   |
| 1   | F     | 52  | TYR  | CB-CG-CD1 | -12.49 | 113.51      | 121.00   |
| 1   | F     | 42  | ARG  | NE-CZ-NH2 | -12.44 | 114.08      | 120.30   |
| 1   | F     | 105 | ARG  | NE-CZ-NH1 | 12.19  | 126.39      | 120.30   |
| 1   | B     | 151 | TYR  | CB-CG-CD2 | -12.14 | 113.71      | 121.00   |
| 1   | A     | 8   | PHE  | CB-CG-CD1 | -12.04 | 112.37      | 120.80   |
| 1   | A     | 151 | TYR  | CB-CG-CD1 | 12.00  | 128.20      | 121.00   |
| 1   | A     | 42  | ARG  | NE-CZ-NH2 | -11.94 | 114.33      | 120.30   |
| 1   | A     | 151 | TYR  | CB-CG-CD2 | -11.94 | 113.84      | 121.00   |
| 1   | B     | 105 | ARG  | NE-CZ-NH1 | -11.85 | 114.38      | 120.30   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | C     | 35  | LEU  | CB-CG-CD2  | 11.78  | 131.03      | 111.00   |
| 1   | D     | 58  | ARG  | NE-CZ-NH2  | -11.71 | 114.44      | 120.30   |
| 1   | A     | 34  | ARG  | NE-CZ-NH2  | 11.68  | 126.14      | 120.30   |
| 1   | E     | 98  | ASP  | CB-CG-OD2  | -11.56 | 107.90      | 118.30   |
| 1   | E     | 36  | VAL  | CA-CB-CG1  | -11.49 | 93.66       | 110.90   |
| 1   | E     | 122 | SER  | N-CA-CB    | 11.47  | 127.70      | 110.50   |
| 1   | C     | 67  | TYR  | CB-CG-CD2  | -11.38 | 114.17      | 121.00   |
| 1   | F     | 134 | PHE  | CB-CG-CD1  | 11.25  | 128.67      | 120.80   |
| 1   | C     | 89  | VAL  | CG1-CB-CG2 | 11.15  | 128.75      | 110.90   |
| 1   | E     | 54  | ASP  | CB-CG-OD1  | -11.13 | 108.28      | 118.30   |
| 1   | A     | 14  | ASP  | CB-CG-OD1  | -11.06 | 108.35      | 118.30   |
| 1   | C     | 97  | ALA  | CB-CA-C    | -11.03 | 93.56       | 110.10   |
| 1   | C     | 41  | MET  | CG-SD-CE   | -10.98 | 82.63       | 100.20   |
| 1   | D     | 67  | TYR  | CB-CG-CD1  | 10.90  | 127.54      | 121.00   |
| 1   | F     | 34  | ARG  | NE-CZ-NH2  | 10.82  | 125.71      | 120.30   |
| 1   | D     | 7   | THR  | CA-CB-CG2  | -10.81 | 97.26       | 112.40   |
| 1   | F     | 46  | ASP  | CB-CG-OD2  | -10.78 | 108.60      | 118.30   |
| 1   | B     | 7   | THR  | CA-CB-CG2  | -10.73 | 97.38       | 112.40   |
| 1   | F     | 151 | TYR  | CB-CG-CD2  | -10.71 | 114.57      | 121.00   |
| 1   | B     | 67  | TYR  | CB-CG-CD2  | -10.67 | 114.60      | 121.00   |
| 1   | C     | 27  | ARG  | NE-CZ-NH2  | -10.49 | 115.06      | 120.30   |
| 1   | E     | 67  | TYR  | CB-CG-CD1  | 10.49  | 127.29      | 121.00   |
| 1   | D     | 6   | ARG  | NE-CZ-NH1  | 10.49  | 125.54      | 120.30   |
| 1   | D     | 90  | MET  | CG-SD-CE   | 10.47  | 116.95      | 100.20   |
| 1   | F     | 35  | LEU  | CB-CA-C    | -10.41 | 90.42       | 110.20   |
| 1   | E     | 6   | ARG  | NE-CZ-NH2  | -10.32 | 115.14      | 120.30   |
| 1   | B     | 151 | TYR  | N-CA-CB    | 10.29  | 129.11      | 110.60   |
| 1   | F     | 132 | LEU  | CB-CG-CD1  | -10.24 | 93.59       | 111.00   |
| 1   | D     | 135 | HIS  | C-N-CD     | -10.03 | 98.54       | 120.60   |
| 1   | B     | 88  | ARG  | NE-CZ-NH1  | -10.01 | 115.29      | 120.30   |
| 1   | F     | 52  | TYR  | CB-CG-CD2  | 10.01  | 127.00      | 121.00   |
| 1   | C     | 115 | ASN  | C-N-CA     | 9.97   | 146.64      | 121.70   |
| 1   | B     | 8   | PHE  | CB-CG-CD2  | 9.94   | 127.76      | 120.80   |
| 1   | A     | 54  | ASP  | CB-CG-OD1  | 9.93   | 127.24      | 118.30   |
| 1   | C     | 67  | TYR  | CB-CG-CD1  | 9.92   | 126.95      | 121.00   |
| 1   | C     | 14  | ASP  | CB-CG-OD2  | -9.90  | 109.39      | 118.30   |
| 1   | E     | 54  | ASP  | CA-CB-CG   | -9.89  | 91.64       | 113.40   |
| 1   | A     | 42  | ARG  | NE-CZ-NH1  | 9.88   | 125.24      | 120.30   |
| 1   | B     | 84  | VAL  | CA-CB-CG1  | -9.81  | 96.18       | 110.90   |
| 1   | E     | 67  | TYR  | CB-CG-CD2  | -9.73  | 115.16      | 121.00   |
| 1   | E     | 103 | THR  | CA-CB-CG2  | 9.65   | 125.92      | 112.40   |
| 1   | E     | 76  | MET  | CG-SD-CE   | -9.65  | 84.76       | 100.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | E     | 126 | ALA  | CB-CA-C     | 9.62  | 124.54      | 110.10   |
| 1   | A     | 114 | ARG  | CG-CD-NE    | -9.59 | 91.65       | 111.80   |
| 1   | A     | 133 | TRP  | CD1-NE1-CE2 | -9.56 | 100.39      | 109.00   |
| 1   | A     | 24  | ILE  | CG1-CB-CG2  | -9.48 | 90.54       | 111.40   |
| 1   | D     | 114 | ARG  | CD-NE-CZ    | 9.46  | 136.85      | 123.60   |
| 1   | C     | 21  | ILE  | CG1-CB-CG2  | -9.44 | 90.64       | 111.40   |
| 1   | D     | 5   | GLU  | CB-CA-C     | -9.44 | 91.53       | 110.40   |
| 1   | E     | 27  | ARG  | NE-CZ-NH1   | 9.33  | 124.97      | 120.30   |
| 1   | E     | 16  | VAL  | CG1-CB-CG2  | -9.33 | 95.98       | 110.90   |
| 1   | B     | 114 | ARG  | NE-CZ-NH1   | 9.28  | 124.94      | 120.30   |
| 1   | F     | 114 | ARG  | NE-CZ-NH1   | 9.17  | 124.88      | 120.30   |
| 1   | C     | 6   | ARG  | NE-CZ-NH1   | 9.16  | 124.88      | 120.30   |
| 1   | C     | 7   | THR  | CA-CB-CG2   | -9.12 | 99.63       | 112.40   |
| 1   | D     | 121 | ASP  | CB-CA-C     | -9.09 | 92.22       | 110.40   |
| 1   | F     | 132 | LEU  | CB-CG-CD2   | 9.05  | 126.39      | 111.00   |
| 1   | B     | 48  | LEU  | CB-CG-CD1   | 9.04  | 126.36      | 111.00   |
| 1   | E     | 35  | LEU  | CB-CG-CD2   | 8.98  | 126.26      | 111.00   |
| 1   | C     | 95  | ASN  | CB-CA-C     | -8.97 | 92.46       | 110.40   |
| 1   | F     | 61  | PHE  | N-CA-CB     | 8.96  | 126.73      | 110.60   |
| 1   | D     | 77  | VAL  | CA-CB-CG1   | -8.95 | 97.48       | 110.90   |
| 1   | B     | 120 | SER  | N-CA-CB     | 8.91  | 123.87      | 110.50   |
| 1   | C     | 140 | VAL  | CG1-CB-CG2  | 8.90  | 125.14      | 110.90   |
| 1   | F     | 122 | SER  | N-CA-CB     | 8.89  | 123.84      | 110.50   |
| 1   | F     | 121 | ASP  | CB-CG-OD1   | 8.89  | 126.30      | 118.30   |
| 1   | B     | 79  | GLU  | OE1-CD-OE2  | -8.88 | 112.64      | 123.30   |
| 1   | A     | 18  | ARG  | NE-CZ-NH1   | 8.79  | 124.69      | 120.30   |
| 1   | E     | 117 | ILE  | CA-CB-CG2   | -8.78 | 93.33       | 110.90   |
| 1   | D     | 34  | ARG  | NE-CZ-NH1   | 8.76  | 124.68      | 120.30   |
| 1   | D     | 38  | MET  | CG-SD-CE    | -8.71 | 86.26       | 100.20   |
| 1   | A     | 18  | ARG  | NE-CZ-NH2   | 8.66  | 124.63      | 120.30   |
| 1   | B     | 100 | LYS  | CB-CA-C     | -8.58 | 93.24       | 110.40   |
| 1   | C     | 6   | ARG  | CA-CB-CG    | -8.55 | 94.58       | 113.40   |
| 1   | F     | 69  | HIS  | CB-CA-C     | 8.55  | 127.50      | 110.40   |
| 1   | F     | 27  | ARG  | NE-CZ-NH1   | -8.50 | 116.05      | 120.30   |
| 1   | E     | 10  | ALA  | CB-CA-C     | -8.46 | 97.41       | 110.10   |
| 1   | E     | 43  | ALA  | N-CA-CB     | 8.41  | 121.88      | 110.10   |
| 1   | B     | 94  | THR  | CA-CB-CG2   | -8.40 | 100.64      | 112.40   |
| 1   | F     | 73  | VAL  | CG1-CB-CG2  | 8.39  | 124.33      | 110.90   |
| 1   | F     | 62  | ALA  | CB-CA-C     | 8.39  | 122.69      | 110.10   |
| 1   | E     | 105 | ARG  | NE-CZ-NH2   | -8.36 | 116.12      | 120.30   |
| 1   | B     | 37  | ALA  | CB-CA-C     | -8.35 | 97.57       | 110.10   |
| 1   | E     | 77  | VAL  | O-C-N       | 8.35  | 136.06      | 122.70   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 127 | GLU  | CG-CD-OE2  | -8.34 | 101.63      | 118.30   |
| 1   | C     | 132 | LEU  | CB-CG-CD1  | -8.26 | 96.95       | 111.00   |
| 1   | C     | 27  | ARG  | NE-CZ-NH1  | 8.26  | 124.43      | 120.30   |
| 1   | E     | 108 | PHE  | CB-CG-CD1  | 8.25  | 126.57      | 120.80   |
| 1   | F     | 27  | ARG  | N-CA-CB    | -8.25 | 95.76       | 110.60   |
| 1   | D     | 67  | TYR  | CB-CG-CD2  | -8.24 | 116.05      | 121.00   |
| 1   | F     | 46  | ASP  | CB-CG-OD1  | 8.24  | 125.72      | 118.30   |
| 1   | B     | 143 | LYS  | CB-CA-C    | -8.22 | 93.95       | 110.40   |
| 1   | C     | 54  | ASP  | CB-CG-OD1  | -8.21 | 110.91      | 118.30   |
| 1   | D     | 68  | MET  | CG-SD-CE   | 8.21  | 113.33      | 100.20   |
| 1   | E     | 95  | ASN  | CB-CA-C    | -8.19 | 94.03       | 110.40   |
| 1   | C     | 67  | TYR  | N-CA-CB    | -8.18 | 95.88       | 110.60   |
| 1   | A     | 16  | VAL  | CA-CB-CG1  | 8.17  | 123.15      | 110.90   |
| 1   | A     | 18  | ARG  | NH1-CZ-NH2 | -8.16 | 110.42      | 119.40   |
| 1   | E     | 123 | VAL  | CA-CB-CG2  | -8.15 | 98.67       | 110.90   |
| 1   | F     | 114 | ARG  | CA-CB-CG   | -8.13 | 95.52       | 113.40   |
| 1   | B     | 125 | SER  | CB-CA-C    | 8.06  | 125.42      | 110.10   |
| 1   | F     | 152 | GLU  | N-CA-CB    | -8.05 | 96.11       | 110.60   |
| 1   | F     | 14  | ASP  | CB-CG-OD1  | 8.02  | 125.52      | 118.30   |
| 1   | F     | 137 | GLU  | CG-CD-OE2  | -8.02 | 102.26      | 118.30   |
| 1   | B     | 67  | TYR  | CB-CG-CD1  | 8.01  | 125.81      | 121.00   |
| 1   | F     | 88  | ARG  | CD-NE-CZ   | 8.00  | 134.80      | 123.60   |
| 1   | C     | 18  | ARG  | N-CA-CB    | -8.00 | 96.20       | 110.60   |
| 1   | C     | 98  | ASP  | CB-CG-OD2  | -7.98 | 111.12      | 118.30   |
| 1   | B     | 134 | PHE  | CB-CG-CD2  | -7.97 | 115.22      | 120.80   |
| 1   | B     | 30  | GLN  | CA-CB-CG   | -7.96 | 95.90       | 113.40   |
| 1   | C     | 46  | ASP  | CB-CG-OD2  | 7.93  | 125.44      | 118.30   |
| 1   | F     | 77  | VAL  | CA-CB-CG2  | -7.93 | 99.01       | 110.90   |
| 1   | E     | 115 | ASN  | CA-CB-CG   | -7.92 | 95.97       | 113.40   |
| 1   | B     | 115 | ASN  | C-N-CA     | 7.91  | 141.49      | 121.70   |
| 1   | E     | 93  | GLU  | N-CA-CB    | 7.90  | 124.83      | 110.60   |
| 1   | B     | 103 | THR  | CA-CB-CG2  | 7.89  | 123.45      | 112.40   |
| 1   | C     | 111 | GLN  | N-CA-CB    | -7.87 | 96.43       | 110.60   |
| 1   | E     | 136 | PRO  | N-CA-CB    | -7.86 | 93.86       | 103.30   |
| 1   | E     | 23  | GLU  | CG-CD-OE1  | 7.84  | 133.98      | 118.30   |
| 1   | C     | 105 | ARG  | NE-CZ-NH2  | -7.82 | 116.39      | 120.30   |
| 1   | C     | 66  | LYS  | CD-CE-NZ   | 7.80  | 129.64      | 111.70   |
| 1   | F     | 105 | ARG  | NE-CZ-NH2  | -7.80 | 116.40      | 120.30   |
| 1   | F     | 123 | VAL  | CG1-CB-CG2 | -7.80 | 98.42       | 110.90   |
| 1   | D     | 151 | TYR  | CB-CG-CD2  | -7.73 | 116.36      | 121.00   |
| 1   | B     | 132 | LEU  | CB-CA-C    | -7.72 | 95.54       | 110.20   |
| 1   | A     | 32  | GLY  | O-C-N      | -7.70 | 110.38      | 122.70   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | E     | 28  | PHE  | CB-CG-CD1  | 7.67  | 126.17      | 120.80   |
| 1   | C     | 134 | PHE  | CB-CA-C    | -7.67 | 95.07       | 110.40   |
| 1   | D     | 73  | VAL  | O-C-N      | 7.67  | 134.96      | 122.70   |
| 1   | D     | 89  | VAL  | CA-CB-CG2  | -7.67 | 99.40       | 110.90   |
| 1   | A     | 50  | GLU  | N-CA-CB    | -7.65 | 96.83       | 110.60   |
| 1   | D     | 97  | ALA  | CB-CA-C    | -7.64 | 98.64       | 110.10   |
| 1   | A     | 83  | VAL  | CB-CA-C    | -7.64 | 96.89       | 111.40   |
| 1   | F     | 67  | TYR  | CG-CD1-CE1 | -7.64 | 115.19      | 121.30   |
| 1   | A     | 142 | TYR  | O-C-N      | 7.63  | 134.91      | 122.70   |
| 1   | F     | 124 | GLU  | CB-CA-C    | -7.63 | 95.14       | 110.40   |
| 1   | B     | 33  | PHE  | N-CA-CB    | -7.62 | 96.88       | 110.60   |
| 1   | B     | 40  | PHE  | CG-CD2-CE2 | 7.62  | 129.18      | 120.80   |
| 1   | A     | 67  | TYR  | CB-CG-CD2  | -7.61 | 116.43      | 121.00   |
| 1   | A     | 18  | ARG  | CA-CB-CG   | -7.60 | 96.67       | 113.40   |
| 1   | A     | 68  | MET  | CG-SD-CE   | 7.60  | 112.36      | 100.20   |
| 1   | C     | 20  | LEU  | CB-CG-CD2  | -7.57 | 98.13       | 111.00   |
| 1   | F     | 61  | PHE  | CB-CG-CD1  | -7.54 | 115.52      | 120.80   |
| 1   | D     | 141 | ASN  | CB-CA-C    | 7.53  | 125.47      | 110.40   |
| 1   | E     | 60  | PHE  | CB-CG-CD1  | 7.52  | 126.06      | 120.80   |
| 1   | A     | 54  | ASP  | CB-CG-OD2  | -7.52 | 111.54      | 118.30   |
| 1   | C     | 70  | SER  | CB-CA-C    | -7.51 | 95.82       | 110.10   |
| 1   | B     | 105 | ARG  | NE-CZ-NH2  | 7.48  | 124.04      | 120.30   |
| 1   | A     | 38  | MET  | CG-SD-CE   | -7.45 | 88.29       | 100.20   |
| 1   | F     | 111 | GLN  | CG-CD-OE1  | -7.43 | 106.74      | 121.60   |
| 1   | D     | 18  | ARG  | NH1-CZ-NH2 | -7.42 | 111.23      | 119.40   |
| 1   | B     | 88  | ARG  | NH1-CZ-NH2 | 7.41  | 127.55      | 119.40   |
| 1   | F     | 10  | ALA  | CB-CA-C    | 7.39  | 121.19      | 110.10   |
| 1   | F     | 98  | ASP  | N-CA-CB    | -7.39 | 97.30       | 110.60   |
| 1   | D     | 35  | LEU  | CB-CA-C    | -7.38 | 96.18       | 110.20   |
| 1   | E     | 129 | GLU  | OE1-CD-OE2 | -7.38 | 114.45      | 123.30   |
| 1   | B     | 108 | PHE  | CB-CG-CD1  | 7.37  | 125.96      | 120.80   |
| 1   | B     | 124 | GLU  | O-C-N      | 7.36  | 134.47      | 122.70   |
| 1   | A     | 91  | LEU  | CB-CA-C    | -7.35 | 96.23       | 110.20   |
| 1   | A     | 134 | PHE  | N-CA-CB    | -7.33 | 97.40       | 110.60   |
| 1   | C     | 112 | VAL  | CA-CB-CG1  | 7.33  | 121.89      | 110.90   |
| 1   | D     | 90  | MET  | CA-CB-CG   | -7.31 | 100.86      | 113.30   |
| 1   | A     | 99  | SER  | CB-CA-C    | -7.31 | 96.21       | 110.10   |
| 1   | A     | 115 | ASN  | N-CA-C     | 7.30  | 130.72      | 111.00   |
| 1   | F     | 10  | ALA  | N-CA-CB    | -7.28 | 99.90       | 110.10   |
| 1   | A     | 13  | PRO  | N-CA-CB    | 7.27  | 112.03      | 103.30   |
| 1   | A     | 132 | LEU  | CB-CG-CD1  | 7.26  | 123.35      | 111.00   |
| 1   | D     | 11  | ILE  | O-C-N      | 7.25  | 134.29      | 122.70   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | C     | 103 | THR  | CA-CB-CG2   | -7.24 | 102.27      | 112.40   |
| 1   | A     | 61  | PHE  | CB-CG-CD1   | 7.22  | 125.86      | 120.80   |
| 1   | C     | 57  | ASP  | CB-CG-OD1   | -7.22 | 111.80      | 118.30   |
| 1   | A     | 103 | THR  | OG1-CB-CG2  | 7.21  | 126.58      | 110.00   |
| 1   | E     | 86  | THR  | CA-CB-CG2   | -7.21 | 102.31      | 112.40   |
| 1   | C     | 127 | GLU  | O-C-N       | 7.21  | 134.23      | 122.70   |
| 1   | B     | 27  | ARG  | NE-CZ-NH1   | 7.20  | 123.90      | 120.30   |
| 1   | F     | 142 | TYR  | CB-CG-CD2   | -7.20 | 116.68      | 121.00   |
| 1   | D     | 38  | MET  | O-C-N       | 7.19  | 134.21      | 122.70   |
| 1   | F     | 20  | LEU  | CB-CG-CD1   | -7.18 | 98.79       | 111.00   |
| 1   | E     | 98  | ASP  | CB-CG-OD1   | 7.17  | 124.75      | 118.30   |
| 1   | B     | 40  | PHE  | CB-CA-C     | -7.16 | 96.07       | 110.40   |
| 1   | C     | 120 | SER  | N-CA-CB     | 7.16  | 121.24      | 110.50   |
| 1   | A     | 34  | ARG  | NH1-CZ-NH2  | -7.12 | 111.56      | 119.40   |
| 1   | A     | 27  | ARG  | NE-CZ-NH2   | -7.12 | 116.74      | 120.30   |
| 1   | F     | 14  | ASP  | CB-CG-OD2   | -7.12 | 111.90      | 118.30   |
| 1   | A     | 142 | TYR  | N-CA-CB     | 7.11  | 123.40      | 110.60   |
| 1   | D     | 90  | MET  | C-N-CA      | 7.10  | 139.44      | 121.70   |
| 1   | B     | 76  | MET  | O-C-N       | 7.09  | 134.04      | 122.70   |
| 1   | D     | 152 | GLU  | CA-C-O      | -7.08 | 105.23      | 120.10   |
| 1   | D     | 133 | TRP  | CD1-NE1-CE2 | -7.08 | 102.63      | 109.00   |
| 1   | E     | 135 | HIS  | N-CA-CB     | 7.07  | 123.33      | 110.60   |
| 1   | B     | 141 | ASN  | CB-CA-C     | 7.07  | 124.54      | 110.40   |
| 1   | A     | 149 | TRP  | CH2-CZ2-CE2 | -7.07 | 110.33      | 117.40   |
| 1   | F     | 86  | THR  | CA-CB-CG2   | -7.05 | 102.53      | 112.40   |
| 1   | F     | 61  | PHE  | C-N-CA      | -7.05 | 104.07      | 121.70   |
| 1   | F     | 88  | ARG  | NE-CZ-NH2   | -7.04 | 116.78      | 120.30   |
| 1   | B     | 134 | PHE  | CA-C-N      | -7.03 | 101.74      | 117.20   |
| 1   | C     | 101 | PRO  | N-CA-CB     | 7.02  | 111.73      | 103.30   |
| 1   | B     | 141 | ASN  | N-CA-CB     | 7.02  | 123.23      | 110.60   |
| 1   | C     | 28  | PHE  | CA-CB-CG    | -7.01 | 97.07       | 113.90   |
| 1   | B     | 73  | VAL  | CA-CB-CG1   | -7.01 | 100.39      | 110.90   |
| 1   | A     | 61  | PHE  | CB-CG-CD2   | -7.00 | 115.90      | 120.80   |
| 1   | E     | 42  | ARG  | O-C-N       | -7.00 | 111.51      | 122.70   |
| 1   | A     | 2   | ALA  | O-C-N       | 6.98  | 133.86      | 122.70   |
| 1   | D     | 35  | LEU  | CB-CG-CD2   | 6.97  | 122.85      | 111.00   |
| 1   | A     | 121 | ASP  | CB-CG-OD2   | -6.96 | 112.04      | 118.30   |
| 1   | D     | 69  | HIS  | O-C-N       | 6.96  | 133.83      | 122.70   |
| 1   | F     | 44  | SER  | N-CA-CB     | 6.93  | 120.90      | 110.50   |
| 1   | A     | 139 | LEU  | O-C-N       | 6.93  | 133.78      | 122.70   |
| 1   | C     | 34  | ARG  | NH1-CZ-NH2  | -6.92 | 111.78      | 119.40   |
| 1   | C     | 84  | VAL  | CA-CB-CG2   | -6.92 | 100.53      | 110.90   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | E     | 118 | HIS  | O-C-N      | 6.92  | 134.96      | 123.20   |
| 1   | B     | 118 | HIS  | CB-CA-C    | -6.92 | 96.57       | 110.40   |
| 1   | F     | 60  | PHE  | CB-CG-CD1  | -6.90 | 115.97      | 120.80   |
| 1   | C     | 29  | GLU  | CG-CD-OE1  | -6.87 | 104.57      | 118.30   |
| 1   | A     | 21  | ILE  | CA-CB-CG2  | 6.86  | 124.62      | 110.90   |
| 1   | E     | 2   | ALA  | N-CA-CB    | 6.84  | 119.67      | 110.10   |
| 1   | B     | 124 | GLU  | CB-CA-C    | -6.83 | 96.74       | 110.40   |
| 1   | A     | 4   | SER  | CB-CA-C    | 6.81  | 123.04      | 110.10   |
| 1   | D     | 143 | LYS  | CD-CE-NZ   | 6.81  | 127.35      | 111.70   |
| 1   | C     | 42  | ARG  | CB-CA-C    | -6.80 | 96.81       | 110.40   |
| 1   | E     | 38  | MET  | CG-SD-CE   | 6.78  | 111.05      | 100.20   |
| 1   | B     | 111 | GLN  | N-CA-CB    | -6.77 | 98.41       | 110.60   |
| 1   | C     | 63  | GLY  | O-C-N      | 6.76  | 133.52      | 122.70   |
| 1   | D     | 139 | LEU  | CB-CG-CD2  | -6.76 | 99.52       | 111.00   |
| 1   | D     | 2   | ALA  | CB-CA-C    | -6.75 | 99.97       | 110.10   |
| 1   | B     | 54  | ASP  | CB-CG-OD1  | -6.75 | 112.22      | 118.30   |
| 1   | C     | 113 | GLY  | CA-C-O     | 6.74  | 132.74      | 120.60   |
| 1   | A     | 85  | LYS  | N-CA-CB    | -6.74 | 98.46       | 110.60   |
| 1   | D     | 134 | PHE  | N-CA-CB    | -6.74 | 98.47       | 110.60   |
| 1   | C     | 136 | PRO  | CB-CA-C    | -6.73 | 95.18       | 112.00   |
| 1   | E     | 116 | ILE  | CA-CB-CG2  | -6.71 | 97.48       | 110.90   |
| 1   | A     | 3   | ASN  | CB-CA-C    | -6.70 | 96.99       | 110.40   |
| 1   | F     | 120 | SER  | N-CA-CB    | 6.70  | 120.55      | 110.50   |
| 1   | E     | 88  | ARG  | CA-CB-CG   | -6.69 | 98.68       | 113.40   |
| 1   | B     | 134 | PHE  | N-CA-CB    | 6.68  | 122.62      | 110.60   |
| 1   | E     | 18  | ARG  | NE-CZ-NH1  | 6.68  | 123.64      | 120.30   |
| 1   | A     | 55  | LEU  | N-CA-CB    | -6.68 | 97.05       | 110.40   |
| 1   | C     | 114 | ARG  | NE-CZ-NH2  | -6.67 | 116.96      | 120.30   |
| 1   | F     | 121 | ASP  | CB-CG-OD2  | -6.67 | 112.30      | 118.30   |
| 1   | C     | 150 | ILE  | CA-CB-CG2  | -6.67 | 97.57       | 110.90   |
| 1   | D     | 10  | ALA  | N-CA-CB    | 6.67  | 119.43      | 110.10   |
| 1   | C     | 151 | TYR  | CB-CG-CD1  | 6.66  | 125.00      | 121.00   |
| 1   | F     | 77  | VAL  | CG1-CB-CG2 | 6.65  | 121.54      | 110.90   |
| 1   | E     | 151 | TYR  | CG-CD2-CE2 | -6.65 | 115.98      | 121.30   |
| 1   | D     | 130 | ILE  | CB-CA-C    | -6.64 | 98.32       | 111.60   |
| 1   | A     | 67  | TYR  | CB-CA-C    | 6.64  | 123.67      | 110.40   |
| 1   | C     | 151 | TYR  | CB-CG-CD2  | -6.63 | 117.02      | 121.00   |
| 1   | C     | 139 | LEU  | CB-CG-CD2  | -6.62 | 99.75       | 111.00   |
| 1   | D     | 18  | ARG  | NE-CZ-NH1  | -6.61 | 117.00      | 120.30   |
| 1   | E     | 39  | LYS  | CD-CE-NZ   | 6.59  | 126.86      | 111.70   |
| 1   | E     | 115 | ASN  | CB-CG-OD1  | -6.59 | 108.43      | 121.60   |
| 1   | C     | 83  | VAL  | CA-CB-CG2  | 6.58  | 120.78      | 110.90   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | F     | 77  | VAL  | N-CA-CB    | 6.58  | 125.98      | 111.50   |
| 1   | E     | 17  | GLN  | CA-CB-CG   | -6.57 | 98.95       | 113.40   |
| 1   | A     | 140 | VAL  | CA-CB-CG2  | 6.56  | 120.74      | 110.90   |
| 1   | C     | 93  | GLU  | CG-CD-OE2  | -6.55 | 105.19      | 118.30   |
| 1   | D     | 102 | GLY  | CA-C-O     | 6.55  | 132.40      | 120.60   |
| 1   | A     | 151 | TYR  | O-C-N      | 6.54  | 133.17      | 122.70   |
| 1   | B     | 148 | ASN  | CB-CA-C    | -6.54 | 97.31       | 110.40   |
| 1   | F     | 34  | ARG  | NH1-CZ-NH2 | -6.53 | 112.21      | 119.40   |
| 1   | D     | 47  | LEU  | CB-CG-CD1  | -6.53 | 99.91       | 111.00   |
| 1   | F     | 5   | GLU  | CG-CD-OE2  | -6.52 | 105.26      | 118.30   |
| 1   | B     | 140 | VAL  | CG1-CB-CG2 | -6.51 | 100.48      | 110.90   |
| 1   | F     | 40  | PHE  | CB-CA-C    | -6.51 | 97.38       | 110.40   |
| 1   | A     | 122 | SER  | N-CA-CB    | 6.51  | 120.26      | 110.50   |
| 1   | E     | 34  | ARG  | NE-CZ-NH1  | 6.51  | 123.55      | 120.30   |
| 1   | D     | 81  | LEU  | CB-CG-CD2  | -6.50 | 99.95       | 111.00   |
| 1   | A     | 151 | TYR  | CA-C-N     | -6.50 | 102.91      | 117.20   |
| 1   | B     | 134 | PHE  | CB-CG-CD1  | 6.49  | 125.34      | 120.80   |
| 1   | E     | 18  | ARG  | CD-NE-CZ   | 6.49  | 132.69      | 123.60   |
| 1   | F     | 57  | ASP  | O-C-N      | 6.49  | 133.09      | 122.70   |
| 1   | F     | 137 | GLU  | CG-CD-OE1  | 6.49  | 131.28      | 118.30   |
| 1   | E     | 30  | GLN  | CA-CB-CG   | -6.49 | 99.13       | 113.40   |
| 1   | F     | 150 | ILE  | CA-C-N     | -6.48 | 102.94      | 117.20   |
| 1   | F     | 100 | LYS  | N-CA-CB    | -6.48 | 98.94       | 110.60   |
| 1   | A     | 37  | ALA  | CB-CA-C    | -6.47 | 100.39      | 110.10   |
| 1   | E     | 85  | LYS  | N-CA-CB    | -6.45 | 98.99       | 110.60   |
| 1   | D     | 42  | ARG  | C-N-CA     | -6.44 | 105.59      | 121.70   |
| 1   | D     | 90  | MET  | O-C-N      | 6.44  | 133.01      | 122.70   |
| 1   | D     | 133 | TRP  | O-C-N      | 6.42  | 132.98      | 122.70   |
| 1   | D     | 86  | THR  | CA-CB-CG2  | -6.42 | 103.42      | 112.40   |
| 1   | D     | 88  | ARG  | CD-NE-CZ   | 6.40  | 132.56      | 123.60   |
| 1   | F     | 27  | ARG  | CG-CD-NE   | 6.40  | 125.23      | 111.80   |
| 1   | D     | 117 | ILE  | CA-CB-CG1  | 6.38  | 123.12      | 111.00   |
| 1   | C     | 124 | GLU  | CA-CB-CG   | -6.37 | 99.39       | 113.40   |
| 1   | F     | 67  | TYR  | CZ-CE2-CD2 | -6.37 | 114.07      | 119.80   |
| 1   | D     | 28  | PHE  | CE1-CZ-CE2 | -6.36 | 108.55      | 120.00   |
| 1   | B     | 59  | PRO  | CB-CA-C    | -6.35 | 96.11       | 112.00   |
| 1   | E     | 151 | TYR  | CZ-CE2-CD2 | 6.35  | 125.51      | 119.80   |
| 1   | B     | 72  | PRO  | N-CD-CG    | 6.33  | 112.70      | 103.20   |
| 1   | C     | 58  | ARG  | CD-NE-CZ   | 6.32  | 132.44      | 123.60   |
| 1   | A     | 121 | ASP  | CB-CA-C    | -6.32 | 97.77       | 110.40   |
| 1   | B     | 88  | ARG  | NE-CZ-NH2  | -6.31 | 117.15      | 120.30   |
| 1   | A     | 114 | ARG  | NH1-CZ-NH2 | 6.30  | 126.33      | 119.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | F     | 65  | VAL  | CA-CB-CG2  | -6.29 | 101.46      | 110.90   |
| 1   | A     | 127 | GLU  | CA-CB-CG   | -6.29 | 99.56       | 113.40   |
| 1   | E     | 118 | HIS  | CA-C-N     | -6.29 | 103.62      | 116.20   |
| 1   | A     | 142 | TYR  | N-CA-C     | -6.29 | 94.02       | 111.00   |
| 1   | B     | 72  | PRO  | CA-N-CD    | -6.29 | 102.70      | 111.50   |
| 1   | C     | 132 | LEU  | N-CA-CB    | -6.28 | 97.85       | 110.40   |
| 1   | C     | 122 | SER  | CA-C-N     | -6.27 | 103.40      | 117.20   |
| 1   | A     | 133 | TRP  | O-C-N      | 6.27  | 132.73      | 122.70   |
| 1   | E     | 37  | ALA  | CB-CA-C    | -6.26 | 100.71      | 110.10   |
| 1   | D     | 80  | GLY  | CA-C-O     | 6.26  | 131.86      | 120.60   |
| 1   | E     | 107 | ASP  | CB-CG-OD2  | -6.25 | 112.68      | 118.30   |
| 1   | C     | 146 | ALA  | N-CA-CB    | -6.24 | 101.36      | 110.10   |
| 1   | D     | 38  | MET  | CB-CA-C    | -6.24 | 97.92       | 110.40   |
| 1   | A     | 63  | GLY  | O-C-N      | 6.24  | 132.68      | 122.70   |
| 1   | F     | 16  | VAL  | CA-CB-CG1  | 6.24  | 120.25      | 110.90   |
| 1   | D     | 40  | PHE  | CB-CG-CD2  | -6.23 | 116.44      | 120.80   |
| 1   | F     | 78  | TRP  | O-C-N      | 6.22  | 132.66      | 122.70   |
| 1   | C     | 29  | GLU  | N-CA-CB    | 6.22  | 121.79      | 110.60   |
| 1   | D     | 133 | TRP  | CA-C-N     | -6.21 | 103.53      | 117.20   |
| 1   | A     | 136 | PRO  | O-C-N      | -6.20 | 112.78      | 122.70   |
| 1   | E     | 136 | PRO  | C-N-CA     | -6.20 | 106.19      | 121.70   |
| 1   | B     | 76  | MET  | CA-C-N     | -6.19 | 103.59      | 117.20   |
| 1   | C     | 91  | LEU  | N-CA-CB    | -6.19 | 98.03       | 110.40   |
| 1   | B     | 58  | ARG  | NE-CZ-NH2  | 6.18  | 123.39      | 120.30   |
| 1   | B     | 55  | LEU  | C-N-CA     | 6.18  | 137.14      | 121.70   |
| 1   | D     | 83  | VAL  | CB-CA-C    | -6.18 | 99.67       | 111.40   |
| 1   | B     | 123 | VAL  | CB-CA-C    | 6.17  | 123.13      | 111.40   |
| 1   | C     | 110 | ILE  | C-N-CA     | -6.17 | 106.28      | 121.70   |
| 1   | C     | 70  | SER  | O-C-N      | 6.16  | 133.67      | 123.20   |
| 1   | F     | 31  | LYS  | N-CA-CB    | -6.16 | 99.52       | 110.60   |
| 1   | B     | 36  | VAL  | CA-CB-CG1  | -6.16 | 101.67      | 110.90   |
| 1   | E     | 81  | LEU  | CB-CG-CD1  | 6.15  | 121.46      | 111.00   |
| 1   | F     | 144 | SER  | CB-CA-C    | -6.14 | 98.43       | 110.10   |
| 1   | D     | 102 | GLY  | O-C-N      | -6.14 | 112.88      | 122.70   |
| 1   | D     | 151 | TYR  | O-C-N      | 6.14  | 132.52      | 122.70   |
| 1   | C     | 46  | ASP  | CB-CA-C    | 6.13  | 122.66      | 110.40   |
| 1   | E     | 140 | VAL  | CA-CB-CG2  | -6.12 | 101.71      | 110.90   |
| 1   | E     | 61  | PHE  | N-CA-CB    | 6.12  | 121.62      | 110.60   |
| 1   | B     | 112 | VAL  | CG1-CB-CG2 | 6.12  | 120.69      | 110.90   |
| 1   | F     | 23  | GLU  | CB-CA-C    | -6.12 | 98.17       | 110.40   |
| 1   | C     | 39  | LYS  | O-C-N      | 6.11  | 132.48      | 122.70   |
| 1   | C     | 108 | PHE  | C-N-CA     | -6.11 | 106.43      | 121.70   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | B     | 137 | GLU  | CG-CD-OE2   | -6.10 | 106.09      | 118.30   |
| 1   | E     | 34  | ARG  | CB-CA-C     | 6.09  | 122.59      | 110.40   |
| 1   | E     | 93  | GLU  | CA-C-O      | 6.09  | 132.88      | 120.10   |
| 1   | E     | 115 | ASN  | O-C-N       | 6.08  | 132.43      | 122.70   |
| 1   | A     | 98  | ASP  | CB-CA-C     | 6.08  | 122.56      | 110.40   |
| 1   | D     | 74  | VAL  | CG1-CB-CG2  | -6.07 | 101.18      | 110.90   |
| 1   | B     | 138 | GLU  | OE1-CD-OE2  | 6.07  | 130.59      | 123.30   |
| 1   | D     | 115 | ASN  | C-N-CA      | 6.07  | 136.88      | 121.70   |
| 1   | F     | 4   | SER  | CB-CA-C     | -6.06 | 98.59       | 110.10   |
| 1   | B     | 131 | ALA  | O-C-N       | 6.05  | 132.39      | 122.70   |
| 1   | E     | 77  | VAL  | CA-CB-CG2   | -6.04 | 101.84      | 110.90   |
| 1   | D     | 27  | ARG  | CG-CD-NE    | 6.04  | 124.48      | 111.80   |
| 1   | D     | 143 | LYS  | CA-CB-CG    | 6.04  | 126.68      | 113.40   |
| 1   | B     | 142 | TYR  | CB-CG-CD2   | 6.03  | 124.62      | 121.00   |
| 1   | E     | 128 | LYS  | CB-CG-CD    | 6.03  | 127.28      | 111.60   |
| 1   | F     | 37  | ALA  | O-C-N       | -6.03 | 113.05      | 122.70   |
| 1   | A     | 101 | PRO  | N-CA-CB     | 6.03  | 110.53      | 103.30   |
| 1   | B     | 40  | PHE  | O-C-N       | 6.03  | 132.35      | 122.70   |
| 1   | B     | 133 | TRP  | CB-CG-CD2   | -6.03 | 118.76      | 126.60   |
| 1   | C     | 86  | THR  | CA-CB-CG2   | -6.02 | 103.97      | 112.40   |
| 1   | D     | 55  | LEU  | CA-CB-CG    | -6.02 | 101.46      | 115.30   |
| 1   | B     | 11  | ILE  | CB-CA-C     | -6.01 | 99.57       | 111.60   |
| 1   | D     | 54  | ASP  | CB-CG-OD2   | -6.01 | 112.89      | 118.30   |
| 1   | B     | 47  | LEU  | CB-CG-CD2   | -5.99 | 100.82      | 111.00   |
| 1   | B     | 122 | SER  | N-CA-CB     | 5.99  | 119.49      | 110.50   |
| 1   | C     | 127 | GLU  | CG-CD-OE1   | 5.98  | 130.26      | 118.30   |
| 1   | C     | 56  | LYS  | CB-CA-C     | 5.98  | 122.36      | 110.40   |
| 1   | B     | 76  | MET  | N-CA-CB     | 5.97  | 121.35      | 110.60   |
| 1   | B     | 26  | LYS  | O-C-N       | -5.97 | 113.14      | 122.70   |
| 1   | E     | 14  | ASP  | N-CA-CB     | 5.97  | 121.35      | 110.60   |
| 1   | E     | 78  | TRP  | CE3-CZ3-CH2 | -5.97 | 114.64      | 121.20   |
| 1   | B     | 86  | THR  | CA-CB-CG2   | -5.96 | 104.05      | 112.40   |
| 1   | E     | 151 | TYR  | CG-CD1-CE1  | 5.96  | 126.07      | 121.30   |
| 1   | C     | 57  | ASP  | CB-CG-OD2   | 5.96  | 123.67      | 118.30   |
| 1   | D     | 127 | GLU  | CG-CD-OE1   | 5.95  | 130.21      | 118.30   |
| 1   | A     | 27  | ARG  | CG-CD-NE    | 5.95  | 124.29      | 111.80   |
| 1   | B     | 35  | LEU  | CD1-CG-CD2  | 5.95  | 128.35      | 110.50   |
| 1   | B     | 123 | VAL  | CA-CB-CG1   | 5.95  | 119.82      | 110.90   |
| 1   | B     | 134 | PHE  | O-C-N       | 5.95  | 132.22      | 122.70   |
| 1   | E     | 21  | ILE  | CA-CB-CG2   | 5.95  | 122.79      | 110.90   |
| 1   | D     | 149 | TRP  | CB-CG-CD2   | -5.94 | 118.87      | 126.60   |
| 1   | E     | 145 | CYS  | CA-C-N      | -5.94 | 104.13      | 117.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 77  | VAL  | CA-CB-CG2   | 5.93  | 119.80      | 110.90   |
| 1   | E     | 110 | ILE  | CB-CA-C     | -5.93 | 99.74       | 111.60   |
| 1   | B     | 60  | PHE  | O-C-N       | 5.92  | 132.17      | 122.70   |
| 1   | B     | 58  | ARG  | O-C-N       | 5.91  | 132.33      | 121.10   |
| 1   | B     | 37  | ALA  | N-CA-CB     | -5.90 | 101.85      | 110.10   |
| 1   | F     | 150 | ILE  | O-C-N       | 5.89  | 132.12      | 122.70   |
| 1   | B     | 117 | ILE  | CG1-CB-CG2  | -5.89 | 98.45       | 111.40   |
| 1   | C     | 65  | VAL  | C-N-CA      | -5.88 | 106.99      | 121.70   |
| 1   | D     | 46  | ASP  | CB-CG-OD2   | 5.88  | 123.59      | 118.30   |
| 1   | A     | 58  | ARG  | CA-CB-CG    | -5.87 | 100.48      | 113.40   |
| 1   | B     | 91  | LEU  | CA-C-N      | -5.87 | 104.46      | 116.20   |
| 1   | C     | 112 | VAL  | O-C-N       | -5.87 | 113.22      | 123.20   |
| 1   | C     | 34  | ARG  | CG-CD-NE    | 5.87  | 124.12      | 111.80   |
| 1   | A     | 94  | THR  | CA-CB-CG2   | -5.86 | 104.19      | 112.40   |
| 1   | F     | 34  | ARG  | CB-CA-C     | -5.86 | 98.69       | 110.40   |
| 1   | B     | 42  | ARG  | NE-CZ-NH2   | -5.85 | 117.38      | 120.30   |
| 1   | B     | 116 | ILE  | CA-CB-CG1   | -5.85 | 99.89       | 111.00   |
| 1   | F     | 27  | ARG  | NE-CZ-NH2   | 5.85  | 123.22      | 120.30   |
| 1   | F     | 26  | LYS  | CB-CG-CD    | -5.84 | 96.40       | 111.60   |
| 1   | E     | 84  | VAL  | CG1-CB-CG2  | 5.84  | 120.25      | 110.90   |
| 1   | B     | 91  | LEU  | C-N-CA      | -5.84 | 110.03      | 122.30   |
| 1   | A     | 107 | ASP  | CB-CG-OD1   | 5.84  | 123.56      | 118.30   |
| 1   | B     | 100 | LYS  | N-CA-CB     | -5.83 | 100.10      | 110.60   |
| 1   | C     | 27  | ARG  | CG-CD-NE    | 5.83  | 124.03      | 111.80   |
| 1   | D     | 93  | GLU  | CA-CB-CG    | -5.83 | 100.58      | 113.40   |
| 1   | E     | 44  | SER  | C-N-CA      | -5.83 | 107.14      | 121.70   |
| 1   | A     | 35  | LEU  | CB-CG-CD1   | 5.82  | 120.90      | 111.00   |
| 1   | B     | 45  | GLU  | OE1-CD-OE2  | 5.81  | 130.27      | 123.30   |
| 1   | D     | 126 | ALA  | CB-CA-C     | 5.81  | 118.81      | 110.10   |
| 1   | D     | 115 | ASN  | CA-CB-CG    | -5.80 | 100.63      | 113.40   |
| 1   | E     | 78  | TRP  | CD2-CE2-CZ2 | -5.80 | 115.33      | 122.30   |
| 1   | E     | 65  | VAL  | CA-CB-CG2   | 5.80  | 119.60      | 110.90   |
| 1   | F     | 29  | GLU  | CA-CB-CG    | -5.80 | 100.65      | 113.40   |
| 1   | C     | 76  | MET  | CB-CA-C     | -5.79 | 98.81       | 110.40   |
| 1   | F     | 42  | ARG  | NH1-CZ-NH2  | 5.79  | 125.77      | 119.40   |
| 1   | A     | 31  | LYS  | N-CA-CB     | 5.79  | 121.02      | 110.60   |
| 1   | D     | 6   | ARG  | NE-CZ-NH2   | -5.78 | 117.41      | 120.30   |
| 1   | C     | 26  | LYS  | O-C-N       | -5.77 | 113.47      | 122.70   |
| 1   | F     | 41  | MET  | CA-CB-CG    | -5.77 | 103.50      | 113.30   |
| 1   | A     | 64  | LEU  | CB-CA-C     | 5.77  | 121.16      | 110.20   |
| 1   | A     | 34  | ARG  | CG-CD-NE    | 5.76  | 123.90      | 111.80   |
| 1   | E     | 121 | ASP  | CB-CG-OD1   | 5.76  | 123.48      | 118.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 40  | PHE  | CZ-CE2-CD2 | -5.76 | 113.19      | 120.10   |
| 1   | F     | 107 | ASP  | N-CA-CB    | -5.76 | 100.24      | 110.60   |
| 1   | C     | 136 | PRO  | O-C-N      | 5.75  | 131.91      | 122.70   |
| 1   | C     | 48  | LEU  | CB-CA-C    | 5.75  | 121.12      | 110.20   |
| 1   | C     | 105 | ARG  | NH1-CZ-NH2 | 5.75  | 125.72      | 119.40   |
| 1   | D     | 132 | LEU  | CB-CG-CD1  | 5.75  | 120.77      | 111.00   |
| 1   | D     | 28  | PHE  | CZ-CE2-CD2 | 5.75  | 127.00      | 120.10   |
| 1   | A     | 73  | VAL  | O-C-N      | 5.74  | 131.89      | 122.70   |
| 1   | A     | 142 | TYR  | CA-C-N     | -5.74 | 104.58      | 117.20   |
| 1   | B     | 138 | GLU  | CG-CD-OE2  | -5.73 | 106.83      | 118.30   |
| 1   | D     | 108 | PHE  | C-N-CA     | -5.73 | 107.37      | 121.70   |
| 1   | C     | 50  | GLU  | CG-CD-OE1  | -5.73 | 106.84      | 118.30   |
| 1   | D     | 57  | ASP  | CB-CG-OD1  | -5.73 | 113.14      | 118.30   |
| 1   | D     | 134 | PHE  | CB-CG-CD2  | -5.73 | 116.79      | 120.80   |
| 1   | F     | 93  | GLU  | CG-CD-OE2  | -5.73 | 106.85      | 118.30   |
| 1   | D     | 100 | LYS  | CA-C-O     | 5.73  | 132.12      | 120.10   |
| 1   | B     | 129 | GLU  | CB-CA-C    | -5.72 | 98.95       | 110.40   |
| 1   | B     | 90  | MET  | O-C-N      | 5.72  | 131.86      | 122.70   |
| 1   | B     | 152 | GLU  | N-CA-CB    | 5.71  | 120.88      | 110.60   |
| 1   | A     | 88  | ARG  | CA-C-N     | -5.70 | 104.65      | 117.20   |
| 1   | E     | 68  | MET  | CA-CB-CG   | -5.70 | 103.60      | 113.30   |
| 1   | A     | 63  | GLY  | CA-C-N     | -5.70 | 104.66      | 117.20   |
| 1   | A     | 112 | VAL  | CA-CB-CG1  | -5.69 | 102.36      | 110.90   |
| 1   | C     | 108 | PHE  | CG-CD1-CE1 | 5.69  | 127.06      | 120.80   |
| 1   | D     | 79  | GLU  | C-N-CA     | -5.69 | 110.34      | 122.30   |
| 1   | F     | 44  | SER  | O-C-N      | 5.69  | 131.81      | 122.70   |
| 1   | C     | 87  | GLY  | C-N-CA     | -5.69 | 107.48      | 121.70   |
| 1   | A     | 35  | LEU  | N-CA-C     | -5.68 | 95.66       | 111.00   |
| 1   | D     | 8   | PHE  | O-C-N      | 5.68  | 131.78      | 122.70   |
| 1   | E     | 38  | MET  | CA-C-O     | 5.67  | 132.02      | 120.10   |
| 1   | E     | 122 | SER  | C-N-CA     | -5.67 | 107.52      | 121.70   |
| 1   | C     | 68  | MET  | CG-SD-CE   | 5.67  | 109.27      | 100.20   |
| 1   | B     | 127 | GLU  | CG-CD-OE2  | -5.67 | 106.97      | 118.30   |
| 1   | C     | 84  | VAL  | O-C-N      | 5.67  | 131.76      | 122.70   |
| 1   | A     | 98  | ASP  | N-CA-CB    | 5.66  | 120.79      | 110.60   |
| 1   | E     | 55  | LEU  | N-CA-CB    | 5.66  | 121.72      | 110.40   |
| 1   | A     | 147 | GLN  | N-CA-CB    | -5.65 | 100.42      | 110.60   |
| 1   | E     | 135 | HIS  | CA-C-O     | 5.65  | 131.97      | 120.10   |
| 1   | E     | 88  | ARG  | O-C-N      | 5.65  | 131.74      | 122.70   |
| 1   | B     | 46  | ASP  | CB-CG-OD2  | 5.65  | 123.38      | 118.30   |
| 1   | B     | 51  | HIS  | CA-CB-CG   | 5.64  | 123.20      | 113.60   |
| 1   | F     | 35  | LEU  | N-CA-CB    | 5.64  | 121.69      | 110.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | F     | 11  | ILE  | CB-CA-C    | -5.64 | 100.32      | 111.60   |
| 1   | C     | 65  | VAL  | O-C-N      | -5.64 | 113.68      | 122.70   |
| 1   | D     | 84  | VAL  | CA-CB-CG2  | 5.63  | 119.35      | 110.90   |
| 1   | D     | 82  | ASN  | CA-CB-CG   | 5.63  | 125.79      | 113.40   |
| 1   | C     | 107 | ASP  | CB-CG-OD2  | -5.63 | 113.23      | 118.30   |
| 1   | B     | 108 | PHE  | CB-CA-C    | -5.62 | 99.16       | 110.40   |
| 1   | E     | 18  | ARG  | O-C-N      | -5.62 | 113.64      | 123.20   |
| 1   | F     | 122 | SER  | CA-C-N     | -5.62 | 104.83      | 117.20   |
| 1   | C     | 121 | ASP  | CB-CG-OD2  | -5.62 | 113.25      | 118.30   |
| 1   | F     | 142 | TYR  | CB-CG-CD1  | 5.60  | 124.36      | 121.00   |
| 1   | B     | 67  | TYR  | CB-CA-C    | -5.59 | 99.22       | 110.40   |
| 1   | A     | 29  | GLU  | CB-CA-C    | -5.59 | 99.23       | 110.40   |
| 1   | C     | 38  | MET  | CG-SD-CE   | 5.59  | 109.14      | 100.20   |
| 1   | E     | 125 | SER  | CA-CB-OG   | -5.58 | 96.12       | 111.20   |
| 1   | B     | 79  | GLU  | CG-CD-OE1  | 5.58  | 129.47      | 118.30   |
| 1   | E     | 149 | TRP  | CA-CB-CG   | -5.58 | 103.09      | 113.70   |
| 1   | A     | 48  | LEU  | C-N-CA     | -5.58 | 107.75      | 121.70   |
| 1   | C     | 28  | PHE  | CB-CG-CD1  | 5.58  | 124.70      | 120.80   |
| 1   | B     | 121 | ASP  | O-C-N      | -5.57 | 113.79      | 122.70   |
| 1   | F     | 119 | GLY  | CA-C-O     | -5.57 | 110.58      | 120.60   |
| 1   | B     | 2   | ALA  | C-N-CA     | 5.57  | 135.62      | 121.70   |
| 1   | D     | 79  | GLU  | N-CA-CB    | 5.57  | 120.62      | 110.60   |
| 1   | D     | 89  | VAL  | CA-CB-CG1  | 5.57  | 119.25      | 110.90   |
| 1   | E     | 65  | VAL  | CA-C-N     | -5.56 | 104.97      | 117.20   |
| 1   | D     | 8   | PHE  | CZ-CE2-CD2 | 5.55  | 126.77      | 120.10   |
| 1   | B     | 31  | LYS  | CA-C-O     | 5.55  | 131.75      | 120.10   |
| 1   | A     | 127 | GLU  | CA-C-N     | -5.55 | 105.00      | 117.20   |
| 1   | D     | 104 | ILE  | O-C-N      | -5.54 | 113.83      | 122.70   |
| 1   | F     | 52  | TYR  | CD1-CE1-CZ | -5.54 | 114.81      | 119.80   |
| 1   | C     | 132 | LEU  | O-C-N      | -5.53 | 113.85      | 122.70   |
| 1   | A     | 98  | ASP  | CB-CG-OD1  | 5.53  | 123.28      | 118.30   |
| 1   | B     | 108 | PHE  | N-CA-C     | 5.52  | 125.92      | 111.00   |
| 1   | D     | 131 | ALA  | O-C-N      | 5.52  | 131.54      | 122.70   |
| 1   | F     | 151 | TYR  | CG-CD2-CE2 | -5.52 | 116.88      | 121.30   |
| 1   | E     | 142 | TYR  | CG-CD2-CE2 | 5.52  | 125.72      | 121.30   |
| 1   | B     | 115 | ASN  | N-CA-C     | 5.51  | 125.88      | 111.00   |
| 1   | C     | 35  | LEU  | CB-CA-C    | -5.51 | 99.73       | 110.20   |
| 1   | C     | 93  | GLU  | CA-CB-CG   | -5.51 | 101.28      | 113.40   |
| 1   | D     | 58  | ARG  | CD-NE-CZ   | 5.51  | 131.32      | 123.60   |
| 1   | D     | 91  | LEU  | C-N-CA     | 5.51  | 133.87      | 122.30   |
| 1   | A     | 150 | ILE  | O-C-N      | 5.51  | 131.51      | 122.70   |
| 1   | D     | 124 | GLU  | CA-C-O     | 5.51  | 131.67      | 120.10   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | F     | 97  | ALA  | O-C-N       | 5.50  | 131.50      | 122.70   |
| 1   | C     | 121 | ASP  | CA-C-N      | -5.50 | 105.10      | 117.20   |
| 1   | E     | 146 | ALA  | N-CA-C      | 5.50  | 125.85      | 111.00   |
| 1   | F     | 129 | GLU  | CG-CD-OE2   | -5.50 | 107.31      | 118.30   |
| 1   | C     | 24  | ILE  | CA-CB-CG2   | -5.50 | 99.91       | 110.90   |
| 1   | E     | 77  | VAL  | CA-C-N      | -5.50 | 105.11      | 117.20   |
| 1   | A     | 110 | ILE  | CA-CB-CG2   | -5.49 | 99.91       | 110.90   |
| 1   | B     | 134 | PHE  | CB-CA-C     | -5.49 | 99.42       | 110.40   |
| 1   | C     | 108 | PHE  | CB-CG-CD1   | 5.49  | 124.64      | 120.80   |
| 1   | A     | 2   | ALA  | N-CA-CB     | 5.49  | 117.78      | 110.10   |
| 1   | A     | 67  | TYR  | CG-CD2-CE2  | -5.49 | 116.91      | 121.30   |
| 1   | A     | 126 | ALA  | CB-CA-C     | 5.49  | 118.33      | 110.10   |
| 1   | A     | 103 | THR  | CB-CA-C     | -5.49 | 96.78       | 111.60   |
| 1   | B     | 103 | THR  | CB-CA-C     | -5.49 | 96.79       | 111.60   |
| 1   | C     | 114 | ARG  | C-N-CA      | -5.49 | 107.99      | 121.70   |
| 1   | A     | 74  | VAL  | C-N-CA      | -5.48 | 107.99      | 121.70   |
| 1   | F     | 128 | LYS  | N-CA-CB     | -5.48 | 100.74      | 110.60   |
| 1   | A     | 26  | LYS  | CA-C-N      | -5.47 | 105.17      | 117.20   |
| 1   | A     | 46  | ASP  | CB-CG-OD2   | 5.47  | 123.22      | 118.30   |
| 1   | D     | 123 | VAL  | CA-CB-CG2   | 5.47  | 119.11      | 110.90   |
| 1   | D     | 98  | ASP  | CB-CG-OD1   | 5.46  | 123.22      | 118.30   |
| 1   | A     | 146 | ALA  | N-CA-CB     | -5.46 | 102.45      | 110.10   |
| 1   | A     | 149 | TRP  | CD2-CE3-CZ3 | -5.46 | 111.70      | 118.80   |
| 1   | C     | 114 | ARG  | CG-CD-NE    | -5.46 | 100.34      | 111.80   |
| 1   | E     | 16  | VAL  | CA-CB-CG2   | 5.46  | 119.08      | 110.90   |
| 1   | F     | 99  | SER  | CB-CA-C     | -5.46 | 99.73       | 110.10   |
| 1   | C     | 34  | ARG  | CD-NE-CZ    | 5.46  | 131.24      | 123.60   |
| 1   | F     | 6   | ARG  | N-CA-CB     | 5.45  | 120.42      | 110.60   |
| 1   | A     | 46  | ASP  | CB-CG-OD1   | -5.45 | 113.39      | 118.30   |
| 1   | A     | 41  | MET  | CB-CA-C     | -5.44 | 99.51       | 110.40   |
| 1   | D     | 124 | GLU  | CA-C-N      | -5.44 | 105.23      | 117.20   |
| 1   | F     | 90  | MET  | O-C-N       | 5.44  | 131.41      | 122.70   |
| 1   | C     | 114 | ARG  | CB-CG-CD    | 5.43  | 125.73      | 111.60   |
| 1   | F     | 36  | VAL  | CA-CB-CG2   | -5.43 | 102.75      | 110.90   |
| 1   | C     | 62  | ALA  | CA-C-N      | -5.43 | 105.34      | 116.20   |
| 1   | A     | 48  | LEU  | CB-CA-C     | -5.43 | 99.89       | 110.20   |
| 1   | B     | 8   | PHE  | CB-CA-C     | 5.42  | 121.25      | 110.40   |
| 1   | E     | 12  | LYS  | CD-CE-NZ    | -5.42 | 99.23       | 111.70   |
| 1   | D     | 130 | ILE  | CA-C-N      | -5.42 | 105.28      | 117.20   |
| 1   | F     | 89  | VAL  | CG1-CB-CG2  | -5.42 | 102.23      | 110.90   |
| 1   | A     | 135 | HIS  | N-CA-CB     | 5.41  | 120.34      | 110.60   |
| 1   | B     | 127 | GLU  | CB-CA-C     | -5.41 | 99.58       | 110.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 147 | GLN  | CA-C-N     | -5.41 | 105.31      | 117.20   |
| 1   | F     | 48  | LEU  | N-CA-CB    | -5.40 | 99.60       | 110.40   |
| 1   | F     | 111 | GLN  | O-C-N      | 5.40  | 131.33      | 122.70   |
| 1   | C     | 34  | ARG  | N-CA-CB    | 5.39  | 120.31      | 110.60   |
| 1   | A     | 133 | TRP  | N-CA-CB    | 5.39  | 120.31      | 110.60   |
| 1   | F     | 138 | GLU  | CA-C-N     | -5.39 | 105.35      | 117.20   |
| 1   | A     | 43  | ALA  | CB-CA-C    | -5.38 | 102.03      | 110.10   |
| 1   | B     | 151 | TYR  | O-C-N      | 5.38  | 131.31      | 122.70   |
| 1   | E     | 82  | ASN  | N-CA-CB    | 5.38  | 120.28      | 110.60   |
| 1   | C     | 127 | GLU  | CB-CG-CD   | 5.38  | 128.71      | 114.20   |
| 1   | D     | 98  | ASP  | O-C-N      | 5.38  | 131.30      | 122.70   |
| 1   | D     | 14  | ASP  | CB-CG-OD2  | -5.37 | 113.47      | 118.30   |
| 1   | F     | 93  | GLU  | CG-CD-OE1  | 5.37  | 129.04      | 118.30   |
| 1   | B     | 77  | VAL  | CA-CB-CG1  | -5.37 | 102.85      | 110.90   |
| 1   | C     | 91  | LEU  | CA-C-O     | 5.37  | 131.37      | 120.10   |
| 1   | E     | 118 | HIS  | CB-CA-C    | -5.37 | 99.67       | 110.40   |
| 1   | C     | 33  | PHE  | C-N-CA     | -5.36 | 108.29      | 121.70   |
| 1   | F     | 112 | VAL  | CB-CA-C    | -5.36 | 101.22      | 111.40   |
| 1   | F     | 61  | PHE  | CD1-CG-CD2 | -5.36 | 111.33      | 118.30   |
| 1   | A     | 35  | LEU  | O-C-N      | 5.35  | 131.27      | 122.70   |
| 1   | D     | 49  | LYS  | O-C-N      | 5.35  | 131.26      | 122.70   |
| 1   | D     | 74  | VAL  | CA-CB-CG1  | -5.35 | 102.88      | 110.90   |
| 1   | A     | 73  | VAL  | CA-CB-CG2  | -5.34 | 102.89      | 110.90   |
| 1   | F     | 88  | ARG  | NE-CZ-NH1  | 5.34  | 122.97      | 120.30   |
| 1   | F     | 104 | ILE  | CA-CB-CG2  | -5.34 | 100.22      | 110.90   |
| 1   | E     | 93  | GLU  | CA-CB-CG   | -5.34 | 101.66      | 113.40   |
| 1   | A     | 68  | MET  | CA-CB-CG   | -5.34 | 104.23      | 113.30   |
| 1   | E     | 55  | LEU  | O-C-N      | 5.33  | 131.23      | 122.70   |
| 1   | A     | 76  | MET  | N-CA-CB    | -5.33 | 101.01      | 110.60   |
| 1   | F     | 40  | PHE  | CB-CG-CD2  | -5.33 | 117.07      | 120.80   |
| 1   | E     | 20  | LEU  | N-CA-CB    | -5.33 | 99.75       | 110.40   |
| 1   | B     | 115 | ASN  | CA-CB-CG   | -5.33 | 101.68      | 113.40   |
| 1   | F     | 81  | LEU  | CB-CA-C    | -5.33 | 100.08      | 110.20   |
| 1   | F     | 145 | CYS  | CA-CB-SG   | -5.32 | 104.42      | 114.00   |
| 1   | F     | 104 | ILE  | CA-C-O     | 5.32  | 131.27      | 120.10   |
| 1   | B     | 145 | CYS  | CB-CA-C    | 5.32  | 121.04      | 110.40   |
| 1   | A     | 110 | ILE  | N-CA-CB    | -5.31 | 98.59       | 110.80   |
| 1   | F     | 6   | ARG  | NE-CZ-NH2  | -5.31 | 117.64      | 120.30   |
| 1   | B     | 47  | LEU  | CA-CB-CG   | -5.31 | 103.09      | 115.30   |
| 1   | C     | 88  | ARG  | NH1-CZ-NH2 | 5.31  | 125.24      | 119.40   |
| 1   | E     | 42  | ARG  | NH1-CZ-NH2 | -5.31 | 113.56      | 119.40   |
| 1   | F     | 112 | VAL  | CA-CB-CG1  | 5.31  | 118.86      | 110.90   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 98  | ASP  | N-CA-CB    | -5.31 | 101.05      | 110.60   |
| 1   | C     | 132 | LEU  | CB-CA-C    | 5.30  | 120.28      | 110.20   |
| 1   | E     | 5   | GLU  | CG-CD-OE2  | -5.30 | 107.69      | 118.30   |
| 1   | B     | 107 | ASP  | CA-CB-CG   | -5.30 | 101.74      | 113.40   |
| 1   | D     | 65  | VAL  | CA-CB-CG2  | -5.30 | 102.95      | 110.90   |
| 1   | E     | 127 | GLU  | O-C-N      | 5.30  | 131.17      | 122.70   |
| 1   | A     | 108 | PHE  | N-CA-C     | 5.29  | 125.29      | 111.00   |
| 1   | C     | 94  | THR  | C-N-CA     | 5.29  | 134.93      | 121.70   |
| 1   | C     | 79  | GLU  | CA-C-N     | -5.29 | 105.63      | 116.20   |
| 1   | F     | 126 | ALA  | CB-CA-C    | -5.29 | 102.17      | 110.10   |
| 1   | A     | 116 | ILE  | N-CA-C     | 5.29  | 125.27      | 111.00   |
| 1   | A     | 3   | ASN  | N-CA-CB    | 5.27  | 120.09      | 110.60   |
| 1   | C     | 27  | ARG  | CD-NE-CZ   | 5.27  | 130.98      | 123.60   |
| 1   | A     | 142 | TYR  | CG-CD1-CE1 | 5.27  | 125.52      | 121.30   |
| 1   | C     | 91  | LEU  | CB-CG-CD1  | 5.27  | 119.96      | 111.00   |
| 1   | B     | 54  | ASP  | CB-CG-OD2  | 5.27  | 123.04      | 118.30   |
| 1   | C     | 100 | LYS  | N-CA-C     | 5.27  | 125.22      | 111.00   |
| 1   | F     | 68  | MET  | CA-CB-CG   | -5.27 | 104.34      | 113.30   |
| 1   | A     | 21  | ILE  | CA-C-O     | -5.27 | 109.04      | 120.10   |
| 1   | A     | 90  | MET  | N-CA-CB    | 5.26  | 120.08      | 110.60   |
| 1   | D     | 48  | LEU  | CA-C-N     | -5.26 | 105.62      | 117.20   |
| 1   | E     | 74  | VAL  | N-CA-C     | -5.26 | 96.80       | 111.00   |
| 1   | E     | 81  | LEU  | CB-CG-CD2  | -5.26 | 102.06      | 111.00   |
| 1   | F     | 148 | ASN  | N-CA-CB    | 5.25  | 120.06      | 110.60   |
| 1   | C     | 60  | PHE  | CB-CG-CD2  | -5.25 | 117.12      | 120.80   |
| 1   | D     | 25  | ILE  | CA-CB-CG1  | 5.25  | 120.97      | 111.00   |
| 1   | D     | 51  | HIS  | CA-CB-CG   | -5.25 | 104.68      | 113.60   |
| 1   | B     | 107 | ASP  | O-C-N      | 5.25  | 131.09      | 122.70   |
| 1   | E     | 46  | ASP  | CB-CG-OD2  | 5.25  | 123.02      | 118.30   |
| 1   | A     | 6   | ARG  | CA-CB-CG   | -5.24 | 101.87      | 113.40   |
| 1   | D     | 62  | ALA  | N-CA-CB    | 5.24  | 117.44      | 110.10   |
| 1   | D     | 136 | PRO  | N-CD-CG    | -5.24 | 95.34       | 103.20   |
| 1   | E     | 142 | TYR  | CB-CG-CD2  | 5.24  | 124.14      | 121.00   |
| 1   | F     | 31  | LYS  | O-C-N      | -5.24 | 114.29      | 123.20   |
| 1   | F     | 107 | ASP  | CB-CG-OD1  | 5.24  | 123.02      | 118.30   |
| 1   | C     | 87  | GLY  | CA-C-O     | 5.24  | 130.03      | 120.60   |
| 1   | E     | 11  | ILE  | CB-CA-C    | -5.24 | 101.12      | 111.60   |
| 1   | A     | 149 | TRP  | CA-CB-CG   | -5.23 | 103.75      | 113.70   |
| 1   | B     | 82  | ASN  | O-C-N      | -5.23 | 114.33      | 122.70   |
| 1   | A     | 8   | PHE  | CG-CD1-CE1 | -5.23 | 115.05      | 120.80   |
| 1   | C     | 47  | LEU  | CA-C-N     | -5.23 | 105.70      | 117.20   |
| 1   | E     | 23  | GLU  | OE1-CD-OE2 | -5.22 | 117.03      | 123.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | F     | 67  | TYR  | N-CA-CB    | -5.22 | 101.21      | 110.60   |
| 1   | A     | 38  | MET  | CA-CB-CG   | 5.21  | 122.16      | 113.30   |
| 1   | A     | 42  | ARG  | CG-CD-NE   | 5.21  | 122.73      | 111.80   |
| 1   | B     | 101 | PRO  | C-N-CA     | -5.21 | 111.37      | 122.30   |
| 1   | F     | 18  | ARG  | NE-CZ-NH1  | 5.21  | 122.90      | 120.30   |
| 1   | F     | 107 | ASP  | C-N-CA     | -5.20 | 108.69      | 121.70   |
| 1   | F     | 144 | SER  | O-C-N      | 5.20  | 131.02      | 122.70   |
| 1   | E     | 60  | PHE  | CA-CB-CG   | 5.20  | 126.38      | 113.90   |
| 1   | A     | 141 | ASN  | CB-CA-C    | 5.20  | 120.79      | 110.40   |
| 1   | A     | 35  | LEU  | CB-CA-C    | -5.19 | 100.34      | 110.20   |
| 1   | F     | 66  | LYS  | CA-C-N     | -5.18 | 105.79      | 117.20   |
| 1   | F     | 108 | PHE  | N-CA-CB    | -5.18 | 101.27      | 110.60   |
| 1   | E     | 151 | TYR  | C-N-CA     | -5.18 | 108.74      | 121.70   |
| 1   | F     | 43  | ALA  | N-CA-CB    | -5.18 | 102.84      | 110.10   |
| 1   | B     | 72  | PRO  | N-CA-CB    | 5.18  | 109.52      | 103.30   |
| 1   | A     | 96  | PRO  | CA-N-CD    | -5.18 | 104.25      | 111.50   |
| 1   | C     | 148 | ASN  | CA-CB-CG   | -5.18 | 102.01      | 113.40   |
| 1   | B     | 129 | GLU  | OE1-CD-OE2 | 5.18  | 129.51      | 123.30   |
| 1   | E     | 104 | ILE  | CA-CB-CG1  | 5.18  | 120.84      | 111.00   |
| 1   | E     | 52  | TYR  | CB-CG-CD2  | 5.18  | 124.11      | 121.00   |
| 1   | F     | 152 | GLU  | CB-CA-C    | 5.18  | 120.75      | 110.40   |
| 1   | F     | 126 | ALA  | C-N-CA     | -5.17 | 108.78      | 121.70   |
| 1   | F     | 132 | LEU  | O-C-N      | -5.17 | 114.44      | 122.70   |
| 1   | C     | 26  | LYS  | CA-C-O     | 5.16  | 130.94      | 120.10   |
| 1   | A     | 108 | PHE  | C-N-CA     | -5.16 | 108.80      | 121.70   |
| 1   | F     | 67  | TYR  | CD1-CG-CD2 | 5.16  | 123.57      | 117.90   |
| 1   | B     | 106 | GLY  | CA-C-O     | 5.15  | 129.88      | 120.60   |
| 1   | D     | 5   | GLU  | OE1-CD-OE2 | -5.15 | 117.12      | 123.30   |
| 1   | D     | 27  | ARG  | NH1-CZ-NH2 | -5.15 | 113.73      | 119.40   |
| 1   | B     | 139 | LEU  | CD1-CG-CD2 | -5.15 | 95.05       | 110.50   |
| 1   | D     | 66  | LYS  | N-CA-CB    | -5.15 | 101.34      | 110.60   |
| 1   | B     | 55  | LEU  | N-CA-CB    | -5.14 | 100.11      | 110.40   |
| 1   | B     | 70  | SER  | CB-CA-C    | -5.14 | 100.33      | 110.10   |
| 1   | C     | 124 | GLU  | OE1-CD-OE2 | 5.14  | 129.47      | 123.30   |
| 1   | A     | 3   | ASN  | O-C-N      | 5.14  | 130.93      | 122.70   |
| 1   | E     | 43  | ALA  | O-C-N      | 5.14  | 130.93      | 122.70   |
| 1   | A     | 62  | ALA  | N-CA-CB    | 5.14  | 117.29      | 110.10   |
| 1   | A     | 46  | ASP  | O-C-N      | 5.13  | 130.92      | 122.70   |
| 1   | D     | 22  | GLY  | CA-C-O     | 5.13  | 129.84      | 120.60   |
| 1   | E     | 34  | ARG  | CA-CB-CG   | 5.13  | 124.69      | 113.40   |
| 1   | D     | 77  | VAL  | CB-CA-C    | -5.13 | 101.65      | 111.40   |
| 1   | A     | 105 | ARG  | CG-CD-NE   | 5.13  | 122.57      | 111.80   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | F     | 28  | PHE  | O-C-N       | 5.13  | 130.91      | 122.70   |
| 1   | A     | 14  | ASP  | CB-CG-OD2   | 5.12  | 122.91      | 118.30   |
| 1   | F     | 111 | GLN  | N-CA-CB     | 5.12  | 119.82      | 110.60   |
| 1   | F     | 131 | ALA  | CB-CA-C     | -5.12 | 102.42      | 110.10   |
| 1   | F     | 33  | PHE  | N-CA-CB     | -5.12 | 101.39      | 110.60   |
| 1   | A     | 109 | CYS  | CA-CB-SG    | -5.12 | 104.79      | 114.00   |
| 1   | D     | 6   | ARG  | CA-CB-CG    | -5.11 | 102.17      | 113.40   |
| 1   | E     | 137 | GLU  | O-C-N       | 5.11  | 130.87      | 122.70   |
| 1   | D     | 64  | LEU  | CB-CA-C     | -5.10 | 100.51      | 110.20   |
| 1   | D     | 149 | TRP  | CH2-CZ2-CE2 | 5.10  | 122.50      | 117.40   |
| 1   | D     | 58  | ARG  | NH1-CZ-NH2  | 5.09  | 125.00      | 119.40   |
| 1   | D     | 127 | GLU  | CB-CA-C     | -5.09 | 100.21      | 110.40   |
| 1   | F     | 86  | THR  | C-N-CA      | -5.09 | 111.60      | 122.30   |
| 1   | F     | 133 | TRP  | N-CA-CB     | 5.09  | 119.77      | 110.60   |
| 1   | B     | 149 | TRP  | CA-CB-CG    | -5.09 | 104.03      | 113.70   |
| 1   | A     | 95  | ASN  | CB-CA-C     | -5.09 | 100.22      | 110.40   |
| 1   | A     | 89  | VAL  | O-C-N       | 5.09  | 130.84      | 122.70   |
| 1   | B     | 86  | THR  | CA-CB-OG1   | -5.09 | 98.32       | 109.00   |
| 1   | F     | 77  | VAL  | CA-CB-CG1   | 5.09  | 118.53      | 110.90   |
| 1   | C     | 142 | TYR  | CB-CG-CD2   | 5.08  | 124.05      | 121.00   |
| 1   | C     | 27  | ARG  | O-C-N       | 5.08  | 130.83      | 122.70   |
| 1   | B     | 106 | GLY  | CA-C-N      | -5.08 | 106.02      | 117.20   |
| 1   | A     | 27  | ARG  | CB-CG-CD    | -5.08 | 98.39       | 111.60   |
| 1   | D     | 40  | PHE  | CB-CA-C     | -5.08 | 100.24      | 110.40   |
| 1   | B     | 152 | GLU  | CA-C-O      | -5.08 | 109.44      | 120.10   |
| 1   | C     | 6   | ARG  | CB-CG-CD    | 5.08  | 124.81      | 111.60   |
| 1   | B     | 109 | CYS  | N-CA-CB     | -5.08 | 101.46      | 110.60   |
| 1   | F     | 132 | LEU  | C-N-CA      | -5.08 | 109.01      | 121.70   |
| 1   | A     | 78  | TRP  | CG-CD2-CE3  | -5.07 | 129.34      | 133.90   |
| 1   | D     | 43  | ALA  | N-CA-CB     | -5.07 | 103.00      | 110.10   |
| 1   | A     | 133 | TRP  | NE1-CE2-CD2 | 5.07  | 112.37      | 107.30   |
| 1   | C     | 106 | GLY  | O-C-N       | -5.07 | 114.59      | 122.70   |
| 1   | A     | 49  | LYS  | CA-CB-CG    | -5.07 | 102.25      | 113.40   |
| 1   | A     | 68  | MET  | N-CA-CB     | -5.07 | 101.48      | 110.60   |
| 1   | A     | 40  | PHE  | N-CA-CB     | -5.07 | 101.48      | 110.60   |
| 1   | A     | 148 | ASN  | CB-CA-C     | 5.07  | 120.53      | 110.40   |
| 1   | D     | 5   | GLU  | CG-CD-OE1   | 5.06  | 128.43      | 118.30   |
| 1   | E     | 139 | LEU  | O-C-N       | 5.06  | 130.80      | 122.70   |
| 1   | A     | 131 | ALA  | CA-C-O      | -5.06 | 109.48      | 120.10   |
| 1   | D     | 47  | LEU  | CB-CA-C     | -5.06 | 100.59      | 110.20   |
| 1   | C     | 28  | PHE  | CA-C-O      | 5.06  | 130.72      | 120.10   |
| 1   | C     | 101 | PRO  | O-C-N       | 5.05  | 131.79      | 123.20   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 52  | TYR  | CB-CG-CD1  | -5.05 | 117.97      | 121.00   |
| 1   | D     | 23  | GLU  | CG-CD-OE1  | -5.05 | 108.20      | 118.30   |
| 1   | D     | 49  | LYS  | CA-C-N     | -5.04 | 106.10      | 117.20   |
| 1   | D     | 67  | TYR  | CD1-CE1-CZ | 5.04  | 124.34      | 119.80   |
| 1   | D     | 125 | SER  | N-CA-C     | -5.04 | 97.38       | 111.00   |
| 1   | E     | 41  | MET  | N-CA-CB    | -5.04 | 101.52      | 110.60   |
| 1   | F     | 133 | TRP  | CB-CA-C    | -5.04 | 100.31      | 110.40   |
| 1   | D     | 29  | GLU  | N-CA-CB    | 5.04  | 119.67      | 110.60   |
| 1   | E     | 18  | ARG  | CA-C-O     | 5.04  | 130.68      | 120.10   |
| 1   | F     | 35  | LEU  | CB-CG-CD2  | 5.04  | 119.56      | 111.00   |
| 1   | B     | 8   | PHE  | CD1-CE1-CZ | -5.03 | 114.06      | 120.10   |
| 1   | F     | 88  | ARG  | CA-C-N     | -5.03 | 106.13      | 117.20   |
| 1   | A     | 80  | GLY  | CA-C-O     | 5.03  | 129.65      | 120.60   |
| 1   | F     | 115 | ASN  | CB-CA-C    | 5.03  | 120.45      | 110.40   |
| 1   | E     | 2   | ALA  | CB-CA-C    | 5.03  | 117.64      | 110.10   |
| 1   | C     | 64  | LEU  | CB-CG-CD2  | 5.02  | 119.54      | 111.00   |
| 1   | F     | 76  | MET  | O-C-N      | 5.01  | 130.72      | 122.70   |
| 1   | F     | 124 | GLU  | CA-CB-CG   | -5.01 | 102.38      | 113.40   |
| 1   | A     | 32  | GLY  | CA-C-N     | 5.00  | 128.21      | 117.20   |
| 1   | F     | 137 | GLU  | C-N-CA     | -5.00 | 109.19      | 121.70   |
| 1   | B     | 23  | GLU  | CG-CD-OE1  | 5.00  | 128.31      | 118.30   |
| 1   | E     | 85  | LYS  | CB-CA-C    | -5.00 | 100.39      | 110.40   |

All (5) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | B     | 115 | ASN  | CA   |
| 1   | B     | 141 | ASN  | CA   |
| 1   | B     | 151 | TYR  | CA   |
| 1   | D     | 140 | VAL  | CA   |
| 1   | D     | 141 | ASN  | CA   |

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | C     | 21  | ILE  | Mainchain |
| 1   | C     | 29  | GLU  | Sidechain |
| 1   | E     | 54  | ASP  | Sidechain |

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1206  | 0        | 1203     | 159     | 0            |
| 1   | B     | 1206  | 0        | 1202     | 174     | 0            |
| 1   | C     | 1206  | 0        | 1203     | 154     | 0            |
| 1   | D     | 1206  | 0        | 1202     | 161     | 0            |
| 1   | E     | 1206  | 0        | 1203     | 182     | 0            |
| 1   | F     | 1206  | 0        | 1203     | 171     | 0            |
| 2   | A     | 51    | 0        | 11       | 8       | 0            |
| 2   | B     | 51    | 0        | 9        | 10      | 0            |
| 2   | C     | 51    | 0        | 9        | 6       | 0            |
| 2   | D     | 51    | 0        | 12       | 6       | 0            |
| 2   | E     | 51    | 0        | 12       | 9       | 0            |
| 2   | F     | 51    | 0        | 10       | 8       | 0            |
| 3   | A     | 49    | 0        | 0        | 12      | 0            |
| 3   | B     | 49    | 0        | 0        | 11      | 0            |
| 3   | C     | 50    | 0        | 0        | 10      | 0            |
| 3   | D     | 40    | 0        | 0        | 8       | 0            |
| 3   | E     | 62    | 0        | 0        | 12      | 0            |
| 3   | F     | 56    | 0        | 0        | 14      | 0            |
| All | All   | 7848  | 0        | 7279     | 974     | 0            |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 66.

All (974) close contacts within the same asymmetric unit are listed below.

| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 2:B:160:35G:O5'  | 2:B:161:GDP:O3B  | 1.59        | 1.21     |
| 1:C:148:ASN:ND2  | 1:C:148:ASN:H    | 1.43        | 1.15     |
| 1:F:41:MET:HE3   | 1:F:133:TRP:HE3  | 1.12        | 1.14     |
| 2:A:160:35G:O5'  | 2:A:161:GDP:O3B  | 1.67        | 1.11     |
| 2:C:160:35G:O2P  | 2:C:161:GDP:O2B  | 1.70        | 1.09     |
| 2:B:160:35G:O5'  | 2:B:161:GDP:PB   | 2.13        | 1.06     |
| 1:C:72:PRO:HG3   | 1:F:140:VAL:HG11 | 1.31        | 1.06     |
| 2:C:160:35G:O2P  | 2:C:161:GDP:O3B  | 1.79        | 1.00     |
| 1:A:147:GLN:HE22 | 1:A:151:TYR:HD2  | 1.12        | 0.98     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:E:16:VAL:HG13  | 1:E:21:ILE:HD11  | 1.42        | 0.97     |
| 1:F:58:ARG:HH11  | 1:F:58:ARG:HG2   | 1.30        | 0.96     |
| 1:F:41:MET:HE3   | 1:F:133:TRP:CE3  | 2.01        | 0.96     |
| 1:C:148:ASN:N    | 1:C:148:ASN:HD22 | 1.64        | 0.95     |
| 1:A:37:ALA:HB3   | 1:A:77:VAL:HG13  | 1.46        | 0.94     |
| 1:B:37:ALA:HB2   | 1:B:139:LEU:HD12 | 1.49        | 0.94     |
| 1:D:136:PRO:HD2  | 1:D:137:GLU:HG3  | 1.48        | 0.93     |
| 1:B:58:ARG:HG3   | 1:B:59:PRO:HD2   | 1.46        | 0.93     |
| 1:A:13:PRO:HD3   | 1:A:73:VAL:HG12  | 1.48        | 0.93     |
| 1:C:140:VAL:HG11 | 1:F:72:PRO:HG3   | 1.51        | 0.92     |
| 1:D:127:GLU:HA   | 1:D:130:ILE:HG13 | 1.48        | 0.92     |
| 1:E:21:ILE:HG23  | 3:E:373:HOH:O    | 1.68        | 0.92     |
| 2:B:160:35G:C5'  | 2:B:161:GDP:PA   | 2.37        | 0.91     |
| 1:C:148:ASN:H    | 1:C:148:ASN:HD22 | 0.91        | 0.91     |
| 1:A:148:ASN:H    | 1:A:148:ASN:HD22 | 0.98        | 0.91     |
| 1:D:143:LYS:HB2  | 1:D:143:LYS:NZ   | 1.84        | 0.91     |
| 1:A:58:ARG:HG3   | 1:A:58:ARG:HH11  | 1.36        | 0.90     |
| 2:B:160:35G:O5'  | 2:B:161:GDP:O3A  | 1.89        | 0.89     |
| 1:C:43:ALA:HB1   | 1:C:47:LEU:HD13  | 1.53        | 0.89     |
| 1:B:48:LEU:HD21  | 1:B:68:MET:HB3   | 1.54        | 0.88     |
| 2:B:160:35G:C5'  | 2:B:161:GDP:O3A  | 2.21        | 0.88     |
| 2:E:160:35G:O2P  | 2:E:161:GDP:O3B  | 1.92        | 0.87     |
| 1:F:48:LEU:CD1   | 1:F:69:HIS:HB2   | 2.05        | 0.86     |
| 2:C:160:35G:O5'  | 2:C:161:GDP:O3B  | 1.93        | 0.86     |
| 2:C:160:35G:O2P  | 2:C:161:GDP:PB   | 2.33        | 0.85     |
| 1:A:37:ALA:HB2   | 1:A:139:LEU:HD12 | 1.59        | 0.85     |
| 1:C:72:PRO:HG3   | 1:F:140:VAL:CG1  | 2.05        | 0.85     |
| 2:C:160:35G:P    | 2:C:161:GDP:O3B  | 2.35        | 0.85     |
| 1:D:24:ILE:O     | 1:D:27:ARG:HB2   | 1.76        | 0.84     |
| 1:A:38:MET:HB2   | 1:A:76:MET:HG2   | 1.56        | 0.84     |
| 1:E:135:HIS:O    | 1:E:138:GLU:HB2  | 1.78        | 0.84     |
| 1:E:40:PHE:CE1   | 1:E:72:PRO:HB2   | 2.12        | 0.84     |
| 1:E:39:LYS:HE3   | 1:E:41:MET:CE    | 2.08        | 0.84     |
| 1:B:49:LYS:NZ    | 1:B:65:VAL:HG11  | 1.93        | 0.83     |
| 1:C:58:ARG:N     | 1:C:58:ARG:HD3   | 1.93        | 0.83     |
| 1:E:140:VAL:HG12 | 1:E:141:ASN:H    | 1.43        | 0.83     |
| 1:C:100:LYS:O    | 1:C:106:GLY:HA3  | 1.79        | 0.82     |
| 2:A:160:35G:P    | 2:A:161:GDP:O3B  | 2.37        | 0.82     |
| 1:C:82:ASN:O     | 1:C:83:VAL:C     | 2.18        | 0.82     |
| 1:A:148:ASN:H    | 1:A:148:ASN:ND2  | 1.72        | 0.81     |
| 1:E:54:ASP:HA    | 3:E:218:HOH:O    | 1.79        | 0.81     |
| 1:F:80:GLY:O     | 1:F:83:VAL:HG22  | 1.80        | 0.81     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:F:86:THR:O     | 1:F:90:MET:HG3   | 1.81        | 0.81     |
| 1:E:46:ASP:HA    | 1:E:49:LYS:HG3   | 1.62        | 0.80     |
| 1:D:138:GLU:C    | 1:D:139:LEU:HD12 | 2.01        | 0.80     |
| 1:B:39:LYS:HE3   | 1:B:41:MET:CE    | 2.11        | 0.80     |
| 1:E:140:VAL:HG12 | 1:E:141:ASN:N    | 1.97        | 0.80     |
| 1:B:45:GLU:O     | 1:B:49:LYS:HB2   | 1.81        | 0.79     |
| 1:C:93:GLU:N     | 1:C:99:SER:HB3   | 1.97        | 0.79     |
| 1:D:110:ILE:HD13 | 1:E:33:PHE:CE1   | 2.17        | 0.79     |
| 1:F:8:PHE:CZ     | 1:F:10:ALA:HB2   | 2.17        | 0.79     |
| 1:C:93:GLU:H     | 1:C:99:SER:HB3   | 1.48        | 0.79     |
| 1:B:13:PRO:HD3   | 1:B:73:VAL:CG1   | 2.14        | 0.78     |
| 1:F:52:TYR:CE1   | 2:F:160:35G:H5'2 | 2.19        | 0.78     |
| 1:E:18:ARG:O     | 1:E:20:LEU:HG    | 1.83        | 0.78     |
| 1:B:13:PRO:HD3   | 1:B:73:VAL:HG12  | 1.64        | 0.78     |
| 1:B:17:GLN:HG3   | 1:C:149:TRP:CE2  | 2.19        | 0.78     |
| 1:B:61:PHE:O     | 1:B:65:VAL:HG23  | 1.82        | 0.78     |
| 1:D:6:ARG:HA     | 1:D:83:VAL:HG21  | 1.65        | 0.77     |
| 1:F:61:PHE:O     | 1:F:65:VAL:HG23  | 1.84        | 0.77     |
| 1:E:25:ILE:O     | 1:E:29:GLU:HG3   | 1.85        | 0.77     |
| 1:A:25:ILE:HG21  | 1:E:21:ILE:HG22  | 1.67        | 0.77     |
| 1:D:128:LYS:O    | 1:D:131:ALA:HB3  | 1.85        | 0.77     |
| 1:F:44:SER:O     | 1:F:47:LEU:N     | 2.18        | 0.77     |
| 1:E:93:GLU:O     | 1:E:94:THR:C     | 2.17        | 0.77     |
| 1:A:148:ASN:N    | 1:A:148:ASN:HD22 | 1.78        | 0.77     |
| 1:F:58:ARG:HG2   | 1:F:58:ARG:NH1   | 1.96        | 0.76     |
| 1:D:139:LEU:HD12 | 1:D:139:LEU:N    | 2.00        | 0.76     |
| 1:E:143:LYS:HA   | 1:E:143:LYS:NZ   | 1.99        | 0.76     |
| 1:A:47:LEU:HD12  | 1:A:47:LEU:O     | 1.86        | 0.76     |
| 1:B:115:ASN:O    | 1:B:116:ILE:HG12 | 1.86        | 0.76     |
| 1:E:39:LYS:HE3   | 1:E:41:MET:HE2   | 1.68        | 0.76     |
| 1:F:48:LEU:HD11  | 1:F:68:MET:O     | 1.86        | 0.76     |
| 1:E:143:LYS:HE2  | 3:E:472:HOH:O    | 1.85        | 0.76     |
| 1:A:31:LYS:HG3   | 1:A:31:LYS:O     | 1.86        | 0.76     |
| 1:A:43:ALA:O     | 1:A:69:HIS:ND1   | 2.17        | 0.76     |
| 1:A:31:LYS:HE3   | 1:C:109:CYS:O    | 1.85        | 0.75     |
| 1:A:45:GLU:O     | 1:A:49:LYS:HG2   | 1.87        | 0.75     |
| 1:F:88:ARG:HD2   | 1:F:121:ASP:HA   | 1.67        | 0.75     |
| 1:F:39:LYS:HE3   | 1:F:41:MET:CE    | 2.16        | 0.75     |
| 1:A:58:ARG:HG3   | 1:A:58:ARG:NH1   | 1.98        | 0.75     |
| 1:D:111:GLN:OE1  | 1:E:151:TYR:HA   | 1.87        | 0.75     |
| 1:A:36:VAL:HB    | 1:A:77:VAL:HG22  | 1.69        | 0.75     |
| 1:E:146:ALA:O    | 1:E:149:TRP:HB2  | 1.87        | 0.75     |

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| Atom-1          | Atom-2           | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:C:53:ILE:O    | 1:C:56:LYS:HB3   | 1.87        | 0.75     |
| 1:C:11:ILE:HG13 | 1:C:76:MET:HE1   | 1.68        | 0.74     |
| 1:B:92:GLY:HA2  | 1:B:103:THR:HG21 | 1.69        | 0.74     |
| 1:D:136:PRO:HD2 | 1:D:137:GLU:H    | 1.53        | 0.74     |
| 1:D:143:LYS:HE3 | 1:D:147:GLN:OE1  | 1.86        | 0.74     |
| 1:D:83:VAL:HG23 | 1:D:84:VAL:H     | 1.51        | 0.74     |
| 1:E:9:ILE:HG22  | 1:E:76:MET:HE3   | 1.70        | 0.74     |
| 1:D:52:TYR:HA   | 3:D:445:HOH:O    | 1.86        | 0.74     |
| 1:E:18:ARG:O    | 1:E:19:GLY:C     | 2.23        | 0.74     |
| 1:B:2:ALA:O     | 1:B:81:LEU:HA    | 1.88        | 0.74     |
| 1:C:23:GLU:HG2  | 3:C:435:HOH:O    | 1.87        | 0.73     |
| 1:B:135:HIS:N   | 1:B:138:GLU:OE2  | 2.20        | 0.73     |
| 1:E:46:ASP:HB2  | 3:E:381:HOH:O    | 1.89        | 0.73     |
| 1:B:39:LYS:HE3  | 1:B:41:MET:HE2   | 1.69        | 0.73     |
| 1:A:131:ALA:HA  | 3:A:356:HOH:O    | 1.88        | 0.73     |
| 1:D:46:ASP:HA   | 1:D:49:LYS:HD3   | 1.71        | 0.73     |
| 1:F:24:ILE:HD13 | 1:F:117:ILE:HD12 | 1.71        | 0.73     |
| 1:A:12:LYS:O    | 1:A:16:VAL:HG23  | 1.89        | 0.73     |
| 1:E:143:LYS:HA  | 1:E:143:LYS:HZ3  | 1.53        | 0.73     |
| 1:B:25:ILE:HG21 | 1:D:21:ILE:HG22  | 1.70        | 0.73     |
| 1:F:82:ASN:HB3  | 3:F:481:HOH:O    | 1.88        | 0.72     |
| 1:B:61:PHE:O    | 1:B:64:LEU:HB3   | 1.90        | 0.72     |
| 1:B:120:SER:OG  | 1:B:126:ALA:HA   | 1.89        | 0.72     |
| 1:E:138:GLU:C   | 1:E:139:LEU:HD12 | 2.09        | 0.72     |
| 1:E:80:GLY:N    | 1:E:83:VAL:HG22  | 2.05        | 0.72     |
| 1:B:135:HIS:O   | 1:B:137:GLU:N    | 2.23        | 0.72     |
| 1:B:135:HIS:O   | 1:B:138:GLU:HG3  | 1.88        | 0.72     |
| 1:C:78:TRP:O    | 1:C:83:VAL:HG11  | 1.90        | 0.72     |
| 1:F:41:MET:O    | 1:F:73:VAL:HG22  | 1.90        | 0.72     |
| 1:F:83:VAL:O    | 1:F:87:GLY:N     | 2.21        | 0.72     |
| 1:E:44:SER:O    | 1:E:45:GLU:C     | 2.21        | 0.71     |
| 1:B:14:ASP:O    | 1:B:18:ARG:HG3   | 1.90        | 0.71     |
| 1:B:33:PHE:CE1  | 1:B:83:VAL:HG13  | 2.25        | 0.71     |
| 1:D:3:ASN:HB3   | 1:D:81:LEU:HB2   | 1.71        | 0.71     |
| 1:A:17:GLN:HG3  | 1:B:149:TRP:CE2  | 2.25        | 0.71     |
| 1:A:7:THR:CB    | 1:A:84:VAL:HG22  | 2.20        | 0.71     |
| 1:A:144:SER:O   | 1:A:147:GLN:HB2  | 1.89        | 0.71     |
| 1:B:115:ASN:C   | 1:B:116:ILE:HG12 | 2.09        | 0.71     |
| 1:A:55:LEU:O    | 1:A:57:ASP:N     | 2.24        | 0.71     |
| 1:D:121:ASP:N   | 1:D:121:ASP:OD1  | 2.20        | 0.71     |
| 1:F:47:LEU:O    | 1:F:48:LEU:C     | 2.24        | 0.71     |
| 1:D:46:ASP:O    | 1:D:50:GLU:HB2   | 1.90        | 0.71     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:E:53:ILE:O     | 1:E:56:LYS:HB2   | 1.91        | 0.70     |
| 1:F:48:LEU:HD11  | 1:F:69:HIS:HB2   | 1.72        | 0.70     |
| 1:C:23:GLU:O     | 1:C:27:ARG:HG2   | 1.92        | 0.70     |
| 1:F:94:THR:O     | 1:F:96:PRO:HD3   | 1.90        | 0.70     |
| 1:F:33:PHE:CD1   | 1:F:83:VAL:HG13  | 2.27        | 0.70     |
| 1:D:78:TRP:O     | 1:D:83:VAL:HG11  | 1.91        | 0.70     |
| 1:D:45:GLU:HG2   | 1:D:65:VAL:HG12  | 1.73        | 0.70     |
| 1:B:139:LEU:N    | 1:B:139:LEU:HD13 | 2.07        | 0.70     |
| 1:B:37:ALA:HB2   | 1:B:139:LEU:CD1  | 2.20        | 0.70     |
| 1:A:7:THR:HB     | 1:A:84:VAL:HG22  | 1.74        | 0.70     |
| 1:A:81:LEU:HD12  | 1:A:82:ASN:HD22  | 1.55        | 0.70     |
| 1:C:12:LYS:HD2   | 1:C:117:ILE:N    | 2.06        | 0.70     |
| 1:B:136:PRO:C    | 1:B:137:GLU:HG3  | 2.12        | 0.69     |
| 1:B:87:GLY:O     | 1:B:88:ARG:C     | 2.29        | 0.69     |
| 1:B:45:GLU:O     | 1:B:49:LYS:NZ    | 2.23        | 0.69     |
| 1:E:115:ASN:O    | 1:E:116:ILE:HG12 | 1.92        | 0.69     |
| 1:E:80:GLY:H     | 1:E:83:VAL:CG2   | 2.06        | 0.69     |
| 1:F:52:TYR:OH    | 2:F:160:35G:O1P  | 2.11        | 0.69     |
| 1:B:88:ARG:HH21  | 1:B:121:ASP:HB2  | 1.57        | 0.69     |
| 1:C:39:LYS:HE2   | 1:C:134:PHE:CE1  | 2.28        | 0.69     |
| 1:E:148:ASN:H    | 1:E:148:ASN:HD22 | 1.40        | 0.69     |
| 1:B:126:ALA:O    | 1:B:130:ILE:HG12 | 1.92        | 0.69     |
| 1:C:140:VAL:CG1  | 1:F:72:PRO:HG3   | 2.21        | 0.69     |
| 1:E:11:ILE:HG13  | 1:E:76:MET:HE2   | 1.73        | 0.69     |
| 1:D:17:GLN:HG3   | 1:E:149:TRP:CE2  | 2.28        | 0.68     |
| 1:D:60:PHE:O     | 1:D:61:PHE:C     | 2.31        | 0.68     |
| 1:A:129:GLU:HA   | 3:A:382:HOH:O    | 1.93        | 0.68     |
| 1:C:148:ASN:ND2  | 1:C:148:ASN:N    | 2.17        | 0.68     |
| 2:A:160:35G:O2P  | 2:A:161:GDP:PB   | 2.51        | 0.68     |
| 1:E:44:SER:HB2   | 3:E:456:HOH:O    | 1.93        | 0.68     |
| 1:F:41:MET:HG3   | 1:F:41:MET:O     | 1.94        | 0.68     |
| 1:B:57:ASP:CG    | 1:B:58:ARG:H     | 1.93        | 0.68     |
| 1:B:94:THR:HA    | 1:B:105:ARG:NH1  | 2.08        | 0.68     |
| 1:D:143:LYS:HB2  | 1:D:143:LYS:HZ2  | 1.58        | 0.68     |
| 1:F:48:LEU:HD12  | 1:F:69:HIS:HB2   | 1.74        | 0.68     |
| 1:B:117:ILE:HG12 | 1:B:118:HIS:N    | 2.09        | 0.68     |
| 1:D:130:ILE:O    | 1:D:134:PHE:HB2  | 1.94        | 0.68     |
| 1:E:7:THR:OG1    | 1:E:120:SER:HB2  | 1.94        | 0.68     |
| 1:A:126:ALA:O    | 1:A:130:ILE:HG13 | 1.94        | 0.68     |
| 1:B:127:GLU:HA   | 1:B:130:ILE:HG13 | 1.75        | 0.67     |
| 1:C:143:LYS:HD3  | 1:C:147:GLN:OE1  | 1.94        | 0.67     |
| 1:E:61:PHE:O     | 1:E:64:LEU:HB3   | 1.94        | 0.67     |

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| Atom-1          | Atom-2           | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:E:86:THR:O    | 1:E:90:MET:HG3   | 1.93        | 0.67     |
| 1:C:91:LEU:HD11 | 1:C:117:ILE:HG12 | 1.76        | 0.67     |
| 1:C:146:ALA:O   | 1:C:149:TRP:HB2  | 1.95        | 0.67     |
| 1:F:53:ILE:HG23 | 1:F:54:ASP:N     | 2.10        | 0.67     |
| 1:E:39:LYS:HE3  | 1:E:41:MET:HE3   | 1.76        | 0.67     |
| 1:A:135:HIS:N   | 1:A:138:GLU:OE2  | 2.27        | 0.67     |
| 1:A:37:ALA:O    | 1:A:77:VAL:N     | 2.25        | 0.67     |
| 1:E:88:ARG:HB3  | 3:E:263:HOH:O    | 1.95        | 0.67     |
| 1:B:143:LYS:NZ  | 1:B:143:LYS:HA   | 2.10        | 0.67     |
| 1:B:88:ARG:O    | 1:B:91:LEU:HB2   | 1.94        | 0.66     |
| 1:D:52:TYR:CE1  | 2:D:160:35G:H5'2 | 2.30        | 0.66     |
| 1:B:34:ARG:NH2  | 1:B:79:GLU:OE2   | 2.27        | 0.66     |
| 1:D:95:ASN:O    | 1:D:98:ASP:N     | 2.26        | 0.66     |
| 1:C:95:ASN:HA   | 1:C:112:VAL:HG13 | 1.76        | 0.66     |
| 1:D:47:LEU:O    | 1:D:51:HIS:N     | 2.27        | 0.66     |
| 1:A:114:ARG:NH2 | 1:B:152:GLU:HB3  | 2.10        | 0.66     |
| 1:E:147:GLN:O   | 1:E:151:TYR:HB2  | 1.95        | 0.66     |
| 1:E:39:LYS:HG3  | 1:E:41:MET:HG2   | 1.77        | 0.66     |
| 1:A:129:GLU:HG2 | 3:A:382:HOH:O    | 1.95        | 0.66     |
| 1:A:81:LEU:CD1  | 1:A:82:ASN:HD22  | 2.09        | 0.66     |
| 1:C:139:LEU:N   | 1:C:139:LEU:HD12 | 2.11        | 0.66     |
| 1:E:27:ARG:HG3  | 1:E:104:ILE:CD1  | 2.26        | 0.66     |
| 1:D:151:TYR:HD1 | 1:F:111:GLN:HE21 | 1.43        | 0.66     |
| 1:F:30:GLN:NE2  | 3:F:331:HOH:O    | 2.29        | 0.66     |
| 1:D:135:HIS:O   | 1:D:138:GLU:N    | 2.27        | 0.65     |
| 1:F:123:VAL:O   | 1:F:126:ALA:N    | 2.29        | 0.65     |
| 1:A:47:LEU:C    | 1:A:47:LEU:HD12  | 2.16        | 0.65     |
| 1:C:128:LYS:O   | 1:C:132:LEU:HB2  | 1.95        | 0.65     |
| 1:A:7:THR:OG1   | 1:A:84:VAL:HG22  | 1.97        | 0.65     |
| 1:B:57:ASP:O    | 1:B:61:PHE:HB3   | 1.96        | 0.65     |
| 1:F:95:ASN:O    | 1:F:97:ALA:N     | 2.29        | 0.65     |
| 1:E:18:ARG:O    | 1:E:20:LEU:N     | 2.30        | 0.65     |
| 1:C:102:GLY:N   | 1:C:107:ASP:OD1  | 2.30        | 0.65     |
| 1:E:80:GLY:H    | 1:E:83:VAL:HG22  | 1.62        | 0.65     |
| 3:A:256:HOH:O   | 1:E:21:ILE:HD12  | 1.96        | 0.65     |
| 1:C:122:SER:O   | 1:C:126:ALA:N    | 2.19        | 0.65     |
| 1:D:58:ARG:O    | 1:D:59:PRO:C     | 2.33        | 0.65     |
| 1:E:55:LEU:H    | 1:E:55:LEU:HD23  | 1.62        | 0.65     |
| 2:B:160:35G:C5' | 2:B:161:GDP:O3B  | 2.44        | 0.64     |
| 1:F:115:ASN:O   | 1:F:117:ILE:N    | 2.26        | 0.64     |
| 1:F:34:ARG:NH1  | 1:F:142:TYR:CE1  | 2.62        | 0.64     |
| 1:E:50:GLU:CG   | 1:E:132:LEU:HD21 | 2.26        | 0.64     |

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| Atom-1          | Atom-2           | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:B:58:ARG:HA   | 3:B:409:HOH:O    | 1.97        | 0.64     |
| 1:E:126:ALA:C   | 1:E:130:ILE:HD12 | 2.16        | 0.64     |
| 1:A:114:ARG:O   | 1:A:116:ILE:N    | 2.30        | 0.64     |
| 1:F:87:GLY:O    | 1:F:90:MET:HB2   | 1.97        | 0.64     |
| 1:B:39:LYS:HE3  | 1:B:41:MET:HE3   | 1.79        | 0.64     |
| 1:D:17:GLN:HG3  | 1:E:149:TRP:CZ2  | 2.32        | 0.64     |
| 1:B:95:ASN:O    | 1:B:97:ALA:N     | 2.31        | 0.64     |
| 1:B:88:ARG:HH21 | 1:B:121:ASP:CB   | 2.10        | 0.64     |
| 1:B:86:THR:HG23 | 3:B:357:HOH:O    | 1.98        | 0.64     |
| 1:C:144:SER:O   | 1:C:147:GLN:HB3  | 1.98        | 0.64     |
| 1:F:143:LYS:HD2 | 1:F:147:GLN:OE1  | 1.98        | 0.64     |
| 1:F:61:PHE:O    | 1:F:64:LEU:HB3   | 1.98        | 0.64     |
| 1:F:33:PHE:CD1  | 1:F:80:GLY:HA3   | 2.33        | 0.64     |
| 1:E:55:LEU:HD22 | 3:E:266:HOH:O    | 1.97        | 0.64     |
| 1:E:115:ASN:C   | 1:E:116:ILE:HG12 | 2.18        | 0.63     |
| 1:A:85:LYS:O    | 1:A:89:VAL:HG23  | 1.98        | 0.63     |
| 1:D:123:VAL:O   | 1:D:126:ALA:HB3  | 1.98        | 0.63     |
| 1:C:53:ILE:HG23 | 1:C:54:ASP:N     | 2.12        | 0.63     |
| 2:A:160:35G:O2P | 2:A:161:GDP:O3B  | 2.16        | 0.63     |
| 1:A:114:ARG:CZ  | 1:B:152:GLU:HB3  | 2.29        | 0.63     |
| 1:B:142:TYR:HA  | 3:B:427:HOH:O    | 1.98        | 0.63     |
| 1:A:13:PRO:HD3  | 1:A:73:VAL:CG1   | 2.23        | 0.63     |
| 1:E:118:HIS:ND1 | 2:E:160:35G:O1P  | 2.30        | 0.63     |
| 1:C:67:TYR:HA   | 1:C:70:SER:OG    | 1.98        | 0.63     |
| 1:B:80:GLY:O    | 1:B:83:VAL:HG22  | 1.97        | 0.63     |
| 1:D:3:ASN:HA    | 1:D:81:LEU:HA    | 1.80        | 0.62     |
| 1:B:48:LEU:O    | 1:B:51:HIS:N     | 2.31        | 0.62     |
| 1:C:115:ASN:N   | 1:C:115:ASN:OD1  | 2.27        | 0.62     |
| 1:E:12:LYS:HE3  | 1:E:117:ILE:O    | 2.00        | 0.62     |
| 1:F:84:VAL:O    | 1:F:85:LYS:C     | 2.34        | 0.62     |
| 1:B:122:SER:OG  | 1:B:125:SER:HB3  | 1.98        | 0.62     |
| 1:F:14:ASP:O    | 1:F:18:ARG:HG3   | 2.00        | 0.62     |
| 1:F:113:GLY:C   | 1:F:114:ARG:HG2  | 2.12        | 0.62     |
| 1:D:122:SER:O   | 1:D:126:ALA:N    | 2.30        | 0.62     |
| 1:C:43:ALA:CB   | 1:C:47:LEU:HD13  | 2.29        | 0.62     |
| 1:E:10:ALA:N    | 1:E:118:HIS:O    | 2.31        | 0.62     |
| 1:D:23:GLU:O    | 1:D:27:ARG:HG2   | 1.99        | 0.62     |
| 2:F:160:35G:O5' | 2:F:161:GDP:O3A  | 2.17        | 0.62     |
| 1:A:23:GLU:O    | 1:A:27:ARG:HG2   | 1.99        | 0.62     |
| 1:A:147:GLN:NE2 | 1:A:151:TYR:HD2  | 1.90        | 0.62     |
| 1:A:34:ARG:NH1  | 1:A:142:TYR:CE1  | 2.68        | 0.62     |
| 1:B:44:SER:OG   | 1:B:47:LEU:HB2   | 1.99        | 0.62     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:F:88:ARG:HD2   | 1:F:120:SER:O    | 2.00        | 0.62     |
| 1:E:39:LYS:NZ    | 1:E:133:TRP:O    | 2.31        | 0.62     |
| 1:E:113:GLY:HA3  | 1:F:152:GLU:OE1  | 1.99        | 0.62     |
| 1:B:139:LEU:N    | 1:B:139:LEU:HD22 | 2.14        | 0.62     |
| 1:C:113:GLY:O    | 1:C:114:ARG:HG2  | 1.99        | 0.62     |
| 1:A:36:VAL:N     | 1:A:77:VAL:O     | 2.29        | 0.62     |
| 1:B:51:HIS:HB2   | 1:B:132:LEU:CD1  | 2.30        | 0.62     |
| 1:C:12:LYS:HB3   | 1:C:13:PRO:CD    | 2.30        | 0.62     |
| 1:C:144:SER:OG   | 1:C:147:GLN:HB2  | 1.99        | 0.62     |
| 2:B:160:35G:H5'2 | 3:B:503:HOH:O    | 2.00        | 0.61     |
| 1:A:135:HIS:O    | 1:A:138:GLU:HG3  | 1.99        | 0.61     |
| 1:E:127:GLU:HA   | 1:E:130:ILE:HD12 | 1.81        | 0.61     |
| 1:C:111:GLN:O    | 1:C:114:ARG:N    | 2.29        | 0.61     |
| 1:A:80:GLY:O     | 1:A:83:VAL:HG22  | 1.99        | 0.61     |
| 1:A:96:PRO:HG3   | 1:A:115:ASN:HB3  | 1.83        | 0.61     |
| 1:A:11:ILE:HG13  | 1:A:76:MET:CE    | 2.30        | 0.61     |
| 1:C:123:VAL:O    | 1:C:126:ALA:HB3  | 2.01        | 0.61     |
| 1:C:101:PRO:HG3  | 3:C:302:HOH:O    | 2.01        | 0.61     |
| 1:C:54:ASP:HB3   | 3:C:358:HOH:O    | 1.99        | 0.61     |
| 2:D:160:35G:O2P  | 2:D:161:GDP:O3B  | 2.18        | 0.61     |
| 1:D:97:ALA:HA    | 3:D:239:HOH:O    | 2.00        | 0.61     |
| 2:B:160:35G:P    | 2:B:161:GDP:O3B  | 2.59        | 0.61     |
| 1:F:85:LYS:HE3   | 3:F:481:HOH:O    | 2.00        | 0.61     |
| 1:D:93:GLU:O     | 1:D:105:ARG:HD2  | 2.00        | 0.61     |
| 1:A:64:LEU:O     | 1:A:68:MET:HG2   | 2.00        | 0.61     |
| 1:A:96:PRO:HB3   | 1:A:105:ARG:HB3  | 1.82        | 0.61     |
| 1:E:150:ILE:HG22 | 1:E:150:ILE:O    | 2.01        | 0.61     |
| 1:D:15:GLY:N     | 1:D:116:ILE:HG22 | 2.15        | 0.61     |
| 1:D:9:ILE:N      | 1:D:76:MET:O     | 2.33        | 0.61     |
| 1:E:50:GLU:HG2   | 1:E:132:LEU:HD21 | 1.83        | 0.61     |
| 1:E:14:ASP:OD1   | 1:E:67:TYR:OH    | 2.14        | 0.60     |
| 1:F:91:LEU:HA    | 1:F:104:ILE:HG13 | 1.82        | 0.60     |
| 1:F:33:PHE:HD1   | 1:F:80:GLY:HA3   | 1.65        | 0.60     |
| 1:B:64:LEU:O     | 1:B:65:VAL:C     | 2.36        | 0.60     |
| 1:B:8:PHE:CZ     | 1:B:10:ALA:HB2   | 2.36        | 0.60     |
| 1:B:136:PRO:O    | 1:B:137:GLU:HG3  | 2.01        | 0.60     |
| 1:A:29:GLU:OE1   | 1:E:19:GLY:HA2   | 2.00        | 0.60     |
| 1:F:5:GLU:OE2    | 1:F:84:VAL:HG23  | 2.01        | 0.60     |
| 1:D:11:ILE:HG22  | 1:D:16:VAL:HG23  | 1.83        | 0.60     |
| 2:B:160:35G:C5'  | 2:B:161:GDP:PB   | 2.89        | 0.60     |
| 1:A:38:MET:HB2   | 1:A:76:MET:CG    | 2.31        | 0.60     |
| 1:B:42:ARG:HA    | 1:B:72:PRO:HA    | 1.84        | 0.60     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:45:GLU:O     | 1:D:48:LEU:HB2   | 2.02        | 0.60     |
| 1:F:33:PHE:CE1   | 1:F:83:VAL:HG13  | 2.36        | 0.60     |
| 1:A:41:MET:CE    | 1:A:133:TRP:CZ3  | 2.85        | 0.60     |
| 1:E:130:ILE:O    | 1:E:134:PHE:N    | 2.31        | 0.59     |
| 1:D:91:LEU:HD11  | 1:D:117:ILE:HD13 | 1.83        | 0.59     |
| 1:A:142:TYR:HA   | 3:A:389:HOH:O    | 2.01        | 0.59     |
| 1:C:34:ARG:NH1   | 1:C:140:VAL:O    | 2.34        | 0.59     |
| 1:C:58:ARG:HD3   | 1:C:58:ARG:H     | 1.67        | 0.59     |
| 1:B:41:MET:O     | 1:B:73:VAL:N     | 2.29        | 0.59     |
| 1:E:80:GLY:O     | 1:E:83:VAL:HG22  | 2.02        | 0.59     |
| 1:F:12:LYS:O     | 1:F:16:VAL:HG23  | 2.01        | 0.59     |
| 1:D:7:THR:HB     | 1:D:84:VAL:HA    | 1.84        | 0.59     |
| 1:E:81:LEU:CD1   | 1:E:82:ASN:HD22  | 2.15        | 0.59     |
| 1:B:6:ARG:HA     | 1:B:78:TRP:O     | 2.02        | 0.59     |
| 1:B:58:ARG:O     | 1:B:61:PHE:N     | 2.32        | 0.59     |
| 1:E:112:VAL:HG23 | 1:E:113:GLY:H    | 1.67        | 0.59     |
| 1:E:125:SER:O    | 1:E:129:GLU:HB2  | 2.03        | 0.59     |
| 2:A:160:35G:O5'  | 2:A:161:GDP:PB   | 2.60        | 0.59     |
| 1:D:45:GLU:HG2   | 1:D:65:VAL:CG1   | 2.32        | 0.59     |
| 1:B:38:MET:HG3   | 1:B:76:MET:HB3   | 1.85        | 0.59     |
| 1:F:129:GLU:O    | 1:F:133:TRP:HD1  | 1.86        | 0.58     |
| 1:B:125:SER:O    | 1:B:126:ALA:C    | 2.39        | 0.58     |
| 1:B:59:PRO:HD3   | 3:B:409:HOH:O    | 2.04        | 0.58     |
| 1:B:6:ARG:HG3    | 1:B:79:GLU:HB2   | 1.84        | 0.58     |
| 1:B:40:PHE:CE1   | 1:B:72:PRO:HB2   | 2.38        | 0.58     |
| 1:F:86:THR:O     | 1:F:87:GLY:C     | 2.36        | 0.58     |
| 1:F:67:TYR:O     | 1:F:70:SER:OG    | 2.19        | 0.58     |
| 1:D:64:LEU:HD12  | 1:D:64:LEU:O     | 2.02        | 0.58     |
| 1:B:58:ARG:CG    | 1:B:59:PRO:HD2   | 2.27        | 0.58     |
| 1:B:49:LYS:HZ2   | 1:B:65:VAL:HG11  | 1.66        | 0.58     |
| 1:D:32:GLY:O     | 1:F:110:ILE:CD1  | 2.51        | 0.58     |
| 1:D:33:PHE:N     | 3:D:352:HOH:O    | 2.36        | 0.58     |
| 1:B:87:GLY:O     | 1:B:90:MET:N     | 2.37        | 0.58     |
| 1:D:52:TYR:O     | 1:D:61:PHE:HE1   | 1.86        | 0.58     |
| 1:A:97:ALA:N     | 3:A:249:HOH:O    | 2.30        | 0.58     |
| 1:B:143:LYS:HZ3  | 1:B:143:LYS:HA   | 1.68        | 0.58     |
| 1:D:35:LEU:HD21  | 1:D:38:MET:HB2   | 1.86        | 0.58     |
| 1:B:40:PHE:HB2   | 1:D:38:MET:HB3   | 1.85        | 0.58     |
| 1:F:14:ASP:OD1   | 1:F:67:TYR:OH    | 2.21        | 0.58     |
| 1:E:80:GLY:N     | 1:E:83:VAL:CG2   | 2.66        | 0.58     |
| 1:B:140:VAL:HG11 | 1:D:72:PRO:HG3   | 1.86        | 0.58     |
| 1:A:87:GLY:O     | 1:A:91:LEU:HD13  | 2.03        | 0.58     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:115:ASN:O    | 1:A:117:ILE:N    | 2.31        | 0.57     |
| 1:D:60:PHE:O     | 1:D:61:PHE:O     | 2.22        | 0.57     |
| 1:F:143:LYS:HZ3  | 1:F:147:GLN:CD   | 2.07        | 0.57     |
| 1:F:44:SER:O     | 1:F:47:LEU:HB3   | 2.03        | 0.57     |
| 1:E:47:LEU:N     | 3:E:456:HOH:O    | 2.37        | 0.57     |
| 1:E:139:LEU:N    | 1:E:139:LEU:HD12 | 2.17        | 0.57     |
| 1:B:89:VAL:O     | 1:B:103:THR:HG22 | 2.04        | 0.57     |
| 1:B:20:LEU:O     | 1:B:24:ILE:HG13  | 2.04        | 0.57     |
| 1:D:44:SER:OG    | 1:D:47:LEU:HB2   | 2.04        | 0.57     |
| 1:F:120:SER:OG   | 1:F:126:ALA:HA   | 2.05        | 0.57     |
| 1:D:81:LEU:O     | 1:D:82:ASN:HB2   | 2.02        | 0.57     |
| 1:E:55:LEU:HD13  | 3:E:266:HOH:O    | 2.03        | 0.57     |
| 1:D:100:LYS:O    | 1:D:106:GLY:HA3  | 2.04        | 0.57     |
| 1:C:140:VAL:HG11 | 1:F:72:PRO:CG    | 2.30        | 0.57     |
| 1:D:32:GLY:O     | 1:F:110:ILE:HD11 | 2.03        | 0.57     |
| 1:D:147:GLN:O    | 1:D:147:GLN:HG3  | 2.04        | 0.57     |
| 1:B:140:VAL:HG11 | 1:D:72:PRO:HB3   | 1.86        | 0.57     |
| 1:B:51:HIS:O     | 1:B:53:ILE:HG22  | 2.04        | 0.56     |
| 1:B:80:GLY:N     | 1:B:83:VAL:HG22  | 2.20        | 0.56     |
| 1:F:8:PHE:HD2    | 1:F:129:GLU:OE1  | 1.88        | 0.56     |
| 1:E:12:LYS:HB3   | 1:E:13:PRO:CD    | 2.34        | 0.56     |
| 1:F:39:LYS:HE3   | 1:F:41:MET:HE1   | 1.86        | 0.56     |
| 1:E:20:LEU:O     | 1:E:24:ILE:HG13  | 2.05        | 0.56     |
| 1:E:47:LEU:HD12  | 1:E:47:LEU:O     | 2.05        | 0.56     |
| 1:A:43:ALA:HB3   | 1:A:48:LEU:HD21  | 1.87        | 0.56     |
| 1:D:80:GLY:HA2   | 3:D:446:HOH:O    | 2.05        | 0.56     |
| 1:F:3:ASN:HA     | 1:F:81:LEU:HA    | 1.87        | 0.56     |
| 1:B:26:LYS:O     | 1:B:27:ARG:C     | 2.42        | 0.56     |
| 1:A:20:LEU:O     | 1:A:21:ILE:C     | 2.39        | 0.56     |
| 1:C:105:ARG:HD3  | 1:C:115:ASN:HB2  | 1.87        | 0.56     |
| 1:F:123:VAL:O    | 1:F:124:GLU:C    | 2.43        | 0.56     |
| 1:F:126:ALA:O    | 1:F:130:ILE:HG13 | 2.05        | 0.56     |
| 1:F:100:LYS:HE3  | 3:F:364:HOH:O    | 2.06        | 0.56     |
| 1:F:53:ILE:HG23  | 1:F:54:ASP:H     | 1.71        | 0.56     |
| 1:D:44:SER:O     | 1:D:48:LEU:HD12  | 2.05        | 0.56     |
| 1:A:80:GLY:O     | 1:A:81:LEU:C     | 2.42        | 0.56     |
| 1:C:48:LEU:HD12  | 1:C:69:HIS:HB2   | 1.88        | 0.56     |
| 1:E:14:ASP:HA    | 1:F:149:TRP:CE3  | 2.41        | 0.56     |
| 1:D:34:ARG:NH1   | 1:D:142:TYR:CD1  | 2.72        | 0.56     |
| 1:B:138:GLU:C    | 1:B:139:LEU:HD13 | 2.26        | 0.56     |
| 1:C:135:HIS:O    | 1:C:138:GLU:HB2  | 2.06        | 0.56     |
| 1:E:6:ARG:HA     | 1:E:78:TRP:O     | 2.06        | 0.56     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:F:72:PRO:HD2   | 3:F:233:HOH:O    | 2.06        | 0.55     |
| 1:B:92:GLY:CA    | 1:B:103:THR:HG21 | 2.35        | 0.55     |
| 1:D:94:THR:OG1   | 2:D:161:GDP:O2B  | 2.22        | 0.55     |
| 1:D:46:ASP:O     | 1:D:47:LEU:C     | 2.44        | 0.55     |
| 1:D:28:PHE:CD1   | 1:D:90:MET:HE1   | 2.41        | 0.55     |
| 1:A:86:THR:O     | 1:A:89:VAL:HB    | 2.06        | 0.55     |
| 1:F:135:HIS:N    | 1:F:138:GLU:OE2  | 2.37        | 0.55     |
| 1:E:43:ALA:HB3   | 1:E:48:LEU:HD21  | 1.89        | 0.55     |
| 1:C:8:PHE:HE1    | 1:C:75:ALA:HB1   | 1.70        | 0.55     |
| 1:C:12:LYS:HE3   | 1:C:117:ILE:O    | 2.07        | 0.55     |
| 1:C:25:ILE:O     | 1:C:28:PHE:HB2   | 2.07        | 0.55     |
| 1:D:83:VAL:O     | 1:D:84:VAL:C     | 2.44        | 0.55     |
| 1:E:12:LYS:HG3   | 1:E:117:ILE:HA   | 1.88        | 0.55     |
| 1:B:123:VAL:O    | 1:B:124:GLU:C    | 2.43        | 0.55     |
| 1:B:45:GLU:HG3   | 1:B:69:HIS:CD2   | 2.42        | 0.55     |
| 1:C:147:GLN:O    | 1:C:147:GLN:HG3  | 1.89        | 0.55     |
| 1:D:2:ALA:O      | 1:D:4:SER:N      | 2.39        | 0.55     |
| 1:D:130:ILE:HG22 | 1:D:130:ILE:O    | 2.06        | 0.55     |
| 1:F:88:ARG:NH1   | 1:F:121:ASP:HB3  | 2.21        | 0.55     |
| 1:A:47:LEU:HD13  | 1:A:132:LEU:CD2  | 2.37        | 0.55     |
| 1:A:79:GLU:HG2   | 1:A:79:GLU:O     | 2.04        | 0.55     |
| 1:D:127:GLU:O    | 1:D:131:ALA:HB2  | 2.07        | 0.55     |
| 1:B:12:LYS:HE3   | 1:B:117:ILE:O    | 2.06        | 0.55     |
| 1:E:54:ASP:C     | 1:E:56:LYS:H     | 2.09        | 0.54     |
| 1:A:80:GLY:N     | 1:A:83:VAL:HG22  | 2.22        | 0.54     |
| 1:D:5:GLU:O      | 1:D:79:GLU:HB2   | 2.07        | 0.54     |
| 1:A:117:ILE:HG12 | 1:A:118:HIS:H    | 1.72        | 0.54     |
| 1:D:38:MET:HA    | 1:D:75:ALA:O     | 2.08        | 0.54     |
| 1:D:83:VAL:HG23  | 1:D:84:VAL:N     | 2.22        | 0.54     |
| 1:E:24:ILE:HG21  | 1:E:117:ILE:HD12 | 1.89        | 0.54     |
| 1:C:83:VAL:O     | 1:C:84:VAL:C     | 2.45        | 0.54     |
| 1:B:145:CYS:SG   | 1:E:146:ALA:HB2  | 2.47        | 0.54     |
| 1:A:130:ILE:O    | 1:A:133:TRP:N    | 2.34        | 0.54     |
| 1:D:132:LEU:O    | 1:D:132:LEU:HD23 | 2.07        | 0.54     |
| 1:C:95:ASN:HB3   | 1:C:98:ASP:HB2   | 1.89        | 0.54     |
| 1:C:29:GLU:OE2   | 1:F:19:GLY:HA2   | 2.07        | 0.54     |
| 1:F:6:ARG:HB3    | 1:F:77:VAL:HG12  | 1.88        | 0.54     |
| 1:B:49:LYS:HB2   | 1:B:49:LYS:HZ3   | 1.73        | 0.54     |
| 1:B:51:HIS:C     | 1:B:53:ILE:H     | 2.10        | 0.54     |
| 1:E:111:GLN:OE1  | 1:F:152:GLU:HB3  | 2.07        | 0.54     |
| 1:E:88:ARG:HH22  | 2:E:161:GDP:PB   | 2.31        | 0.54     |
| 1:C:67:TYR:O     | 1:C:70:SER:OG    | 2.24        | 0.54     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:16:VAL:HG22  | 1:D:21:ILE:HD11  | 1.90        | 0.54     |
| 1:A:41:MET:HE2   | 1:A:133:TRP:CZ3  | 2.43        | 0.54     |
| 1:A:96:PRO:HD3   | 1:A:112:VAL:HA   | 1.89        | 0.54     |
| 1:F:143:LYS:HE3  | 3:F:369:HOH:O    | 2.08        | 0.54     |
| 1:B:117:ILE:CG1  | 1:B:118:HIS:N    | 2.70        | 0.54     |
| 1:B:49:LYS:HB2   | 1:B:49:LYS:NZ    | 2.22        | 0.54     |
| 1:C:140:VAL:HG12 | 1:C:142:TYR:HD1  | 1.73        | 0.54     |
| 1:A:104:ILE:HG13 | 3:A:306:HOH:O    | 2.08        | 0.54     |
| 1:B:108:PHE:HE1  | 1:C:30:GLN:NE2   | 2.06        | 0.54     |
| 1:A:41:MET:CE    | 1:A:133:TRP:HZ3  | 2.21        | 0.54     |
| 1:D:115:ASN:C    | 1:D:117:ILE:H    | 2.10        | 0.53     |
| 1:D:11:ILE:O     | 1:D:73:VAL:HB    | 2.08        | 0.53     |
| 1:A:152:GLU:HB3  | 1:C:111:GLN:CD   | 2.27        | 0.53     |
| 1:D:15:GLY:CA    | 1:D:116:ILE:HG22 | 2.38        | 0.53     |
| 1:A:6:ARG:HG2    | 1:A:79:GLU:HB2   | 1.90        | 0.53     |
| 1:B:117:ILE:HG12 | 1:B:118:HIS:H    | 1.74        | 0.53     |
| 1:F:45:GLU:O     | 1:F:49:LYS:HG3   | 2.08        | 0.53     |
| 1:D:114:ARG:CZ   | 1:E:152:GLU:HB3  | 2.38        | 0.53     |
| 1:C:136:PRO:HG2  | 1:C:137:GLU:HG3  | 1.90        | 0.53     |
| 1:E:125:SER:O    | 1:E:126:ALA:C    | 2.46        | 0.53     |
| 2:F:160:35G:O5'  | 2:F:161:GDP:PB   | 2.66        | 0.53     |
| 1:D:4:SER:HA     | 1:D:79:GLU:HG3   | 1.90        | 0.53     |
| 1:B:51:HIS:O     | 1:B:53:ILE:N     | 2.41        | 0.53     |
| 1:B:88:ARG:HE    | 1:B:121:ASP:HA   | 1.73        | 0.53     |
| 1:C:138:GLU:C    | 1:C:139:LEU:HD12 | 2.28        | 0.53     |
| 1:F:27:ARG:HG2   | 3:F:326:HOH:O    | 2.08        | 0.53     |
| 1:B:52:TYR:OH    | 2:B:160:35G:O1P  | 2.25        | 0.53     |
| 1:E:81:LEU:HD11  | 1:E:82:ASN:HD22  | 1.73        | 0.53     |
| 1:D:6:ARG:CA     | 1:D:83:VAL:HG21  | 2.38        | 0.53     |
| 1:B:117:ILE:CG1  | 1:B:118:HIS:H    | 2.22        | 0.53     |
| 1:B:108:PHE:HA   | 1:C:31:LYS:HA    | 1.91        | 0.53     |
| 1:D:3:ASN:HA     | 1:D:81:LEU:CA    | 2.38        | 0.53     |
| 1:A:11:ILE:HG13  | 1:A:76:MET:HE2   | 1.91        | 0.53     |
| 1:C:38:MET:HG3   | 1:C:76:MET:HG3   | 1.90        | 0.53     |
| 1:B:79:GLU:HA    | 1:B:83:VAL:HG21  | 1.89        | 0.53     |
| 1:B:33:PHE:CZ    | 1:B:83:VAL:HG13  | 2.43        | 0.53     |
| 1:A:125:SER:O    | 1:A:129:GLU:HB2  | 2.09        | 0.53     |
| 1:A:80:GLY:H     | 1:A:83:VAL:CG2   | 2.21        | 0.53     |
| 1:D:34:ARG:NH1   | 1:D:140:VAL:O    | 2.31        | 0.53     |
| 1:C:121:ASP:N    | 1:C:121:ASP:OD1  | 2.31        | 0.53     |
| 1:A:139:LEU:N    | 1:A:139:LEU:HD13 | 2.24        | 0.53     |
| 1:D:139:LEU:N    | 1:D:139:LEU:CD1  | 2.71        | 0.53     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:95:ASN:C     | 1:B:97:ALA:H     | 2.12        | 0.53     |
| 1:B:27:ARG:NH2   | 1:B:107:ASP:OD2  | 2.31        | 0.53     |
| 1:A:105:ARG:HE   | 1:A:115:ASN:HB2  | 1.73        | 0.53     |
| 1:D:85:LYS:O     | 1:D:88:ARG:HB2   | 2.09        | 0.53     |
| 1:E:120:SER:OG   | 1:E:126:ALA:HA   | 2.09        | 0.53     |
| 1:A:128:LYS:HG2  | 1:A:129:GLU:N    | 2.24        | 0.53     |
| 1:F:34:ARG:NH1   | 1:F:142:TYR:CD1  | 2.77        | 0.53     |
| 1:E:58:ARG:HG3   | 1:E:59:PRO:HD2   | 1.91        | 0.53     |
| 2:F:160:35G:H3'  | 2:F:161:GDP:O3A  | 2.08        | 0.52     |
| 1:C:14:ASP:OD1   | 1:C:67:TYR:OH    | 2.24        | 0.52     |
| 1:F:35:LEU:HD21  | 1:F:76:MET:HG2   | 1.89        | 0.52     |
| 1:F:58:ARG:CG    | 1:F:58:ARG:HH11  | 2.14        | 0.52     |
| 1:A:38:MET:HA    | 1:A:75:ALA:O     | 2.09        | 0.52     |
| 1:F:11:ILE:HG12  | 1:F:24:ILE:HD12  | 1.91        | 0.52     |
| 1:F:96:PRO:HD2   | 1:F:112:VAL:HA   | 1.90        | 0.52     |
| 1:C:12:LYS:HD2   | 1:C:116:ILE:C    | 2.28        | 0.52     |
| 1:F:67:TYR:C     | 1:F:69:HIS:H     | 2.13        | 0.52     |
| 1:A:22:GLY:HA2   | 1:E:22:GLY:HA2   | 1.91        | 0.52     |
| 1:A:9:ILE:O      | 1:A:76:MET:N     | 2.39        | 0.52     |
| 1:F:88:ARG:CD    | 1:F:121:ASP:HA   | 2.38        | 0.52     |
| 1:B:23:GLU:O     | 1:B:26:LYS:HB3   | 2.09        | 0.52     |
| 2:A:161:GDP:O1A  | 2:A:161:GDP:O1B  | 2.28        | 0.52     |
| 1:E:115:ASN:N    | 1:E:115:ASN:OD1  | 2.28        | 0.52     |
| 1:C:12:LYS:HD2   | 1:C:117:ILE:CA   | 2.38        | 0.52     |
| 1:B:35:LEU:HD21  | 1:B:38:MET:HE2   | 1.91        | 0.52     |
| 1:C:143:LYS:NZ   | 1:C:143:LYS:HA   | 2.25        | 0.52     |
| 1:A:147:GLN:NE2  | 1:A:151:TYR:HB2  | 2.25        | 0.52     |
| 1:A:100:LYS:O    | 1:A:106:GLY:HA3  | 2.10        | 0.52     |
| 1:D:108:PHE:HD2  | 1:E:30:GLN:HB2   | 1.75        | 0.52     |
| 1:E:135:HIS:O    | 1:E:137:GLU:N    | 2.42        | 0.52     |
| 1:D:17:GLN:HA    | 1:D:17:GLN:OE1   | 2.10        | 0.52     |
| 1:A:53:ILE:O     | 1:A:56:LYS:HB2   | 2.10        | 0.52     |
| 1:B:84:VAL:O     | 1:B:88:ARG:HG2   | 2.10        | 0.52     |
| 1:C:113:GLY:C    | 1:C:114:ARG:HG2  | 2.30        | 0.52     |
| 1:A:110:ILE:HG22 | 1:A:110:ILE:O    | 2.09        | 0.52     |
| 1:F:31:LYS:HG3   | 1:F:31:LYS:O     | 2.08        | 0.52     |
| 1:C:53:ILE:CG2   | 1:C:54:ASP:N     | 2.73        | 0.51     |
| 1:C:87:GLY:O     | 1:C:91:LEU:HB2   | 2.10        | 0.51     |
| 2:D:161:GDP:O1A  | 2:D:161:GDP:O1B  | 2.29        | 0.51     |
| 1:E:34:ARG:NH1   | 1:E:36:VAL:HG22  | 2.26        | 0.51     |
| 1:B:51:HIS:HB2   | 1:B:132:LEU:HD11 | 1.91        | 0.51     |
| 1:E:117:ILE:HG12 | 1:E:118:HIS:N    | 2.25        | 0.51     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:85:LYS:O     | 1:B:89:VAL:HG23  | 2.10        | 0.51     |
| 1:C:123:VAL:CG2  | 1:C:124:GLU:N    | 2.74        | 0.51     |
| 1:F:51:HIS:O     | 1:F:53:ILE:HG22  | 2.10        | 0.51     |
| 1:E:50:GLU:HG3   | 1:E:132:LEU:HD21 | 1.90        | 0.51     |
| 1:F:122:SER:O    | 1:F:126:ALA:N    | 2.42        | 0.51     |
| 1:D:54:ASP:N     | 1:D:54:ASP:OD1   | 2.44        | 0.51     |
| 1:F:61:PHE:CE1   | 1:F:65:VAL:HG21  | 2.44        | 0.51     |
| 1:C:67:TYR:HA    | 1:C:70:SER:HG    | 1.75        | 0.51     |
| 1:D:9:ILE:O      | 1:D:76:MET:N     | 2.40        | 0.51     |
| 1:F:127:GLU:HB3  | 3:F:496:HOH:O    | 2.11        | 0.51     |
| 1:D:42:ARG:HD3   | 1:D:69:HIS:CE1   | 2.45        | 0.51     |
| 1:C:104:ILE:O    | 1:C:108:PHE:HD2  | 1.94        | 0.51     |
| 1:E:34:ARG:HH12  | 1:E:36:VAL:HG22  | 1.75        | 0.51     |
| 1:F:129:GLU:O    | 1:F:133:TRP:N    | 2.43        | 0.51     |
| 1:E:25:ILE:HD11  | 3:E:373:HOH:O    | 2.11        | 0.51     |
| 1:A:38:MET:HA    | 1:A:76:MET:HA    | 1.92        | 0.51     |
| 1:E:60:PHE:O     | 1:E:61:PHE:C     | 2.49        | 0.51     |
| 1:E:140:VAL:CG1  | 1:E:141:ASN:H    | 2.18        | 0.51     |
| 1:B:5:GLU:HB3    | 1:B:80:GLY:O     | 2.10        | 0.51     |
| 1:D:150:ILE:HG22 | 1:D:150:ILE:O    | 2.10        | 0.51     |
| 1:C:72:PRO:CG    | 1:F:140:VAL:HG11 | 2.23        | 0.51     |
| 1:D:123:VAL:HA   | 1:D:126:ALA:HB3  | 1.93        | 0.51     |
| 1:C:113:GLY:O    | 1:C:114:ARG:NE   | 2.39        | 0.51     |
| 1:E:11:ILE:HD12  | 1:E:74:VAL:HB    | 1.92        | 0.51     |
| 1:F:20:LEU:O     | 1:F:24:ILE:HG13  | 2.11        | 0.51     |
| 1:D:12:LYS:HG2   | 1:D:68:MET:SD    | 2.50        | 0.51     |
| 1:F:56:LYS:HD2   | 3:F:297:HOH:O    | 2.10        | 0.51     |
| 1:F:5:GLU:HG2    | 1:F:83:VAL:HG23  | 1.92        | 0.51     |
| 1:D:6:ARG:O      | 1:D:84:VAL:HG23  | 2.12        | 0.50     |
| 1:E:140:VAL:CG1  | 1:E:141:ASN:N    | 2.69        | 0.50     |
| 1:C:137:GLU:OE1  | 1:C:137:GLU:O    | 2.30        | 0.50     |
| 1:A:148:ASN:N    | 1:A:148:ASN:ND2  | 2.39        | 0.50     |
| 1:E:142:TYR:N    | 1:E:142:TYR:CD1  | 2.80        | 0.50     |
| 1:A:23:GLU:OE1   | 1:E:26:LYS:NZ    | 2.36        | 0.50     |
| 1:F:122:SER:O    | 1:F:125:SER:HB2  | 2.11        | 0.50     |
| 1:F:64:LEU:O     | 1:F:65:VAL:C     | 2.48        | 0.50     |
| 1:C:12:LYS:HB3   | 1:C:13:PRO:HD2   | 1.94        | 0.50     |
| 1:D:2:ALA:C      | 1:D:4:SER:H      | 2.15        | 0.50     |
| 1:F:32:GLY:HA2   | 3:F:252:HOH:O    | 2.11        | 0.50     |
| 1:D:110:ILE:HD13 | 1:E:33:PHE:CD1   | 2.46        | 0.50     |
| 1:C:39:LYS:HE2   | 1:C:134:PHE:CD1  | 2.46        | 0.50     |
| 1:F:6:ARG:HB3    | 1:F:77:VAL:CG1   | 2.41        | 0.50     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:F:39:LYS:HE3   | 1:F:41:MET:HE2   | 1.92        | 0.50     |
| 1:E:88:ARG:CZ    | 1:E:121:ASP:HB2  | 2.41        | 0.50     |
| 1:E:127:GLU:CA   | 1:E:130:ILE:HD12 | 2.42        | 0.50     |
| 1:B:39:LYS:HG3   | 1:B:41:MET:HG2   | 1.94        | 0.50     |
| 1:A:130:ILE:HG22 | 1:A:131:ALA:N    | 2.26        | 0.50     |
| 1:A:94:THR:HG23  | 1:A:95:ASN:N     | 2.25        | 0.50     |
| 1:A:139:LEU:CD1  | 1:A:139:LEU:N    | 2.74        | 0.50     |
| 1:F:135:HIS:O    | 1:F:138:GLU:HG3  | 2.10        | 0.49     |
| 1:A:30:GLN:NE2   | 3:A:325:HOH:O    | 2.43        | 0.49     |
| 1:B:33:PHE:CD1   | 1:B:83:VAL:HG13  | 2.47        | 0.49     |
| 1:C:45:GLU:HA    | 1:C:48:LEU:HB2   | 1.94        | 0.49     |
| 1:D:28:PHE:HD1   | 1:D:90:MET:HE1   | 1.77        | 0.49     |
| 1:E:60:PHE:CZ    | 2:E:161:GDP:C8   | 2.99        | 0.49     |
| 1:E:139:LEU:N    | 1:E:139:LEU:CD1  | 2.75        | 0.49     |
| 1:C:99:SER:O     | 1:C:106:GLY:HA2  | 2.12        | 0.49     |
| 1:A:14:ASP:OD2   | 1:A:114:ARG:O    | 2.29        | 0.49     |
| 1:E:33:PHE:CE1   | 1:E:83:VAL:HG13  | 2.48        | 0.49     |
| 1:A:110:ILE:HG23 | 3:B:399:HOH:O    | 2.12        | 0.49     |
| 1:A:112:VAL:O    | 1:A:112:VAL:HG12 | 2.12        | 0.49     |
| 1:E:50:GLU:O     | 1:E:53:ILE:HG22  | 2.12        | 0.49     |
| 1:E:140:VAL:HG22 | 3:E:375:HOH:O    | 2.12        | 0.49     |
| 1:A:22:GLY:O     | 1:E:22:GLY:HA3   | 2.12        | 0.49     |
| 1:E:60:PHE:HE2   | 2:E:161:GDP:O4'  | 1.96        | 0.49     |
| 1:C:143:LYS:CE   | 1:C:143:LYS:HA   | 2.42        | 0.49     |
| 1:A:61:PHE:O     | 1:A:62:ALA:C     | 2.51        | 0.49     |
| 1:C:129:GLU:O    | 1:C:133:TRP:N    | 2.46        | 0.49     |
| 1:C:14:ASP:O     | 1:C:18:ARG:HB2   | 2.12        | 0.49     |
| 1:A:85:LYS:HB2   | 3:A:396:HOH:O    | 2.12        | 0.49     |
| 1:F:40:PHE:CE1   | 1:F:72:PRO:HB2   | 2.47        | 0.49     |
| 1:A:47:LEU:CD1   | 1:A:132:LEU:HD22 | 2.42        | 0.49     |
| 1:D:47:LEU:HD11  | 1:D:132:LEU:CD2  | 2.43        | 0.49     |
| 1:C:139:LEU:N    | 1:C:139:LEU:CD1  | 2.74        | 0.49     |
| 1:C:134:PHE:HD1  | 1:C:138:GLU:OE1  | 1.96        | 0.49     |
| 1:F:96:PRO:HB2   | 1:F:110:ILE:O    | 2.13        | 0.48     |
| 1:D:64:LEU:HD12  | 1:D:64:LEU:C     | 2.33        | 0.48     |
| 1:B:102:GLY:N    | 3:B:415:HOH:O    | 2.45        | 0.48     |
| 1:D:135:HIS:O    | 1:D:137:GLU:N    | 2.46        | 0.48     |
| 1:B:14:ASP:OD1   | 1:B:67:TYR:OH    | 2.30        | 0.48     |
| 1:E:14:ASP:HA    | 1:F:149:TRP:HE3  | 1.78        | 0.48     |
| 1:B:93:GLU:N     | 1:B:99:SER:OG    | 2.45        | 0.48     |
| 1:D:152:GLU:HG3  | 1:D:152:GLU:OXT  | 2.13        | 0.48     |
| 1:C:74:VAL:HG12  | 1:C:74:VAL:O     | 2.14        | 0.48     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:140:VAL:CG1  | 1:D:141:ASN:N    | 2.76        | 0.48     |
| 1:F:9:ILE:O      | 1:F:76:MET:HB2   | 2.13        | 0.48     |
| 1:C:46:ASP:O     | 1:C:50:GLU:HB2   | 2.13        | 0.48     |
| 1:D:77:VAL:HG12  | 1:D:78:TRP:N     | 2.27        | 0.48     |
| 1:F:42:ARG:HA    | 1:F:72:PRO:HA    | 1.94        | 0.48     |
| 1:E:43:ALA:O     | 1:E:69:HIS:ND1   | 2.29        | 0.48     |
| 1:B:4:SER:O      | 1:B:5:GLU:C      | 2.52        | 0.48     |
| 1:C:96:PRO:HA    | 1:C:99:SER:OG    | 2.13        | 0.48     |
| 1:F:11:ILE:HD13  | 1:F:21:ILE:HA    | 1.96        | 0.48     |
| 1:B:109:CYS:HB3  | 1:B:116:ILE:HD13 | 1.95        | 0.48     |
| 1:B:48:LEU:CB    | 1:B:65:VAL:HG13  | 2.44        | 0.48     |
| 1:E:88:ARG:O     | 1:E:91:LEU:HB2   | 2.13        | 0.48     |
| 1:D:52:TYR:OH    | 2:D:160:35G:O1P  | 2.24        | 0.48     |
| 1:E:81:LEU:HG    | 1:E:81:LEU:O     | 2.14        | 0.48     |
| 1:D:87:GLY:O     | 1:D:90:MET:HB2   | 2.12        | 0.48     |
| 1:C:150:ILE:HG22 | 1:C:150:ILE:O    | 2.10        | 0.48     |
| 1:B:49:LYS:HZ1   | 1:B:65:VAL:HG11  | 1.73        | 0.48     |
| 1:D:143:LYS:HB2  | 1:D:143:LYS:HZ3  | 1.74        | 0.48     |
| 1:D:46:ASP:HA    | 1:D:49:LYS:CD    | 2.43        | 0.48     |
| 1:D:86:THR:O     | 1:D:87:GLY:C     | 2.51        | 0.48     |
| 1:C:5:GLU:O      | 1:C:83:VAL:HG22  | 2.13        | 0.48     |
| 1:C:7:THR:CB     | 1:C:84:VAL:HG22  | 2.44        | 0.48     |
| 1:D:110:ILE:CD1  | 1:E:33:PHE:CD1   | 2.96        | 0.48     |
| 1:A:56:LYS:HD2   | 1:A:57:ASP:OD1   | 2.13        | 0.48     |
| 1:B:118:HIS:CG   | 1:B:119:GLY:N    | 2.80        | 0.48     |
| 1:E:67:TYR:O     | 1:E:68:MET:C     | 2.49        | 0.48     |
| 1:F:87:GLY:O     | 1:F:91:LEU:HD13  | 2.14        | 0.48     |
| 1:B:2:ALA:O      | 1:B:5:GLU:HB2    | 2.13        | 0.48     |
| 1:B:128:LYS:HG2  | 1:B:129:GLU:N    | 2.29        | 0.48     |
| 1:C:6:ARG:HG3    | 1:C:6:ARG:H      | 1.22        | 0.48     |
| 1:E:33:PHE:CD1   | 1:E:83:VAL:HG13  | 2.48        | 0.48     |
| 1:A:41:MET:HE2   | 1:A:133:TRP:HZ3  | 1.78        | 0.48     |
| 1:F:95:ASN:C     | 1:F:97:ALA:H     | 2.17        | 0.48     |
| 1:A:34:ARG:NH2   | 1:A:36:VAL:HG22  | 2.29        | 0.47     |
| 1:D:27:ARG:NH1   | 1:D:102:GLY:O    | 2.46        | 0.47     |
| 1:E:38:MET:HA    | 1:E:75:ALA:O     | 2.14        | 0.47     |
| 1:E:143:LYS:HA   | 1:E:143:LYS:HZ2  | 1.77        | 0.47     |
| 1:A:17:GLN:HG3   | 1:B:149:TRP:CZ2  | 2.49        | 0.47     |
| 1:A:35:LEU:O     | 1:A:142:TYR:OH   | 2.27        | 0.47     |
| 1:E:34:ARG:O     | 1:E:78:TRP:HA    | 2.13        | 0.47     |
| 1:C:25:ILE:HG21  | 1:C:25:ILE:HD13  | 1.69        | 0.47     |
| 1:C:118:HIS:CG   | 1:C:119:GLY:N    | 2.82        | 0.47     |

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| Atom-1          | Atom-2           | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:A:11:ILE:HA   | 1:A:117:ILE:HG13 | 1.95        | 0.47     |
| 1:F:124:GLU:HB2 | 3:F:485:HOH:O    | 2.15        | 0.47     |
| 1:F:141:ASN:OD1 | 1:F:141:ASN:N    | 2.46        | 0.47     |
| 1:C:145:CYS:HB2 | 1:D:145:CYS:O    | 2.14        | 0.47     |
| 1:C:40:PHE:CE2  | 1:F:140:VAL:HB   | 2.49        | 0.47     |
| 1:B:133:TRP:CD1 | 1:B:133:TRP:N    | 2.83        | 0.47     |
| 1:F:67:TYR:O    | 1:F:69:HIS:N     | 2.46        | 0.47     |
| 1:C:83:VAL:HG23 | 1:C:84:VAL:H     | 1.79        | 0.47     |
| 1:F:123:VAL:HB  | 1:F:124:GLU:H    | 1.48        | 0.47     |
| 1:D:51:HIS:HD2  | 1:D:52:TYR:CD2   | 2.32        | 0.47     |
| 1:C:24:ILE:O    | 1:C:27:ARG:HB2   | 2.14        | 0.47     |
| 1:E:127:GLU:N   | 1:E:130:ILE:HD12 | 2.29        | 0.47     |
| 1:E:129:GLU:O   | 1:E:133:TRP:HD1  | 1.98        | 0.47     |
| 1:C:111:GLN:N   | 3:C:209:HOH:O    | 2.30        | 0.47     |
| 1:B:59:PRO:N    | 3:B:365:HOH:O    | 2.47        | 0.47     |
| 1:E:124:GLU:O   | 1:E:127:GLU:N    | 2.48        | 0.47     |
| 1:C:26:LYS:O    | 1:C:27:ARG:C     | 2.53        | 0.47     |
| 1:A:80:GLY:H    | 1:A:83:VAL:HG22  | 1.79        | 0.47     |
| 1:C:95:ASN:C    | 1:C:97:ALA:H     | 2.18        | 0.47     |
| 1:A:135:HIS:HB3 | 1:A:137:GLU:OE2  | 2.15        | 0.47     |
| 1:F:113:GLY:O   | 1:F:114:ARG:NE   | 2.48        | 0.47     |
| 1:F:143:LYS:HZ3 | 1:F:147:GLN:NE2  | 2.12        | 0.47     |
| 1:E:85:LYS:HB3  | 3:E:354:HOH:O    | 2.14        | 0.47     |
| 1:B:144:SER:HB3 | 3:D:303:HOH:O    | 2.15        | 0.47     |
| 1:A:118:HIS:HA  | 3:A:502:HOH:O    | 2.14        | 0.47     |
| 1:F:145:CYS:O   | 1:F:147:GLN:N    | 2.48        | 0.47     |
| 1:B:64:LEU:O    | 1:B:67:TYR:HB3   | 2.15        | 0.47     |
| 1:E:40:PHE:CZ   | 1:E:72:PRO:HB2   | 2.49        | 0.47     |
| 1:A:60:PHE:N    | 1:A:60:PHE:CD1   | 2.81        | 0.47     |
| 1:F:12:LYS:HB3  | 1:F:13:PRO:CD    | 2.45        | 0.46     |
| 1:B:24:ILE:O    | 1:B:25:ILE:C     | 2.52        | 0.46     |
| 1:B:88:ARG:HH11 | 1:B:88:ARG:HD2   | 1.54        | 0.46     |
| 3:A:232:HOH:O   | 1:E:144:SER:HB3  | 2.13        | 0.46     |
| 1:F:45:GLU:O    | 1:F:46:ASP:C     | 2.50        | 0.46     |
| 1:D:114:ARG:NH2 | 3:D:226:HOH:O    | 2.48        | 0.46     |
| 1:E:66:LYS:HE3  | 1:E:67:TYR:N     | 2.31        | 0.46     |
| 1:E:135:HIS:HB3 | 1:E:137:GLU:OE2  | 2.16        | 0.46     |
| 1:F:49:LYS:HA   | 1:F:61:PHE:HZ    | 1.80        | 0.46     |
| 1:C:54:ASP:C    | 1:C:55:LEU:HD12  | 2.36        | 0.46     |
| 1:E:22:GLY:O    | 1:E:26:LYS:HB2   | 2.14        | 0.46     |
| 1:D:126:ALA:O   | 1:D:130:ILE:HG13 | 2.16        | 0.46     |
| 1:B:48:LEU:CD2  | 1:B:68:MET:HB3   | 2.35        | 0.46     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:D:40:PHE:CZ    | 1:D:72:PRO:HG2   | 2.51        | 0.46     |
| 1:F:58:ARG:O     | 1:F:59:PRO:C     | 2.53        | 0.46     |
| 1:B:47:LEU:O     | 1:B:48:LEU:C     | 2.54        | 0.46     |
| 1:E:126:ALA:O    | 1:E:130:ILE:HD12 | 2.16        | 0.46     |
| 1:C:55:LEU:HD12  | 1:C:55:LEU:N     | 2.29        | 0.46     |
| 1:A:51:HIS:ND1   | 1:A:133:TRP:NE1  | 2.62        | 0.46     |
| 1:B:40:PHE:CZ    | 1:B:72:PRO:HB2   | 2.49        | 0.46     |
| 2:C:160:35G:P    | 2:C:161:GDP:PB   | 3.11        | 0.46     |
| 1:D:81:LEU:HG    | 1:D:81:LEU:O     | 2.15        | 0.46     |
| 1:C:18:ARG:NH1   | 1:C:108:PHE:O    | 2.47        | 0.46     |
| 1:C:45:GLU:HB3   | 1:C:49:LYS:HE2   | 1.97        | 0.46     |
| 1:F:36:VAL:HB    | 1:F:77:VAL:HB    | 1.96        | 0.46     |
| 1:B:53:ILE:CG2   | 1:B:128:LYS:NZ   | 2.79        | 0.46     |
| 1:A:58:ARG:NH1   | 1:A:58:ARG:CG    | 2.76        | 0.46     |
| 1:F:65:VAL:H     | 1:F:65:VAL:HG23  | 1.40        | 0.46     |
| 1:D:34:ARG:CG    | 1:D:142:TYR:CZ   | 2.98        | 0.46     |
| 1:F:53:ILE:CG2   | 1:F:54:ASP:N     | 2.78        | 0.46     |
| 1:C:89:VAL:HG12  | 1:C:90:MET:N     | 2.30        | 0.46     |
| 1:F:48:LEU:HA    | 1:F:48:LEU:HD23  | 1.72        | 0.46     |
| 1:A:81:LEU:HD12  | 1:A:82:ASN:N     | 2.30        | 0.46     |
| 1:B:139:LEU:HD22 | 1:B:139:LEU:H    | 1.80        | 0.45     |
| 1:D:134:PHE:HD1  | 1:D:138:GLU:OE1  | 1.98        | 0.45     |
| 1:B:128:LYS:CG   | 1:B:129:GLU:N    | 2.80        | 0.45     |
| 1:D:108:PHE:CD2  | 1:E:30:GLN:HB2   | 2.52        | 0.45     |
| 1:F:127:GLU:O    | 1:F:128:LYS:C    | 2.53        | 0.45     |
| 1:D:56:LYS:NZ    | 1:D:57:ASP:OD2   | 2.49        | 0.45     |
| 1:C:41:MET:O     | 1:C:73:VAL:HG22  | 2.16        | 0.45     |
| 1:E:109:CYS:HB3  | 1:E:116:ILE:HD13 | 1.98        | 0.45     |
| 1:F:67:TYR:C     | 1:F:69:HIS:N     | 2.70        | 0.45     |
| 1:E:134:PHE:O    | 1:E:136:PRO:HD3  | 2.16        | 0.45     |
| 1:F:111:GLN:C    | 1:F:113:GLY:H    | 2.19        | 0.45     |
| 1:E:81:LEU:HD12  | 1:E:81:LEU:C     | 2.35        | 0.45     |
| 1:D:42:ARG:O     | 1:D:43:ALA:C     | 2.52        | 0.45     |
| 1:F:51:HIS:C     | 1:F:53:ILE:H     | 2.18        | 0.45     |
| 1:D:67:TYR:O     | 1:D:70:SER:HB2   | 2.17        | 0.45     |
| 1:C:6:ARG:HA     | 1:C:83:VAL:HG21  | 1.97        | 0.45     |
| 1:D:44:SER:O     | 1:D:48:LEU:HB2   | 2.16        | 0.45     |
| 1:D:61:PHE:O     | 1:D:62:ALA:HB3   | 2.16        | 0.45     |
| 1:F:137:GLU:H    | 1:F:137:GLU:HG3  | 1.39        | 0.45     |
| 2:A:160:35G:P    | 2:A:161:GDP:PB   | 3.15        | 0.45     |
| 1:A:10:ALA:HA    | 1:A:74:VAL:O     | 2.17        | 0.45     |
| 1:B:12:LYS:HD2   | 3:B:404:HOH:O    | 2.16        | 0.45     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:E:64:LEU:O     | 1:E:68:MET:HG2   | 2.16        | 0.45     |
| 1:F:88:ARG:NH1   | 1:F:121:ASP:CB   | 2.79        | 0.45     |
| 2:F:161:GDP:O6   | 3:F:377:HOH:O    | 2.20        | 0.45     |
| 1:C:26:LYS:O     | 1:C:30:GLN:HG2   | 2.16        | 0.45     |
| 1:E:60:PHE:CE2   | 2:E:161:GDP:N9   | 2.85        | 0.45     |
| 1:B:80:GLY:N     | 1:B:83:VAL:CG2   | 2.79        | 0.45     |
| 1:C:27:ARG:HD3   | 3:C:247:HOH:O    | 2.16        | 0.45     |
| 1:A:110:ILE:HD11 | 1:B:31:LYS:O     | 2.17        | 0.45     |
| 1:C:21:ILE:HG21  | 1:C:21:ILE:HD13  | 1.71        | 0.45     |
| 1:B:48:LEU:O     | 1:B:49:LYS:C     | 2.55        | 0.45     |
| 1:F:85:LYS:HB3   | 1:F:85:LYS:HE3   | 1.62        | 0.45     |
| 1:B:38:MET:HB3   | 1:B:38:MET:HE3   | 1.74        | 0.45     |
| 1:A:129:GLU:O    | 1:A:130:ILE:C    | 2.55        | 0.45     |
| 1:F:6:ARG:HA     | 1:F:78:TRP:O     | 2.17        | 0.45     |
| 1:D:12:LYS:O     | 1:D:13:PRO:C     | 2.53        | 0.45     |
| 1:B:129:GLU:O    | 1:B:133:TRP:HD1  | 2.00        | 0.45     |
| 1:E:40:PHE:HD1   | 1:E:73:VAL:O     | 2.00        | 0.45     |
| 1:B:35:LEU:N     | 1:B:78:TRP:CE3   | 2.85        | 0.45     |
| 1:B:5:GLU:OE2    | 1:B:82:ASN:HA    | 2.17        | 0.45     |
| 1:A:55:LEU:HA    | 1:A:55:LEU:HD13  | 1.37        | 0.45     |
| 1:F:145:CYS:C    | 1:F:147:GLN:H    | 2.20        | 0.45     |
| 1:C:55:LEU:CD1   | 1:C:55:LEU:N     | 2.80        | 0.44     |
| 1:D:91:LEU:HA    | 1:D:91:LEU:HD12  | 1.71        | 0.44     |
| 1:C:4:SER:HA     | 1:C:79:GLU:HG3   | 1.99        | 0.44     |
| 1:D:136:PRO:CD   | 1:D:137:GLU:H    | 2.26        | 0.44     |
| 1:B:12:LYS:HD3   | 1:B:68:MET:SD    | 2.57        | 0.44     |
| 1:E:14:ASP:OD2   | 1:E:116:ILE:HG22 | 2.18        | 0.44     |
| 1:D:94:THR:HA    | 1:D:105:ARG:NH1  | 2.31        | 0.44     |
| 1:B:94:THR:O     | 1:B:96:PRO:HD3   | 2.17        | 0.44     |
| 1:E:5:GLU:OE2    | 1:E:84:VAL:HG23  | 2.17        | 0.44     |
| 1:D:6:ARG:NH1    | 3:D:294:HOH:O    | 2.50        | 0.44     |
| 1:F:70:SER:H     | 1:F:70:SER:HG    | 1.59        | 0.44     |
| 1:E:47:LEU:HD12  | 1:E:47:LEU:C     | 2.38        | 0.44     |
| 1:F:23:GLU:O     | 1:F:24:ILE:C     | 2.53        | 0.44     |
| 1:F:8:PHE:CE2    | 1:F:10:ALA:HB2   | 2.52        | 0.44     |
| 1:E:135:HIS:C    | 1:E:137:GLU:N    | 2.70        | 0.44     |
| 1:F:5:GLU:O      | 1:F:83:VAL:HG21  | 2.18        | 0.44     |
| 1:C:8:PHE:C      | 1:C:9:ILE:HG12   | 2.36        | 0.44     |
| 1:D:47:LEU:O     | 1:D:50:GLU:HB2   | 2.18        | 0.44     |
| 1:A:84:VAL:HG13  | 1:A:120:SER:O    | 2.16        | 0.44     |
| 1:C:91:LEU:HD11  | 1:C:117:ILE:CG1  | 2.46        | 0.44     |
| 1:A:47:LEU:CD1   | 1:A:132:LEU:CD2  | 2.95        | 0.44     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:129:GLU:O    | 1:A:133:TRP:HD1  | 1.99        | 0.44     |
| 1:B:91:LEU:O     | 1:B:105:ARG:HG3  | 2.17        | 0.44     |
| 1:A:14:ASP:O     | 1:A:18:ARG:HG3   | 2.18        | 0.44     |
| 1:A:38:MET:HG3   | 1:A:74:VAL:CG1   | 2.48        | 0.44     |
| 1:A:39:LYS:N     | 1:A:75:ALA:O     | 2.43        | 0.44     |
| 1:F:47:LEU:O     | 1:F:48:LEU:O     | 2.34        | 0.44     |
| 1:E:8:PHE:HE1    | 1:E:75:ALA:HB1   | 1.83        | 0.44     |
| 1:A:132:LEU:HD23 | 1:A:132:LEU:O    | 2.18        | 0.44     |
| 1:A:48:LEU:HD13  | 1:A:48:LEU:HA    | 1.53        | 0.44     |
| 1:C:8:PHE:CE1    | 1:C:75:ALA:HB1   | 2.50        | 0.44     |
| 1:E:30:GLN:HG2   | 1:E:30:GLN:H     | 1.49        | 0.44     |
| 1:A:59:PRO:O     | 1:A:60:PHE:C     | 2.56        | 0.44     |
| 1:A:31:LYS:HE2   | 1:C:110:ILE:HG23 | 2.00        | 0.44     |
| 1:F:100:LYS:O    | 1:F:106:GLY:HA3  | 2.17        | 0.44     |
| 1:A:140:VAL:HG12 | 1:A:141:ASN:H    | 1.82        | 0.44     |
| 1:A:37:ALA:HB2   | 1:A:139:LEU:CD1  | 2.40        | 0.44     |
| 1:C:6:ARG:HD2    | 3:C:380:HOH:O    | 2.17        | 0.44     |
| 1:E:44:SER:O     | 1:E:47:LEU:HB3   | 2.18        | 0.44     |
| 1:E:52:TYR:O     | 1:E:53:ILE:C     | 2.56        | 0.44     |
| 1:E:48:LEU:CD1   | 1:E:69:HIS:HB2   | 2.47        | 0.44     |
| 1:A:7:THR:HB     | 1:A:84:VAL:CG2   | 2.46        | 0.44     |
| 1:C:77:VAL:HG23  | 1:C:134:PHE:CE2  | 2.53        | 0.44     |
| 1:D:28:PHE:CD1   | 1:D:90:MET:CE    | 3.01        | 0.44     |
| 1:B:134:PHE:HB3  | 1:B:138:GLU:OE2  | 2.18        | 0.43     |
| 1:B:125:SER:HB3  | 3:B:422:HOH:O    | 2.18        | 0.43     |
| 1:E:60:PHE:CE2   | 2:E:161:GDP:O4'  | 2.70        | 0.43     |
| 1:B:29:GLU:OE2   | 1:D:21:ILE:HB    | 2.18        | 0.43     |
| 1:B:42:ARG:NH1   | 3:B:257:HOH:O    | 2.50        | 0.43     |
| 1:C:44:SER:O     | 1:C:48:LEU:N     | 2.43        | 0.43     |
| 1:C:40:PHE:HE2   | 1:F:140:VAL:HB   | 1.83        | 0.43     |
| 1:E:117:ILE:HG12 | 1:E:118:HIS:H    | 1.82        | 0.43     |
| 1:F:69:HIS:O     | 1:F:69:HIS:CD2   | 2.71        | 0.43     |
| 1:A:31:LYS:CG    | 1:A:31:LYS:O     | 2.62        | 0.43     |
| 1:D:108:PHE:O    | 1:D:109:CYS:HB3  | 2.17        | 0.43     |
| 1:F:88:ARG:O     | 1:F:91:LEU:HB2   | 2.19        | 0.43     |
| 1:D:37:ALA:O     | 1:D:76:MET:HA    | 2.18        | 0.43     |
| 1:C:29:GLU:OE2   | 3:C:321:HOH:O    | 2.21        | 0.43     |
| 1:D:8:PHE:HB3    | 1:D:120:SER:OG   | 2.18        | 0.43     |
| 1:E:12:LYS:HB3   | 1:E:13:PRO:HD2   | 2.01        | 0.43     |
| 1:F:85:LYS:HB2   | 3:F:280:HOH:O    | 2.19        | 0.43     |
| 1:D:47:LEU:HD11  | 1:D:132:LEU:HD22 | 2.01        | 0.43     |
| 1:A:41:MET:CE    | 1:A:133:TRP:CE3  | 3.01        | 0.43     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:C:104:ILE:O    | 1:C:108:PHE:CD2  | 2.71        | 0.43     |
| 1:F:60:PHE:CD1   | 1:F:60:PHE:N     | 2.80        | 0.43     |
| 1:D:41:MET:HB2   | 1:D:41:MET:HE2   | 1.62        | 0.43     |
| 1:F:27:ARG:NH2   | 1:F:107:ASP:OD2  | 2.48        | 0.43     |
| 1:A:37:ALA:O     | 1:A:76:MET:HA    | 2.19        | 0.43     |
| 1:B:122:SER:OG   | 1:B:124:GLU:HG3  | 2.17        | 0.43     |
| 1:E:37:ALA:O     | 1:E:76:MET:HA    | 2.18        | 0.43     |
| 1:E:58:ARG:HA    | 1:E:59:PRO:HD3   | 1.78        | 0.43     |
| 1:D:144:SER:C    | 1:D:146:ALA:H    | 2.22        | 0.43     |
| 1:D:18:ARG:NH1   | 3:D:473:HOH:O    | 2.38        | 0.43     |
| 1:D:89:VAL:H     | 1:D:89:VAL:HG23  | 1.55        | 0.43     |
| 1:A:117:ILE:HG12 | 1:A:118:HIS:N    | 2.33        | 0.43     |
| 1:D:124:GLU:O    | 1:D:128:LYS:HB2  | 2.19        | 0.43     |
| 1:B:109:CYS:CB   | 1:B:116:ILE:HD13 | 2.49        | 0.43     |
| 1:B:45:GLU:HG3   | 1:B:69:HIS:HD2   | 1.82        | 0.43     |
| 1:C:100:LYS:HD3  | 3:C:348:HOH:O    | 2.17        | 0.43     |
| 1:D:48:LEU:O     | 1:D:52:TYR:N     | 2.51        | 0.43     |
| 1:A:7:THR:OG1    | 3:A:397:HOH:O    | 2.20        | 0.43     |
| 1:B:95:ASN:O     | 1:B:98:ASP:N     | 2.40        | 0.43     |
| 1:A:108:PHE:O    | 1:A:109:CYS:HB3  | 2.19        | 0.43     |
| 1:E:12:LYS:HG3   | 1:E:117:ILE:CA   | 2.48        | 0.43     |
| 1:F:12:LYS:NZ    | 2:F:160:35G:O3'  | 2.48        | 0.43     |
| 1:A:14:ASP:OD1   | 1:A:67:TYR:OH    | 2.23        | 0.43     |
| 1:A:14:ASP:OD2   | 1:A:116:ILE:N    | 2.51        | 0.43     |
| 1:D:149:TRP:O    | 1:F:114:ARG:HB3  | 2.18        | 0.43     |
| 1:C:61:PHE:O     | 1:C:63:GLY:N     | 2.51        | 0.43     |
| 1:C:40:PHE:HD1   | 1:C:74:VAL:HG22  | 1.84        | 0.43     |
| 1:B:117:ILE:HG21 | 1:B:117:ILE:HD13 | 1.57        | 0.43     |
| 1:C:7:THR:HB     | 1:C:84:VAL:HG22  | 2.01        | 0.43     |
| 1:E:80:GLY:O     | 1:E:83:VAL:CG2   | 2.66        | 0.43     |
| 1:A:80:GLY:O     | 1:A:83:VAL:CG2   | 2.66        | 0.43     |
| 1:A:12:LYS:HE3   | 1:A:117:ILE:O    | 2.19        | 0.43     |
| 1:F:53:ILE:O     | 1:F:56:LYS:HB2   | 2.19        | 0.43     |
| 1:C:125:SER:O    | 1:C:126:ALA:C    | 2.57        | 0.43     |
| 1:F:152:GLU:HG2  | 1:F:152:GLU:O    | 2.18        | 0.43     |
| 1:A:152:GLU:HB3  | 1:C:111:GLN:OE1  | 2.19        | 0.43     |
| 1:F:44:SER:O     | 1:F:48:LEU:N     | 2.47        | 0.42     |
| 1:E:40:PHE:O     | 1:E:41:MET:HB3   | 2.19        | 0.42     |
| 1:A:14:ASP:OD2   | 1:A:116:ILE:HA   | 2.19        | 0.42     |
| 1:F:2:ALA:O      | 1:F:81:LEU:HA    | 2.19        | 0.42     |
| 1:A:11:ILE:HG13  | 1:A:76:MET:HE1   | 2.00        | 0.42     |
| 1:D:11:ILE:HG21  | 1:D:11:ILE:HD13  | 1.46        | 0.42     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:C:20:LEU:O     | 1:C:24:ILE:HG13  | 2.19        | 0.42     |
| 1:A:136:PRO:C    | 1:A:138:GLU:H    | 2.19        | 0.42     |
| 1:F:3:ASN:HA     | 1:F:81:LEU:CA    | 2.48        | 0.42     |
| 1:B:16:VAL:HG13  | 1:B:21:ILE:HD11  | 2.01        | 0.42     |
| 1:D:25:ILE:HD13  | 1:D:25:ILE:HG21  | 1.80        | 0.42     |
| 1:C:65:VAL:H     | 1:C:65:VAL:HG23  | 1.62        | 0.42     |
| 1:A:9:ILE:HG23   | 1:A:9:ILE:HD12   | 1.71        | 0.42     |
| 1:E:45:GLU:O     | 1:E:48:LEU:HB2   | 2.19        | 0.42     |
| 1:A:82:ASN:O     | 1:A:83:VAL:C     | 2.57        | 0.42     |
| 1:C:18:ARG:NH1   | 3:C:264:HOH:O    | 2.28        | 0.42     |
| 1:B:93:GLU:O     | 1:B:99:SER:OG    | 2.38        | 0.42     |
| 1:D:136:PRO:HD2  | 1:D:137:GLU:CG   | 2.34        | 0.42     |
| 1:B:127:GLU:O    | 1:B:128:LYS:C    | 2.51        | 0.42     |
| 1:E:7:THR:O      | 1:E:77:VAL:HA    | 2.20        | 0.42     |
| 1:F:95:ASN:C     | 1:F:97:ALA:N     | 2.73        | 0.42     |
| 1:A:30:GLN:C     | 1:A:32:GLY:H     | 2.23        | 0.42     |
| 1:C:118:HIS:CD2  | 1:C:119:GLY:N    | 2.88        | 0.42     |
| 1:F:95:ASN:HA    | 1:F:112:VAL:HG13 | 2.01        | 0.42     |
| 1:C:12:LYS:CB    | 1:C:13:PRO:CD    | 2.94        | 0.42     |
| 1:B:104:ILE:O    | 1:B:105:ARG:C    | 2.57        | 0.42     |
| 1:D:149:TRP:CE2  | 1:F:17:GLN:HG3   | 2.55        | 0.42     |
| 1:F:143:LYS:NZ   | 1:F:147:GLN:OE1  | 2.47        | 0.42     |
| 1:B:15:GLY:O     | 1:B:16:VAL:C     | 2.57        | 0.42     |
| 1:B:135:HIS:HA   | 1:B:136:PRO:HD2  | 1.79        | 0.42     |
| 1:F:45:GLU:O     | 1:F:49:LYS:HB2   | 2.19        | 0.42     |
| 1:B:110:ILE:HD11 | 1:C:32:GLY:C     | 2.39        | 0.42     |
| 1:B:115:ASN:C    | 1:B:117:ILE:H    | 2.23        | 0.42     |
| 1:E:53:ILE:HD11  | 1:E:56:LYS:NZ    | 2.35        | 0.42     |
| 1:D:94:THR:O     | 1:D:96:PRO:HD3   | 2.19        | 0.42     |
| 1:E:26:LYS:O     | 1:E:26:LYS:HG2   | 2.19        | 0.42     |
| 2:E:161:GDP:O1B  | 2:E:161:GDP:O1A  | 2.38        | 0.42     |
| 1:E:135:HIS:HA   | 1:E:136:PRO:HD2  | 1.46        | 0.42     |
| 1:E:45:GLU:O     | 1:E:49:LYS:HG2   | 2.20        | 0.42     |
| 1:F:49:LYS:HG2   | 1:F:61:PHE:HZ    | 1.85        | 0.42     |
| 1:F:100:LYS:HA   | 1:F:100:LYS:HD3  | 1.95        | 0.42     |
| 1:D:56:LYS:HB3   | 1:D:56:LYS:NZ    | 2.34        | 0.42     |
| 1:D:31:LYS:HE2   | 1:F:109:CYS:O    | 2.19        | 0.42     |
| 1:B:127:GLU:HA   | 1:B:130:ILE:CG1  | 2.45        | 0.42     |
| 1:E:124:GLU:O    | 1:E:127:GLU:HB2  | 2.20        | 0.42     |
| 2:D:160:35G:O2P  | 2:D:161:GDP:PB   | 2.78        | 0.42     |
| 1:A:36:VAL:HG23  | 1:A:79:GLU:HB3   | 2.02        | 0.41     |
| 1:D:135:HIS:O    | 1:D:138:GLU:HB2  | 2.19        | 0.41     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:B:58:ARG:O     | 1:B:61:PHE:CB    | 2.68        | 0.41     |
| 1:B:39:LYS:CE    | 1:B:41:MET:HE3   | 2.49        | 0.41     |
| 1:B:29:GLU:HG3   | 1:B:78:TRP:HH2   | 1.85        | 0.41     |
| 1:A:41:MET:HE1   | 1:A:133:TRP:CE3  | 2.55        | 0.41     |
| 1:D:15:GLY:HA2   | 1:D:116:ILE:HG22 | 2.02        | 0.41     |
| 1:C:61:PHE:O     | 1:C:62:ALA:C     | 2.57        | 0.41     |
| 1:E:128:LYS:O    | 1:E:131:ALA:HB3  | 2.19        | 0.41     |
| 1:C:93:GLU:H     | 1:C:99:SER:CB    | 2.25        | 0.41     |
| 1:C:81:LEU:HB3   | 1:C:151:TYR:CE1  | 2.55        | 0.41     |
| 1:C:53:ILE:HG23  | 1:C:54:ASP:H     | 1.84        | 0.41     |
| 1:D:47:LEU:HA    | 1:D:47:LEU:HD12  | 1.57        | 0.41     |
| 1:E:58:ARG:HG3   | 1:E:59:PRO:CD    | 2.50        | 0.41     |
| 1:B:129:GLU:H    | 1:B:129:GLU:HG2  | 1.53        | 0.41     |
| 1:F:123:VAL:HG23 | 3:F:485:HOH:O    | 2.19        | 0.41     |
| 1:C:14:ASP:OD2   | 1:C:116:ILE:HG23 | 2.21        | 0.41     |
| 1:C:64:LEU:HD13  | 1:C:64:LEU:HA    | 1.71        | 0.41     |
| 1:B:126:ALA:O    | 1:B:127:GLU:C    | 2.57        | 0.41     |
| 1:F:46:ASP:O     | 1:F:49:LYS:HB2   | 2.21        | 0.41     |
| 1:E:9:ILE:HG22   | 1:E:76:MET:CE    | 2.46        | 0.41     |
| 1:D:135:HIS:O    | 1:D:136:PRO:C    | 2.59        | 0.41     |
| 1:B:129:GLU:O    | 1:B:133:TRP:CD1  | 2.74        | 0.41     |
| 1:E:132:LEU:HB3  | 1:E:133:TRP:CD1  | 2.56        | 0.41     |
| 1:E:8:PHE:H      | 1:E:120:SER:HB2  | 1.85        | 0.41     |
| 1:C:28:PHE:O     | 1:C:29:GLU:C     | 2.58        | 0.41     |
| 1:A:140:VAL:HG12 | 1:A:141:ASN:N    | 2.36        | 0.41     |
| 1:C:146:ALA:C    | 1:C:148:ASN:N    | 2.74        | 0.41     |
| 1:A:142:TYR:N    | 1:A:142:TYR:CD1  | 2.88        | 0.41     |
| 1:E:17:GLN:HG3   | 1:F:149:TRP:CE2  | 2.56        | 0.41     |
| 1:E:45:GLU:HB3   | 1:E:49:LYS:HE2   | 2.03        | 0.41     |
| 1:A:100:LYS:HD2  | 1:A:100:LYS:HA   | 1.93        | 0.41     |
| 1:F:60:PHE:O     | 1:F:63:GLY:N     | 2.29        | 0.41     |
| 1:A:146:ALA:O    | 1:A:149:TRP:N    | 2.48        | 0.41     |
| 1:F:12:LYS:HZ1   | 2:F:160:35G:P    | 2.43        | 0.41     |
| 1:B:81:LEU:O     | 1:B:82:ASN:C     | 2.59        | 0.41     |
| 1:A:135:HIS:O    | 1:A:138:GLU:HB2  | 2.21        | 0.41     |
| 1:A:88:ARG:NH2   | 2:A:161:GDP:O1B  | 2.46        | 0.41     |
| 1:B:67:TYR:HA    | 1:B:70:SER:HG    | 1.85        | 0.41     |
| 1:C:140:VAL:HG12 | 1:C:142:TYR:CD1  | 2.54        | 0.41     |
| 2:E:160:35G:C5'  | 2:E:161:GDP:PA   | 2.84        | 0.41     |
| 1:F:67:TYR:C     | 1:F:67:TYR:CD1   | 2.89        | 0.41     |
| 1:D:24:ILE:HA    | 1:D:27:ARG:HG3   | 2.03        | 0.41     |
| 1:A:8:PHE:HD2    | 1:A:129:GLU:OE1  | 2.03        | 0.41     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:17:GLN:NE2   | 1:E:142:TYR:HD2  | 2.19        | 0.41     |
| 1:A:112:VAL:HG12 | 1:A:115:ASN:ND2  | 2.36        | 0.41     |
| 1:F:123:VAL:C    | 1:F:125:SER:N    | 2.72        | 0.41     |
| 1:E:48:LEU:O     | 1:E:49:LYS:C     | 2.56        | 0.41     |
| 1:B:4:SER:C      | 1:B:79:GLU:HG3   | 2.42        | 0.41     |
| 1:A:83:VAL:O     | 1:A:84:VAL:C     | 2.57        | 0.41     |
| 1:B:140:VAL:HG11 | 1:D:72:PRO:CB    | 2.51        | 0.41     |
| 1:D:41:MET:O     | 1:D:72:PRO:HA    | 2.21        | 0.41     |
| 1:B:111:GLN:OE1  | 1:C:151:TYR:HD1  | 2.04        | 0.41     |
| 1:D:84:VAL:HG21  | 1:D:123:VAL:HA   | 2.01        | 0.40     |
| 1:F:53:ILE:CG2   | 1:F:54:ASP:H     | 2.34        | 0.40     |
| 1:E:137:GLU:H    | 1:E:137:GLU:HG3  | 1.29        | 0.40     |
| 1:E:39:LYS:CE    | 1:E:41:MET:HE3   | 2.48        | 0.40     |
| 1:E:94:THR:O     | 1:E:96:PRO:HD3   | 2.21        | 0.40     |
| 1:B:86:THR:O     | 1:B:87:GLY:C     | 2.60        | 0.40     |
| 1:E:23:GLU:O     | 1:E:27:ARG:HG2   | 2.21        | 0.40     |
| 1:E:112:VAL:HG23 | 1:E:113:GLY:N    | 2.33        | 0.40     |
| 1:B:140:VAL:HG11 | 1:D:72:PRO:CG    | 2.50        | 0.40     |
| 1:C:94:THR:HG22  | 3:C:499:HOH:O    | 2.20        | 0.40     |
| 1:C:149:TRP:CE3  | 1:C:149:TRP:HA   | 2.57        | 0.40     |
| 1:C:100:LYS:HA   | 1:C:101:PRO:HD3  | 1.89        | 0.40     |
| 1:D:47:LEU:CD1   | 1:D:132:LEU:CD2  | 2.99        | 0.40     |
| 1:E:81:LEU:HD12  | 1:E:82:ASN:HD22  | 1.85        | 0.40     |
| 1:C:45:GLU:O     | 1:C:48:LEU:N     | 2.55        | 0.40     |
| 1:A:6:ARG:HD2    | 1:A:36:VAL:HG21  | 2.03        | 0.40     |
| 1:C:34:ARG:NH1   | 1:C:36:VAL:HG22  | 2.36        | 0.40     |
| 1:E:12:LYS:HB3   | 1:E:13:PRO:HD3   | 2.03        | 0.40     |
| 1:F:48:LEU:O     | 1:F:51:HIS:HB3   | 2.21        | 0.40     |
| 1:F:46:ASP:O     | 1:F:50:GLU:HB2   | 2.20        | 0.40     |
| 1:C:9:ILE:O      | 1:C:76:MET:HE2   | 2.21        | 0.40     |
| 1:B:93:GLU:O     | 1:B:95:ASN:N     | 2.54        | 0.40     |
| 1:A:152:GLU:N    | 1:C:111:GLN:OE1  | 2.31        | 0.40     |
| 1:B:123:VAL:O    | 1:B:126:ALA:N    | 2.55        | 0.40     |
| 1:E:64:LEU:HD12  | 1:E:64:LEU:O     | 2.22        | 0.40     |
| 1:E:51:HIS:ND1   | 1:E:133:TRP:NE1  | 2.63        | 0.40     |
| 1:A:47:LEU:HD13  | 1:A:132:LEU:HD21 | 2.03        | 0.40     |
| 1:D:55:LEU:HA    | 1:D:55:LEU:HD23  | 1.48        | 0.40     |
| 1:D:84:VAL:HG12  | 1:D:85:LYS:N     | 2.37        | 0.40     |
| 1:E:72:PRO:C     | 1:E:73:VAL:HG13  | 2.41        | 0.40     |
| 1:E:40:PHE:HE1   | 1:E:72:PRO:HB2   | 1.80        | 0.40     |
| 1:B:9:ILE:HD13   | 1:B:9:ILE:HA     | 1.79        | 0.40     |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 149/152 (98%) | 126 (85%) | 16 (11%)  | 7 (5%)   | 4           | 2 |
| 1   | B     | 149/152 (98%) | 118 (79%) | 17 (11%)  | 14 (9%)  | 1           | 0 |
| 1   | C     | 149/152 (98%) | 122 (82%) | 18 (12%)  | 9 (6%)   | 2           | 1 |
| 1   | D     | 149/152 (98%) | 119 (80%) | 25 (17%)  | 5 (3%)   | 6           | 4 |
| 1   | E     | 149/152 (98%) | 122 (82%) | 21 (14%)  | 6 (4%)   | 5           | 3 |
| 1   | F     | 149/152 (98%) | 117 (78%) | 21 (14%)  | 11 (7%)  | 2           | 0 |
| All | All   | 894/912 (98%) | 724 (81%) | 118 (13%) | 52 (6%)  | 3           | 1 |

All (52) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 56  | LYS  |
| 1   | A     | 59  | PRO  |
| 1   | A     | 61  | PHE  |
| 1   | A     | 115 | ASN  |
| 1   | A     | 116 | ILE  |
| 1   | B     | 56  | LYS  |
| 1   | B     | 58  | ARG  |
| 1   | B     | 59  | PRO  |
| 1   | B     | 96  | PRO  |
| 1   | B     | 116 | ILE  |
| 1   | C     | 83  | VAL  |
| 1   | C     | 100 | LYS  |
| 1   | C     | 116 | ILE  |
| 1   | D     | 61  | PHE  |
| 1   | D     | 116 | ILE  |
| 1   | E     | 116 | ILE  |
| 1   | F     | 58  | ARG  |
| 1   | F     | 61  | PHE  |
| 1   | F     | 84  | VAL  |
| 1   | F     | 116 | ILE  |
| 1   | A     | 104 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 130 | ILE  |
| 1   | B     | 52  | TYR  |
| 1   | B     | 53  | ILE  |
| 1   | B     | 61  | PHE  |
| 1   | B     | 94  | THR  |
| 1   | B     | 136 | PRO  |
| 1   | C     | 84  | VAL  |
| 1   | C     | 147 | GLN  |
| 1   | E     | 19  | GLY  |
| 1   | E     | 59  | PRO  |
| 1   | E     | 61  | PHE  |
| 1   | F     | 68  | MET  |
| 1   | B     | 5   | GLU  |
| 1   | F     | 59  | PRO  |
| 1   | F     | 146 | ALA  |
| 1   | C     | 112 | VAL  |
| 1   | E     | 53  | ILE  |
| 1   | C     | 61  | PHE  |
| 1   | C     | 96  | PRO  |
| 1   | C     | 136 | PRO  |
| 1   | F     | 96  | PRO  |
| 1   | F     | 120 | SER  |
| 1   | B     | 48  | LEU  |
| 1   | B     | 104 | ILE  |
| 1   | B     | 84  | VAL  |
| 1   | D     | 21  | ILE  |
| 1   | E     | 83  | VAL  |
| 1   | F     | 123 | VAL  |
| 1   | D     | 84  | VAL  |
| 1   | D     | 136 | PRO  |
| 1   | F     | 112 | VAL  |

### 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     | 128/129 (99%) | 95 (74%)  | 33 (26%) | <b>1</b> <b>1</b> |

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| Mol | Chain | Analysed      | Rotameric | Outliers  | Percentiles |   |
|-----|-------|---------------|-----------|-----------|-------------|---|
| 1   | B     | 128/129 (99%) | 91 (71%)  | 37 (29%)  | 0           | 0 |
| 1   | C     | 128/129 (99%) | 93 (73%)  | 35 (27%)  | 0           | 0 |
| 1   | D     | 128/129 (99%) | 100 (78%) | 28 (22%)  | 1           | 1 |
| 1   | E     | 128/129 (99%) | 93 (73%)  | 35 (27%)  | 0           | 0 |
| 1   | F     | 128/129 (99%) | 99 (77%)  | 29 (23%)  | 1           | 1 |
| All | All   | 768/774 (99%) | 571 (74%) | 197 (26%) | 1           | 1 |

All (197) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 7   | THR  |
| 1   | A     | 14  | ASP  |
| 1   | A     | 23  | GLU  |
| 1   | A     | 35  | LEU  |
| 1   | A     | 38  | MET  |
| 1   | A     | 48  | LEU  |
| 1   | A     | 53  | ILE  |
| 1   | A     | 54  | ASP  |
| 1   | A     | 55  | LEU  |
| 1   | A     | 56  | LYS  |
| 1   | A     | 58  | ARG  |
| 1   | A     | 66  | LYS  |
| 1   | A     | 70  | SER  |
| 1   | A     | 77  | VAL  |
| 1   | A     | 81  | LEU  |
| 1   | A     | 83  | VAL  |
| 1   | A     | 85  | LYS  |
| 1   | A     | 88  | ARG  |
| 1   | A     | 93  | GLU  |
| 1   | A     | 98  | ASP  |
| 1   | A     | 100 | LYS  |
| 1   | A     | 108 | PHE  |
| 1   | A     | 112 | VAL  |
| 1   | A     | 116 | ILE  |
| 1   | A     | 128 | LYS  |
| 1   | A     | 137 | GLU  |
| 1   | A     | 139 | LEU  |
| 1   | A     | 140 | VAL  |
| 1   | A     | 142 | TYR  |
| 1   | A     | 143 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 147 | GLN  |
| 1   | A     | 148 | ASN  |
| 1   | A     | 150 | ILE  |
| 1   | B     | 3   | ASN  |
| 1   | B     | 4   | SER  |
| 1   | B     | 6   | ARG  |
| 1   | B     | 20  | LEU  |
| 1   | B     | 35  | LEU  |
| 1   | B     | 38  | MET  |
| 1   | B     | 41  | MET  |
| 1   | B     | 44  | SER  |
| 1   | B     | 48  | LEU  |
| 1   | B     | 49  | LYS  |
| 1   | B     | 50  | GLU  |
| 1   | B     | 51  | HIS  |
| 1   | B     | 53  | ILE  |
| 1   | B     | 56  | LYS  |
| 1   | B     | 57  | ASP  |
| 1   | B     | 64  | LEU  |
| 1   | B     | 66  | LYS  |
| 1   | B     | 70  | SER  |
| 1   | B     | 79  | GLU  |
| 1   | B     | 83  | VAL  |
| 1   | B     | 88  | ARG  |
| 1   | B     | 93  | GLU  |
| 1   | B     | 109 | CYS  |
| 1   | B     | 115 | ASN  |
| 1   | B     | 116 | ILE  |
| 1   | B     | 124 | GLU  |
| 1   | B     | 125 | SER  |
| 1   | B     | 128 | LYS  |
| 1   | B     | 129 | GLU  |
| 1   | B     | 132 | LEU  |
| 1   | B     | 134 | PHE  |
| 1   | B     | 137 | GLU  |
| 1   | B     | 139 | LEU  |
| 1   | B     | 143 | LYS  |
| 1   | B     | 144 | SER  |
| 1   | B     | 145 | CYS  |
| 1   | B     | 151 | TYR  |
| 1   | C     | 4   | SER  |
| 1   | C     | 6   | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 9   | ILE  |
| 1   | C     | 12  | LYS  |
| 1   | C     | 30  | GLN  |
| 1   | C     | 35  | LEU  |
| 1   | C     | 41  | MET  |
| 1   | C     | 47  | LEU  |
| 1   | C     | 50  | GLU  |
| 1   | C     | 56  | LYS  |
| 1   | C     | 58  | ARG  |
| 1   | C     | 64  | LEU  |
| 1   | C     | 66  | LYS  |
| 1   | C     | 76  | MET  |
| 1   | C     | 79  | GLU  |
| 1   | C     | 83  | VAL  |
| 1   | C     | 94  | THR  |
| 1   | C     | 98  | ASP  |
| 1   | C     | 100 | LYS  |
| 1   | C     | 104 | ILE  |
| 1   | C     | 107 | ASP  |
| 1   | C     | 110 | ILE  |
| 1   | C     | 112 | VAL  |
| 1   | C     | 114 | ARG  |
| 1   | C     | 120 | SER  |
| 1   | C     | 121 | ASP  |
| 1   | C     | 123 | VAL  |
| 1   | C     | 124 | GLU  |
| 1   | C     | 132 | LEU  |
| 1   | C     | 137 | GLU  |
| 1   | C     | 141 | ASN  |
| 1   | C     | 143 | LYS  |
| 1   | C     | 144 | SER  |
| 1   | C     | 147 | GLN  |
| 1   | C     | 148 | ASN  |
| 1   | D     | 4   | SER  |
| 1   | D     | 6   | ARG  |
| 1   | D     | 20  | LEU  |
| 1   | D     | 31  | LYS  |
| 1   | D     | 35  | LEU  |
| 1   | D     | 39  | LYS  |
| 1   | D     | 41  | MET  |
| 1   | D     | 49  | LYS  |
| 1   | D     | 50  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 54  | ASP  |
| 1   | D     | 56  | LYS  |
| 1   | D     | 64  | LEU  |
| 1   | D     | 66  | LYS  |
| 1   | D     | 67  | TYR  |
| 1   | D     | 79  | GLU  |
| 1   | D     | 83  | VAL  |
| 1   | D     | 88  | ARG  |
| 1   | D     | 91  | LEU  |
| 1   | D     | 94  | THR  |
| 1   | D     | 104 | ILE  |
| 1   | D     | 112 | VAL  |
| 1   | D     | 121 | ASP  |
| 1   | D     | 124 | GLU  |
| 1   | D     | 130 | ILE  |
| 1   | D     | 137 | GLU  |
| 1   | D     | 143 | LYS  |
| 1   | D     | 144 | SER  |
| 1   | D     | 152 | GLU  |
| 1   | E     | 6   | ARG  |
| 1   | E     | 18  | ARG  |
| 1   | E     | 35  | LEU  |
| 1   | E     | 41  | MET  |
| 1   | E     | 44  | SER  |
| 1   | E     | 46  | ASP  |
| 1   | E     | 47  | LEU  |
| 1   | E     | 49  | LYS  |
| 1   | E     | 53  | ILE  |
| 1   | E     | 55  | LEU  |
| 1   | E     | 56  | LYS  |
| 1   | E     | 64  | LEU  |
| 1   | E     | 66  | LYS  |
| 1   | E     | 67  | TYR  |
| 1   | E     | 76  | MET  |
| 1   | E     | 81  | LEU  |
| 1   | E     | 83  | VAL  |
| 1   | E     | 85  | LYS  |
| 1   | E     | 91  | LEU  |
| 1   | E     | 93  | GLU  |
| 1   | E     | 94  | THR  |
| 1   | E     | 100 | LYS  |
| 1   | E     | 112 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 120 | SER  |
| 1   | E     | 121 | ASP  |
| 1   | E     | 124 | GLU  |
| 1   | E     | 132 | LEU  |
| 1   | E     | 136 | PRO  |
| 1   | E     | 137 | GLU  |
| 1   | E     | 141 | ASN  |
| 1   | E     | 142 | TYR  |
| 1   | E     | 143 | LYS  |
| 1   | E     | 144 | SER  |
| 1   | E     | 147 | GLN  |
| 1   | E     | 148 | ASN  |
| 1   | F     | 6   | ARG  |
| 1   | F     | 7   | THR  |
| 1   | F     | 14  | ASP  |
| 1   | F     | 30  | GLN  |
| 1   | F     | 35  | LEU  |
| 1   | F     | 39  | LYS  |
| 1   | F     | 41  | MET  |
| 1   | F     | 46  | ASP  |
| 1   | F     | 54  | ASP  |
| 1   | F     | 57  | ASP  |
| 1   | F     | 58  | ARG  |
| 1   | F     | 60  | PHE  |
| 1   | F     | 66  | LYS  |
| 1   | F     | 69  | HIS  |
| 1   | F     | 70  | SER  |
| 1   | F     | 83  | VAL  |
| 1   | F     | 85  | LYS  |
| 1   | F     | 96  | PRO  |
| 1   | F     | 112 | VAL  |
| 1   | F     | 120 | SER  |
| 1   | F     | 123 | VAL  |
| 1   | F     | 127 | GLU  |
| 1   | F     | 129 | GLU  |
| 1   | F     | 132 | LEU  |
| 1   | F     | 137 | GLU  |
| 1   | F     | 139 | LEU  |
| 1   | F     | 147 | GLN  |
| 1   | F     | 148 | ASN  |
| 1   | F     | 152 | GLU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such

sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 30  | GLN  |
| 1   | A     | 82  | ASN  |
| 1   | A     | 141 | ASN  |
| 1   | A     | 147 | GLN  |
| 1   | A     | 148 | ASN  |
| 1   | B     | 30  | GLN  |
| 1   | B     | 69  | HIS  |
| 1   | C     | 30  | GLN  |
| 1   | C     | 51  | HIS  |
| 1   | C     | 148 | ASN  |
| 1   | D     | 141 | ASN  |
| 1   | E     | 30  | GLN  |
| 1   | E     | 82  | ASN  |
| 1   | E     | 148 | ASN  |
| 1   | F     | 30  | GLN  |
| 1   | F     | 69  | HIS  |
| 1   | F     | 135 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 2   | 35G  | A     | 160 | -    | 26,26,26     | 1.62 | 6 (23%)     | 38,41,41    | 6.82 | 12 (31%)    |
| 2   | GDP  | A     | 161 | -    | 30,30,30     | 1.16 | 3 (10%)     | 44,47,47    | 4.54 | 9 (20%)     |
| 2   | 35G  | B     | 160 | -    | 26,26,26     | 1.44 | 3 (11%)     | 38,41,41    | 3.72 | 9 (23%)     |
| 2   | GDP  | B     | 161 | -    | 30,30,30     | 1.21 | 3 (10%)     | 44,47,47    | 5.70 | 10 (22%)    |
| 2   | 35G  | C     | 160 | -    | 26,26,26     | 1.75 | 7 (26%)     | 38,41,41    | 4.43 | 13 (34%)    |
| 2   | GDP  | C     | 161 | -    | 30,30,30     | 1.15 | 3 (10%)     | 44,47,47    | 7.12 | 14 (31%)    |
| 2   | 35G  | D     | 160 | -    | 26,26,26     | 1.38 | 2 (7%)      | 38,41,41    | 4.90 | 8 (21%)     |
| 2   | GDP  | D     | 161 | -    | 30,30,30     | 0.93 | 0           | 44,47,47    | 5.16 | 14 (31%)    |
| 2   | 35G  | E     | 160 | -    | 26,26,26     | 1.27 | 3 (11%)     | 38,41,41    | 6.35 | 13 (34%)    |
| 2   | GDP  | E     | 161 | -    | 30,30,30     | 1.08 | 2 (6%)      | 44,47,47    | 5.38 | 15 (34%)    |
| 2   | 35G  | F     | 160 | -    | 26,26,26     | 1.86 | 6 (23%)     | 38,41,41    | 4.13 | 15 (39%)    |
| 2   | GDP  | F     | 161 | -    | 30,30,30     | 1.16 | 3 (10%)     | 44,47,47    | 4.23 | 14 (31%)    |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | 35G  | A     | 160 | -    | -       | 0/4/31/31  | 0/0/4/4 |
| 2   | GDP  | A     | 161 | -    | -       | 0/16/32/32 | 0/1/3/3 |
| 2   | 35G  | B     | 160 | -    | -       | 0/4/31/31  | 0/0/4/4 |
| 2   | GDP  | B     | 161 | -    | -       | 0/16/32/32 | 0/1/3/3 |
| 2   | 35G  | C     | 160 | -    | -       | 0/4/31/31  | 0/0/4/4 |
| 2   | GDP  | C     | 161 | -    | -       | 0/16/32/32 | 0/1/3/3 |
| 2   | 35G  | D     | 160 | -    | -       | 0/4/31/31  | 0/0/4/4 |
| 2   | GDP  | D     | 161 | -    | -       | 0/16/32/32 | 0/1/3/3 |
| 2   | 35G  | E     | 160 | -    | -       | 0/4/31/31  | 0/0/4/4 |
| 2   | GDP  | E     | 161 | -    | -       | 0/16/32/32 | 0/1/3/3 |
| 2   | 35G  | F     | 160 | -    | -       | 0/4/31/31  | 0/0/4/4 |
| 2   | GDP  | F     | 161 | -    | -       | 0/16/32/32 | 0/1/3/3 |

All (41) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | F     | 160 | 35G  | P-O3' | -5.21 | 1.48        | 1.58     |
| 2   | F     | 160 | 35G  | P-O5' | -4.28 | 1.50        | 1.58     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | C     | 160 | 35G  | P-O5'   | -4.09 | 1.50        | 1.58     |
| 2   | A     | 160 | 35G  | P-O3'   | -4.08 | 1.50        | 1.58     |
| 2   | B     | 160 | 35G  | P-O3'   | -4.02 | 1.50        | 1.58     |
| 2   | B     | 160 | 35G  | P-O5'   | -3.92 | 1.50        | 1.58     |
| 2   | A     | 160 | 35G  | P-O5'   | -3.85 | 1.50        | 1.58     |
| 2   | D     | 160 | 35G  | P-O5'   | -3.80 | 1.51        | 1.58     |
| 2   | C     | 160 | 35G  | P-O3'   | -3.67 | 1.51        | 1.58     |
| 2   | E     | 160 | 35G  | P-O3'   | -3.48 | 1.51        | 1.58     |
| 2   | D     | 160 | 35G  | P-O3'   | -3.37 | 1.51        | 1.58     |
| 2   | C     | 160 | 35G  | C2-N1   | 3.32  | 1.42        | 1.36     |
| 2   | F     | 160 | 35G  | O3'-C3' | -3.08 | 1.39        | 1.44     |
| 2   | C     | 160 | 35G  | C2-N2   | 2.97  | 1.37        | 1.32     |
| 2   | B     | 161 | GDP  | PA-O3A  | 2.97  | 1.65        | 1.59     |
| 2   | E     | 160 | 35G  | P-O5'   | -2.97 | 1.52        | 1.58     |
| 2   | F     | 161 | GDP  | PA-O3A  | 2.90  | 1.65        | 1.59     |
| 2   | B     | 161 | GDP  | PB-O3A  | 2.85  | 1.65        | 1.60     |
| 2   | A     | 160 | 35G  | C2-N2   | 2.84  | 1.36        | 1.32     |
| 2   | C     | 160 | 35G  | C6-N1   | 2.54  | 1.41        | 1.37     |
| 2   | F     | 161 | GDP  | PB-O3A  | 2.52  | 1.64        | 1.60     |
| 2   | C     | 161 | GDP  | C6-N1   | 2.43  | 1.41        | 1.37     |
| 2   | A     | 160 | 35G  | C2-N1   | 2.43  | 1.40        | 1.36     |
| 2   | E     | 161 | GDP  | C2-N2   | 2.35  | 1.36        | 1.32     |
| 2   | B     | 161 | GDP  | PA-O5'  | -2.34 | 1.48        | 1.59     |
| 2   | C     | 160 | 35G  | O5'-C5' | -2.33 | 1.42        | 1.46     |
| 2   | C     | 161 | GDP  | PA-O5'  | -2.33 | 1.48        | 1.59     |
| 2   | E     | 161 | GDP  | C6-N1   | 2.23  | 1.41        | 1.37     |
| 2   | F     | 160 | 35G  | C6-C5   | 2.18  | 1.44        | 1.41     |
| 2   | C     | 160 | 35G  | C8-N7   | -2.16 | 1.30        | 1.34     |
| 2   | F     | 161 | GDP  | PA-O5'  | -2.16 | 1.49        | 1.59     |
| 2   | A     | 161 | GDP  | PA-O5'  | -2.13 | 1.49        | 1.59     |
| 2   | A     | 161 | GDP  | C6-N1   | 2.13  | 1.40        | 1.37     |
| 2   | A     | 160 | 35G  | C6-N1   | 2.11  | 1.40        | 1.37     |
| 2   | A     | 161 | GDP  | PA-O3A  | 2.11  | 1.63        | 1.59     |
| 2   | C     | 161 | GDP  | PA-O3A  | 2.09  | 1.63        | 1.59     |
| 2   | A     | 160 | 35G  | O3'-C3' | -2.09 | 1.41        | 1.44     |
| 2   | F     | 160 | 35G  | C2-N2   | 2.07  | 1.35        | 1.32     |
| 2   | B     | 160 | 35G  | C6-N1   | 2.02  | 1.40        | 1.37     |
| 2   | F     | 160 | 35G  | C2-N1   | 2.02  | 1.39        | 1.36     |
| 2   | E     | 160 | 35G  | C8-N7   | -2.02 | 1.30        | 1.34     |

All (146) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 2   | C     | 161 | GDP  | C6-C5-N7    | -44.68 | 128.12      | 134.14   |
| 2   | B     | 161 | GDP  | C6-C5-N7    | -36.60 | 129.21      | 134.14   |
| 2   | A     | 160 | 35G  | C6-C5-N7    | -33.29 | 129.66      | 134.14   |
| 2   | E     | 160 | 35G  | C6-C5-N7    | -32.06 | 129.82      | 134.14   |
| 2   | E     | 161 | GDP  | C6-C5-N7    | -31.29 | 129.93      | 134.14   |
| 2   | A     | 161 | GDP  | C6-C5-N7    | -27.73 | 130.41      | 134.14   |
| 2   | D     | 161 | GDP  | C6-C5-N7    | -26.79 | 130.53      | 134.14   |
| 2   | F     | 161 | GDP  | C6-C5-N7    | -22.49 | 131.11      | 134.14   |
| 2   | F     | 160 | 35G  | C6-C5-N7    | -19.73 | 131.48      | 134.14   |
| 2   | B     | 160 | 35G  | C6-C5-N7    | -17.89 | 131.73      | 134.14   |
| 2   | D     | 160 | 35G  | C6-C5-N7    | -17.34 | 131.81      | 134.14   |
| 2   | D     | 160 | 35G  | C1'-N9-C4   | -16.95 | 97.36       | 126.64   |
| 2   | A     | 160 | 35G  | C1'-N9-C4   | -16.57 | 98.01       | 126.64   |
| 2   | D     | 160 | 35G  | C8-N9-C1'   | 15.62  | 157.16      | 126.38   |
| 2   | A     | 160 | 35G  | C8-N9-C1'   | 14.58  | 155.10      | 126.38   |
| 2   | E     | 160 | 35G  | C1'-N9-C4   | -14.14 | 102.21      | 126.64   |
| 2   | C     | 160 | 35G  | C1'-N9-C4   | -13.08 | 104.04      | 126.64   |
| 2   | C     | 160 | 35G  | C8-N9-C1'   | 13.02  | 152.02      | 126.38   |
| 2   | C     | 160 | 35G  | C6-C5-N7    | -12.76 | 132.42      | 134.14   |
| 2   | E     | 160 | 35G  | C8-N9-C1'   | 11.33  | 148.70      | 126.38   |
| 2   | E     | 161 | GDP  | O3B-PB-O1B  | 11.08  | 146.66      | 110.44   |
| 2   | D     | 161 | GDP  | O3B-PB-O1B  | 10.90  | 146.09      | 110.44   |
| 2   | F     | 161 | GDP  | O3B-PB-O2B  | 9.38   | 144.13      | 107.61   |
| 2   | D     | 161 | GDP  | C1'-N9-C4   | -9.32  | 110.54      | 126.64   |
| 2   | D     | 161 | GDP  | C8-N9-C1'   | 8.88   | 143.87      | 126.38   |
| 2   | C     | 161 | GDP  | O4'-C1'-N9  | 8.20   | 116.07      | 108.44   |
| 2   | C     | 160 | 35G  | N2-C2-N1    | 8.05   | 126.72      | 117.86   |
| 2   | A     | 160 | 35G  | O3'-C3'-C4' | -8.04  | 104.27      | 110.73   |
| 2   | D     | 161 | GDP  | O3B-PB-O2B  | -7.93  | 76.72       | 107.61   |
| 2   | F     | 160 | 35G  | O5'-P-O3'   | 7.85   | 116.60      | 105.81   |
| 2   | F     | 161 | GDP  | O3B-PB-O1B  | -7.49  | 85.96       | 110.44   |
| 2   | E     | 160 | 35G  | O4'-C1'-N9  | -7.21  | 101.74      | 108.44   |
| 2   | E     | 161 | GDP  | O3B-PB-O2B  | -6.94  | 80.59       | 107.61   |
| 2   | B     | 160 | 35G  | C1'-N9-C4   | -6.71  | 115.04      | 126.64   |
| 2   | B     | 160 | 35G  | O3'-C3'-C2' | 6.62   | 123.23      | 115.62   |
| 2   | B     | 160 | 35G  | C8-N9-C1'   | 6.32   | 138.83      | 126.38   |
| 2   | C     | 160 | 35G  | O5'-P-O3'   | 6.18   | 114.31      | 105.81   |
| 2   | A     | 161 | GDP  | O2A-PA-O3A  | 5.90   | 133.11      | 105.14   |
| 2   | C     | 160 | 35G  | O3'-C3'-C4' | -5.69  | 106.16      | 110.73   |
| 2   | F     | 160 | 35G  | O4'-C1'-N9  | 5.68   | 113.72      | 108.44   |
| 2   | E     | 160 | 35G  | O5'-P-O3'   | 5.25   | 113.03      | 105.81   |
| 2   | C     | 161 | GDP  | C1'-N9-C4   | -5.20  | 117.66      | 126.64   |
| 2   | F     | 160 | 35G  | C8-N9-C1'   | 5.18   | 136.58      | 126.38   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | F     | 160 | 35G  | O3'-P-O1P   | -5.16 | 98.95       | 109.99   |
| 2   | F     | 161 | GDP  | O2A-PA-O3A  | 5.16  | 129.63      | 105.14   |
| 2   | C     | 161 | GDP  | O3B-PB-O1B  | 5.11  | 127.14      | 110.44   |
| 2   | A     | 160 | 35G  | O5'-P-O3'   | 5.09  | 112.81      | 105.81   |
| 2   | C     | 161 | GDP  | C8-N9-C1'   | 5.06  | 136.34      | 126.38   |
| 2   | F     | 161 | GDP  | O4'-C1'-N9  | 4.97  | 113.06      | 108.44   |
| 2   | C     | 160 | 35G  | N2-C2-N3    | -4.84 | 113.75      | 120.30   |
| 2   | E     | 161 | GDP  | PA-O3A-PB   | -4.46 | 118.59      | 131.68   |
| 2   | D     | 160 | 35G  | O3'-C3'-C2' | 4.37  | 120.64      | 115.62   |
| 2   | A     | 161 | GDP  | O3B-PB-O2B  | 4.33  | 124.49      | 107.61   |
| 2   | E     | 160 | 35G  | O3'-C3'-C4' | -4.25 | 107.32      | 110.73   |
| 2   | F     | 161 | GDP  | C1'-N9-C4   | -4.19 | 119.39      | 126.64   |
| 2   | F     | 160 | 35G  | C1'-N9-C4   | -4.17 | 119.43      | 126.64   |
| 2   | D     | 161 | GDP  | O2A-PA-O3A  | -4.12 | 85.59       | 105.14   |
| 2   | F     | 161 | GDP  | C8-N9-C1'   | 4.06  | 134.37      | 126.38   |
| 2   | D     | 161 | GDP  | O4'-C1'-N9  | 4.04  | 112.20      | 108.44   |
| 2   | F     | 160 | 35G  | C8-N9-C4    | -3.95 | 103.88      | 106.90   |
| 2   | A     | 160 | 35G  | O4'-C1'-N9  | -3.94 | 104.78      | 108.44   |
| 2   | E     | 161 | GDP  | O4'-C1'-N9  | 3.93  | 112.10      | 108.44   |
| 2   | C     | 160 | 35G  | C8-N9-C4    | -3.91 | 103.91      | 106.90   |
| 2   | A     | 160 | 35G  | C6-N1-C2    | 3.84  | 126.22      | 119.51   |
| 2   | C     | 160 | 35G  | C6-N1-C2    | 3.83  | 126.20      | 119.51   |
| 2   | C     | 160 | 35G  | C2'-C3'-C4' | -3.80 | 95.77       | 103.16   |
| 2   | B     | 160 | 35G  | O5'-P-O3'   | 3.77  | 110.98      | 105.81   |
| 2   | C     | 161 | GDP  | C6-N1-C2    | 3.73  | 126.04      | 119.51   |
| 2   | B     | 160 | 35G  | O2'-C2'-C3' | 3.65  | 121.94      | 111.20   |
| 2   | E     | 160 | 35G  | C4'-O4'-C1' | -3.63 | 105.81      | 109.75   |
| 2   | F     | 160 | 35G  | O3'-C3'-C2' | -3.62 | 111.45      | 115.62   |
| 2   | D     | 160 | 35G  | O2P-P-O3'   | 3.51  | 114.59      | 107.39   |
| 2   | B     | 161 | GDP  | O3B-PB-O1B  | 3.46  | 121.76      | 110.44   |
| 2   | E     | 161 | GDP  | C6-N1-C2    | 3.43  | 125.52      | 119.51   |
| 2   | A     | 161 | GDP  | C6-N1-C2    | 3.38  | 125.42      | 119.51   |
| 2   | A     | 161 | GDP  | O3B-PB-O1B  | -3.37 | 99.42       | 110.44   |
| 2   | F     | 160 | 35G  | C6-N1-C2    | 3.37  | 125.40      | 119.51   |
| 2   | A     | 161 | GDP  | C4-C5-N7    | 3.34  | 112.38      | 109.52   |
| 2   | E     | 161 | GDP  | C4-C5-N7    | 3.27  | 112.32      | 109.52   |
| 2   | B     | 161 | GDP  | C8-N9-C1'   | 3.26  | 132.80      | 126.38   |
| 2   | B     | 161 | GDP  | C1'-N9-C4   | -3.19 | 121.12      | 126.64   |
| 2   | A     | 161 | GDP  | O3A-PA-O1A  | -3.12 | 88.86       | 111.28   |
| 2   | E     | 160 | 35G  | C6-N1-C2    | 3.11  | 124.94      | 119.51   |
| 2   | C     | 161 | GDP  | O3B-PB-O2B  | -3.06 | 95.68       | 107.61   |
| 2   | E     | 160 | 35G  | C4-C5-N7    | 3.02  | 112.11      | 109.52   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | F     | 160 | 35G  | O3'-C3'-C4' | -2.99 | 108.33      | 110.73   |
| 2   | B     | 160 | 35G  | N2-C2-N3    | -2.98 | 116.26      | 120.30   |
| 2   | D     | 161 | GDP  | C6-N1-C2    | 2.93  | 124.63      | 119.51   |
| 2   | C     | 160 | 35G  | O4'-C1'-N9  | 2.92  | 111.15      | 108.44   |
| 2   | D     | 160 | 35G  | C6-N1-C2    | 2.89  | 124.56      | 119.51   |
| 2   | C     | 161 | GDP  | PA-O3A-PB   | -2.81 | 123.44      | 131.68   |
| 2   | C     | 161 | GDP  | C2-N3-C4    | -2.80 | 111.15      | 115.09   |
| 2   | D     | 161 | GDP  | PA-O3A-PB   | -2.80 | 123.47      | 131.68   |
| 2   | E     | 161 | GDP  | C1'-N9-C4   | -2.78 | 121.84      | 126.64   |
| 2   | B     | 161 | GDP  | C6-N1-C2    | 2.77  | 124.35      | 119.51   |
| 2   | C     | 161 | GDP  | C8-N9-C4    | -2.75 | 104.80      | 106.90   |
| 2   | A     | 160 | 35G  | C5-C4-N3    | 2.67  | 129.82      | 125.94   |
| 2   | D     | 161 | GDP  | N2-C2-N1    | -2.67 | 114.92      | 117.86   |
| 2   | E     | 161 | GDP  | C3'-C2'-C1' | 2.66  | 105.08      | 100.91   |
| 2   | B     | 161 | GDP  | N2-C2-N1    | -2.65 | 114.94      | 117.86   |
| 2   | B     | 160 | 35G  | C6-N1-C2    | 2.58  | 124.03      | 119.51   |
| 2   | A     | 160 | 35G  | N2-C2-N3    | -2.58 | 116.81      | 120.30   |
| 2   | D     | 161 | GDP  | O2B-PB-O3A  | -2.57 | 92.94       | 105.14   |
| 2   | E     | 161 | GDP  | C4'-O4'-C1' | 2.50  | 112.47      | 109.75   |
| 2   | A     | 160 | 35G  | C2-N3-C4    | -2.50 | 111.58      | 115.09   |
| 2   | E     | 160 | 35G  | C5-C4-N9    | -2.50 | 103.55      | 107.16   |
| 2   | D     | 160 | 35G  | O5'-P-O1P   | -2.48 | 104.68      | 109.99   |
| 2   | A     | 161 | GDP  | C5-C4-N3    | 2.47  | 129.52      | 125.94   |
| 2   | B     | 161 | GDP  | C2-N3-C4    | -2.44 | 111.66      | 115.09   |
| 2   | C     | 161 | GDP  | C4-C5-N7    | 2.37  | 111.55      | 109.52   |
| 2   | D     | 161 | GDP  | C8-N9-C4    | -2.32 | 105.12      | 106.90   |
| 2   | C     | 161 | GDP  | O2A-PA-O3A  | -2.28 | 94.31       | 105.14   |
| 2   | A     | 160 | 35G  | N2-C2-N1    | 2.28  | 120.37      | 117.86   |
| 2   | A     | 160 | 35G  | C4-C5-N7    | 2.28  | 111.47      | 109.52   |
| 2   | D     | 161 | GDP  | O2A-PA-O1A  | 2.27  | 124.91      | 112.21   |
| 2   | C     | 161 | GDP  | O2B-PB-O1B  | 2.27  | 117.85      | 110.44   |
| 2   | F     | 161 | GDP  | N2-C2-N1    | -2.26 | 115.36      | 117.86   |
| 2   | A     | 161 | GDP  | C8-N9-C4    | -2.26 | 105.17      | 106.90   |
| 2   | E     | 160 | 35G  | C2-N3-C4    | -2.24 | 111.94      | 115.09   |
| 2   | D     | 160 | 35G  | O5'-P-O3'   | 2.24  | 108.89      | 105.81   |
| 2   | F     | 161 | GDP  | O3A-PA-O1A  | -2.24 | 95.24       | 111.28   |
| 2   | F     | 161 | GDP  | C2'-C1'-N9  | -2.23 | 107.53      | 113.27   |
| 2   | C     | 160 | 35G  | C4'-O4'-C1' | -2.23 | 107.33      | 109.75   |
| 2   | B     | 161 | GDP  | O4'-C1'-N9  | 2.22  | 110.50      | 108.44   |
| 2   | E     | 161 | GDP  | C5-C4-N9    | -2.22 | 103.96      | 107.16   |
| 2   | E     | 160 | 35G  | C5-C4-N3    | 2.21  | 129.15      | 125.94   |
| 2   | F     | 160 | 35G  | P-O3'-C3'   | -2.20 | 106.62      | 117.72   |

*Continued on next page...*

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | E     | 160 | 35G  | P-O5'-C5'   | 2.19  | 126.02      | 118.66   |
| 2   | E     | 161 | GDP  | C2'-C1'-N9  | -2.19 | 107.66      | 113.27   |
| 2   | F     | 161 | GDP  | C8-N9-C4    | -2.17 | 105.24      | 106.90   |
| 2   | F     | 160 | 35G  | O2P-P-O5'   | 2.16  | 111.82      | 107.39   |
| 2   | C     | 161 | GDP  | O3A-PA-O1A  | 2.13  | 126.60      | 111.28   |
| 2   | F     | 161 | GDP  | C6-N1-C2    | 2.13  | 123.24      | 119.51   |
| 2   | E     | 161 | GDP  | O2'-C2'-C3' | 2.13  | 118.76      | 111.83   |
| 2   | F     | 160 | 35G  | C4'-O4'-C1' | -2.13 | 107.44      | 109.75   |
| 2   | F     | 160 | 35G  | C2'-C1'-N9  | 2.09  | 118.64      | 113.27   |
| 2   | E     | 161 | GDP  | C8-N9-C1'   | 2.08  | 130.48      | 126.38   |
| 2   | D     | 161 | GDP  | C2-N3-C4    | -2.08 | 112.18      | 115.09   |
| 2   | E     | 161 | GDP  | O5'-C5'-C4' | 2.07  | 116.54      | 108.94   |
| 2   | B     | 161 | GDP  | O2A-PA-O3A  | 2.04  | 114.82      | 105.14   |
| 2   | F     | 161 | GDP  | O5'-C5'-C4' | 2.04  | 116.42      | 108.94   |
| 2   | F     | 160 | 35G  | C2-N3-C4    | -2.01 | 112.27      | 115.09   |
| 2   | B     | 161 | GDP  | N1-C2-N3    | 2.01  | 124.60      | 121.78   |
| 2   | B     | 160 | 35G  | C5'-C4'-C3' | -2.01 | 108.37      | 112.62   |
| 2   | C     | 160 | 35G  | C5-C4-N3    | 2.00  | 128.85      | 125.94   |
| 2   | F     | 161 | GDP  | N1-C2-N3    | 2.00  | 124.59      | 121.78   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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     | 151/152 (99%) | -0.82  | 0       | 100 100 | 7, 25, 54, 76         | 0     |
| 1   | B     | 151/152 (99%) | -0.72  | 0       | 100 100 | 13, 28, 67, 81        | 0     |
| 1   | C     | 151/152 (99%) | -0.87  | 0       | 100 100 | 12, 25, 55, 71        | 0     |
| 1   | D     | 151/152 (99%) | -0.82  | 0       | 100 100 | 7, 26, 55, 70         | 0     |
| 1   | E     | 151/152 (99%) | -0.83  | 0       | 100 100 | 11, 24, 58, 92        | 0     |
| 1   | F     | 151/152 (99%) | -0.80  | 2 (1%)  | 74 73   | 10, 25, 61, 75        | 0     |
| All | All   | 906/912 (99%) | -0.81  | 2 (0%)  | 93 94   | 7, 26, 60, 92         | 0     |

All (2) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 61  | PHE  | 4.1  |
| 1   | F     | 2   | ALA  | 2.7  |

### 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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | GDP  | F     | 161 | 28/28 | 0.22 | 2.28 | 2,99,99,99                  | 28    |
| 2   | GDP  | C     | 161 | 28/28 | 0.12 | 1.67 | 5,32,99,99                  | 28    |
| 2   | 35G  | C     | 160 | 23/23 | 0.12 | 1.52 | 1,39,99,99                  | 23    |
| 2   | GDP  | B     | 161 | 28/28 | 0.19 | 1.45 | 23,99,99,99                 | 28    |
| 2   | 35G  | A     | 160 | 23/23 | 0.14 | 1.23 | 6,70,99,99                  | 23    |
| 2   | GDP  | A     | 161 | 28/28 | 0.15 | 1.15 | 9,78,99,99                  | 28    |
| 2   | 35G  | B     | 160 | 23/23 | 0.17 | 0.99 | 13,99,99,99                 | 23    |
| 2   | GDP  | E     | 161 | 28/28 | 0.15 | 0.96 | 16,79,99,99                 | 28    |
| 2   | 35G  | E     | 160 | 23/23 | 0.14 | 0.76 | 12,53,99,99                 | 23    |
| 2   | GDP  | D     | 161 | 28/28 | 0.12 | 0.40 | 4,38,99,99                  | 28    |
| 2   | 35G  | D     | 160 | 23/23 | 0.12 | 0.36 | 1,69,99,99                  | 23    |
| 2   | 35G  | F     | 160 | 23/23 | 0.14 | 0.35 | 11,52,99,99                 | 23    |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.