



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:08 AM UTC

PDB ID : 2YHM / pdb\_00002yhm  
Title : Structure of respiratory syncytial virus nucleocapsid protein, P212121 crystal form  
Authors : El Omari, K.; Dhaliwal, B.; Ren, J.; Abrescia, N.G.A.; Lockyer, M.; Powell, K.L.; Hawkins, A.R.; Stammers, D.K.  
Deposited on : 2011-05-04  
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

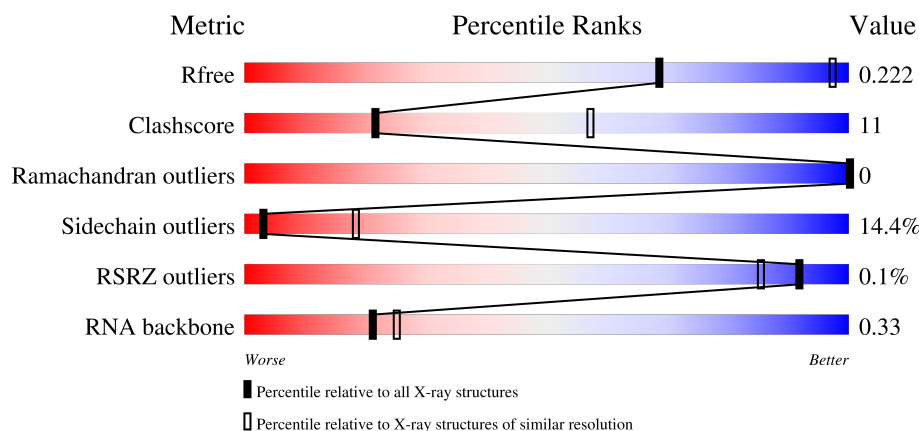
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 Å.

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



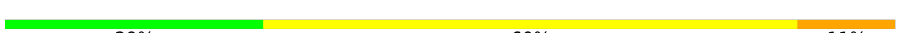
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1747 (3.70-3.50)                                      |
| Clashscore            | 190562                      | 1827 (3.70-3.50)                                      |
| Ramachandran outliers | 187476                      | 1773 (3.70-3.50)                                      |
| Sidechain outliers    | 187428                      | 1772 (3.70-3.50)                                      |
| RSRZ outliers         | 180081                      | 1745 (3.70-3.50)                                      |
| RNA backbone          | 3983                        | 1014 (4.14-3.06)                                      |

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 375    |                  |
| 1   | B     | 375    |                  |
| 1   | C     | 375    |                  |
| 1   | D     | 375    |                  |

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| Mol | Chain | Length | Quality of chain                                                                             |
|-----|-------|--------|----------------------------------------------------------------------------------------------|
| 1   | E     | 375    |  69%26%6%  |
| 1   | F     | 375    |  67%29%4%  |
| 1   | G     | 375    |  70%25%5%  |
| 1   | H     | 375    |  71%25%5%  |
| 1   | I     | 375    |  71%23%5%  |
| 1   | J     | 375    |  68%27%5%  |
| 2   | K     | 70     |  29%60%11% |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 30600 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NUCLEOPROTEIN.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 375      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2920  | 1848 | 506 | 549 | 17 |         |         |       |
| 1   | B     | 375      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2920  | 1848 | 506 | 549 | 17 |         |         |       |
| 1   | C     | 375      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2920  | 1848 | 506 | 549 | 17 |         |         |       |
| 1   | D     | 375      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2920  | 1848 | 506 | 549 | 17 |         |         |       |
| 1   | E     | 375      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2920  | 1848 | 506 | 549 | 17 |         |         |       |
| 1   | F     | 375      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2920  | 1848 | 506 | 549 | 17 |         |         |       |
| 1   | G     | 375      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2920  | 1848 | 506 | 549 | 17 |         |         |       |
| 1   | H     | 375      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2920  | 1848 | 506 | 549 | 17 |         |         |       |
| 1   | I     | 375      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2920  | 1848 | 506 | 549 | 17 |         |         |       |
| 1   | J     | 375      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2920  | 1848 | 506 | 549 | 17 |         |         |       |

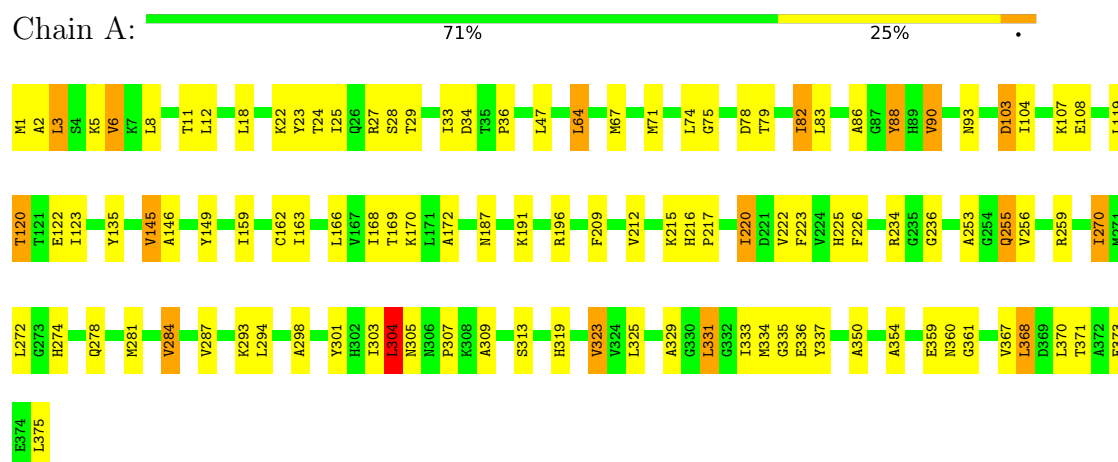
- Molecule 2 is a RNA chain called RNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 2   | K     | 70       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1400  | 630 | 210 | 490 | 70 |         |         |       |

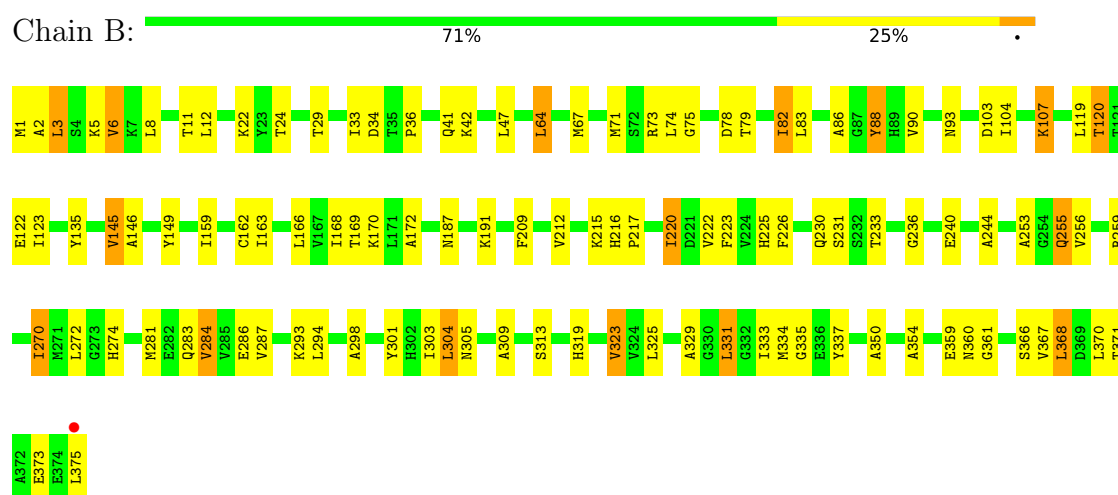
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

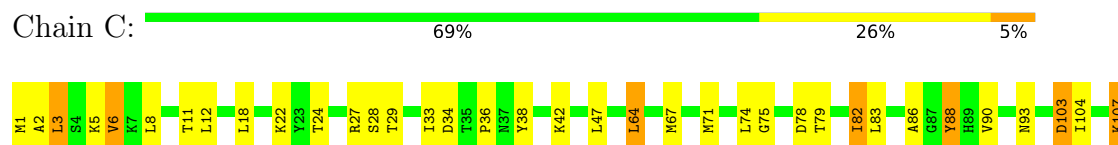
#### • Molecule 1: NUCLEOPROTEIN

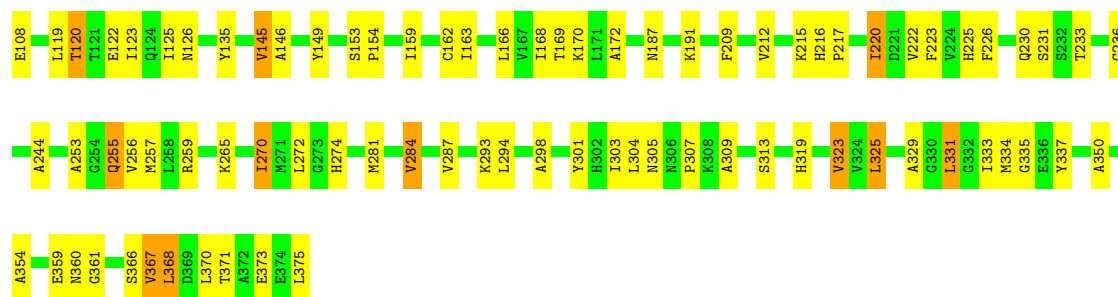


#### • Molecule 1: NUCLEOPROTEIN



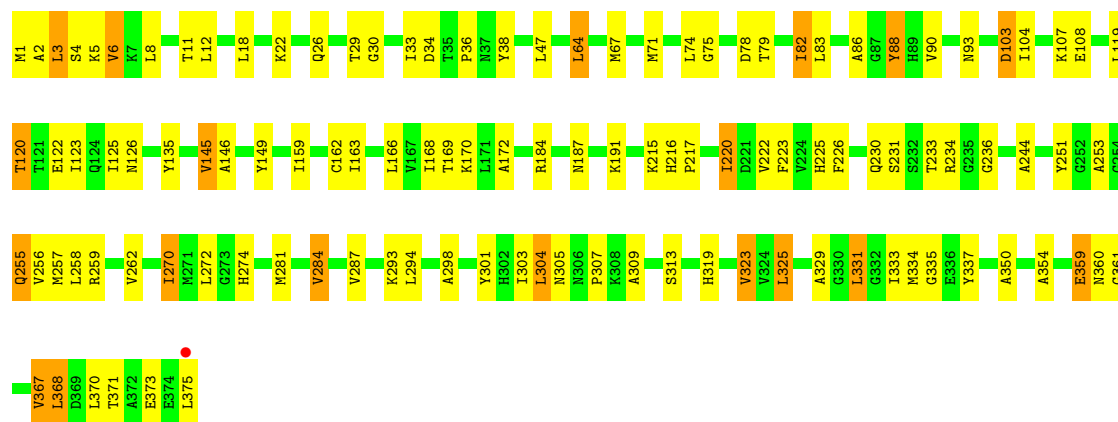
#### • Molecule 1: NUCLEOPROTEIN





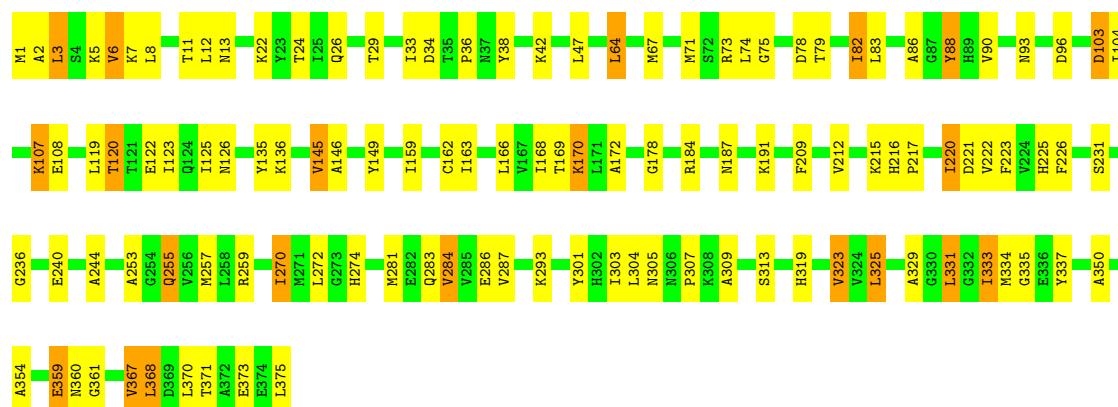
• Molecule 1: NUCLEOPROTEIN

Chain D: 69% 26% 5%



• Molecule 1: NUCLEOPROTEIN

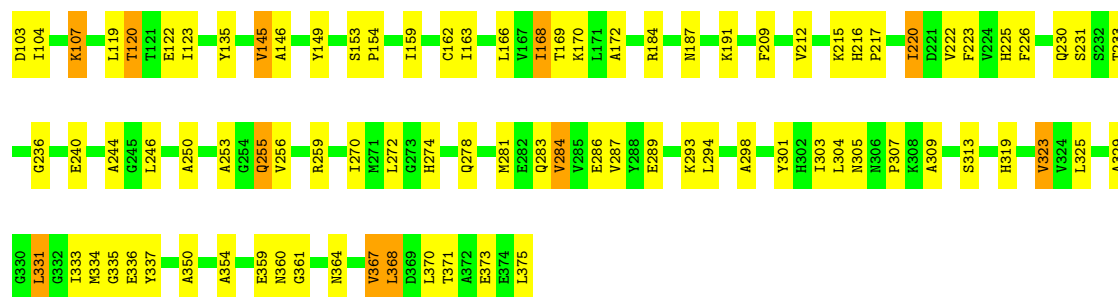
Chain E: 69% 26% 6%



• Molecule 1: NUCLEOPROTEIN

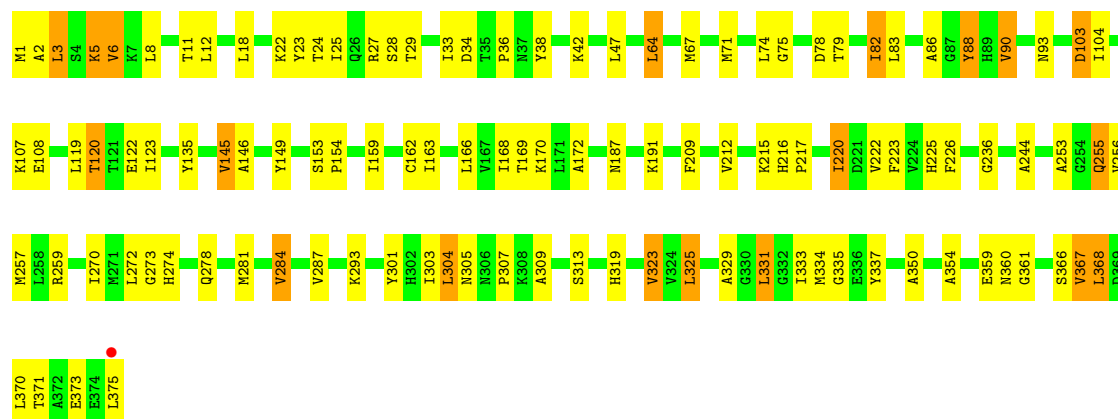
Chain F: 67% 29% .





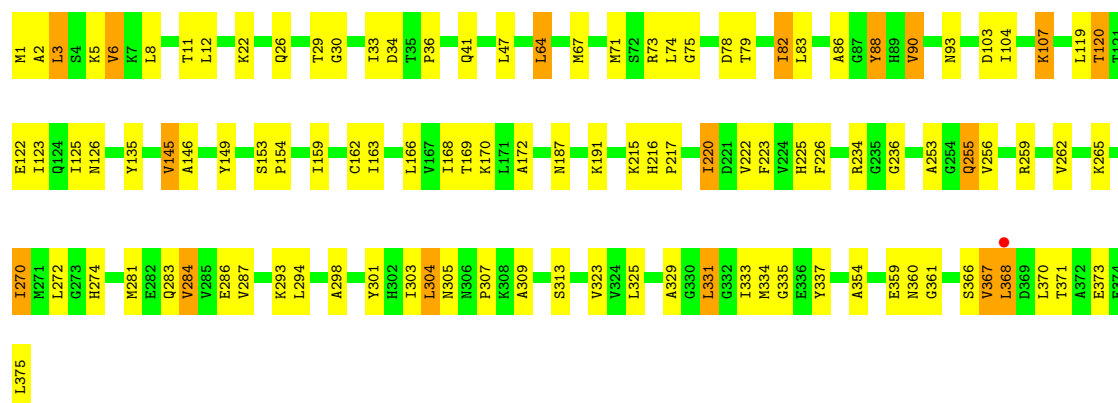
• Molecule 1: NUCLEOPROTEIN

Chain G: 70% 25% 5%



• Molecule 1: NUCLEOPROTEIN

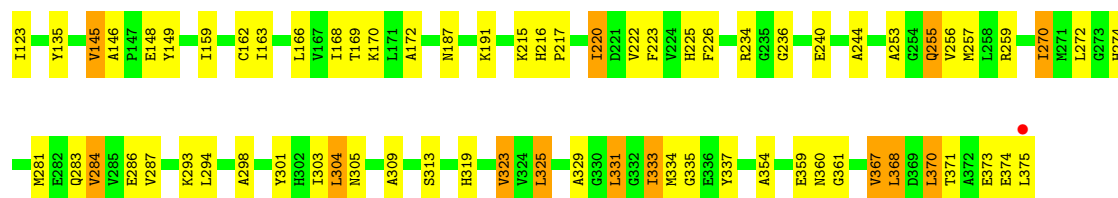
Chain H: 71% 25% 5%



• Molecule 1: NUCLEOPROTEIN

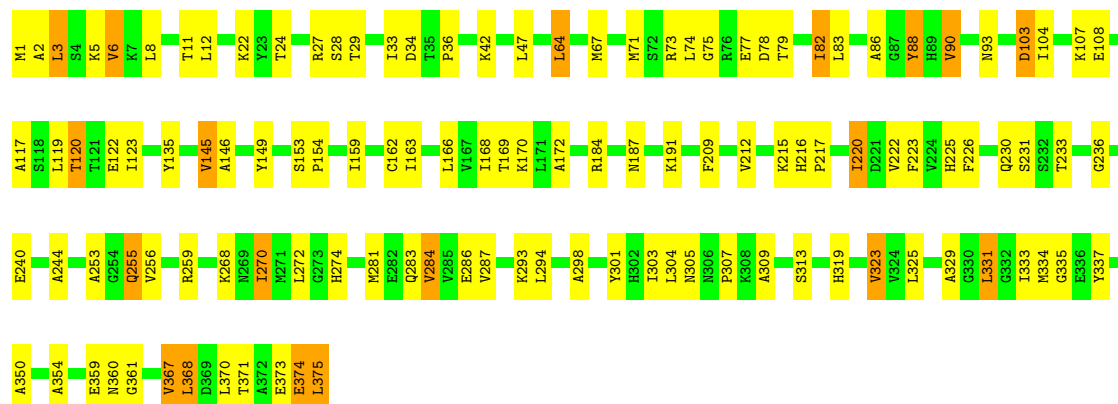
Chain I: 71% 23% 5%





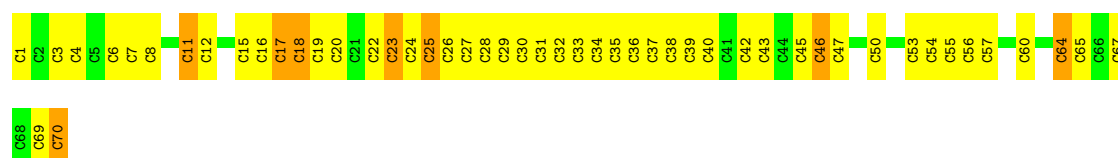
• Molecule 1: NUCLEOPROTEIN

Chain J: 68% 27% 5%



• Molecule 2: RNA

Chain K: 29% 60% 11%



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 133.61Å 149.91Å 255.20Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 50.00 – 3.60<br>50.00 – 3.60                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 83.4 (50.00-3.60)<br>83.4 (50.00-3.60)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.14                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.70 (at 3.47Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.6.0077                                             | Depositor        |
| R, $R_{free}$                                                           | 0.196 , 0.224<br>0.196 , 0.222                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2682 reflections (5.06%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 82.1                                                        | Xtriage          |
| Anisotropy                                                              | 0.491                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 51.3                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 30600                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 102.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 1   | A     | 0.46         | 0/2968  | 0.88        | 2/3998 (0.1%)  |
| 1   | B     | 0.45         | 0/2968  | 0.87        | 0/3998         |
| 1   | C     | 0.46         | 0/2968  | 0.88        | 0/3998         |
| 1   | D     | 0.46         | 0/2968  | 0.87        | 1/3998 (0.0%)  |
| 1   | E     | 0.47         | 0/2968  | 0.88        | 0/3998         |
| 1   | F     | 0.48         | 0/2968  | 0.88        | 0/3998         |
| 1   | G     | 0.47         | 0/2968  | 0.87        | 1/3998 (0.0%)  |
| 1   | H     | 0.47         | 0/2968  | 0.89        | 1/3998 (0.0%)  |
| 1   | I     | 0.47         | 0/2968  | 0.88        | 0/3998         |
| 1   | J     | 0.47         | 0/2968  | 0.87        | 1/3998 (0.0%)  |
| 2   | K     | 0.38         | 0/1539  | 0.82        | 0/2376         |
| All | All   | 0.46         | 0/31219 | 0.87        | 6/42356 (0.0%) |

There are no bond length outliers.

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | D     | 304 | LEU  | N-CA-C | -5.32 | 103.01      | 110.50   |
| 1   | A     | 304 | LEU  | N-CA-C | -5.31 | 103.13      | 110.35   |
| 1   | J     | 90  | VAL  | N-CA-C | 5.30  | 115.71      | 107.28   |
| 1   | G     | 90  | VAL  | N-CA-C | 5.06  | 115.33      | 107.28   |
| 1   | H     | 90  | VAL  | N-CA-C | 5.06  | 115.33      | 107.28   |
| 1   | A     | 90  | VAL  | N-CA-C | 5.03  | 115.28      | 107.28   |

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2920  | 0        | 2955     | 68      | 0            |
| 1   | B     | 2920  | 0        | 2955     | 69      | 0            |
| 1   | C     | 2920  | 0        | 2955     | 82      | 0            |
| 1   | D     | 2920  | 0        | 2955     | 75      | 1            |
| 1   | E     | 2920  | 0        | 2955     | 92      | 13           |
| 1   | F     | 2920  | 0        | 2955     | 89      | 4            |
| 1   | G     | 2920  | 0        | 2955     | 73      | 0            |
| 1   | H     | 2920  | 0        | 2955     | 67      | 0            |
| 1   | I     | 2920  | 0        | 2955     | 73      | 8            |
| 1   | J     | 2920  | 0        | 2955     | 78      | 10           |
| 2   | K     | 1400  | 0        | 771      | 28      | 0            |
| All | All   | 30600 | 0        | 30321    | 658     | 18           |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (658) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:F:82:ILE:HD11  | 1:F:222:VAL:HA  | 1.32                     | 1.10              |
| 1:J:82:ILE:HD11  | 1:J:222:VAL:HA  | 1.34                     | 1.10              |
| 1:H:82:ILE:HD11  | 1:H:222:VAL:HA  | 1.34                     | 1.09              |
| 1:G:82:ILE:HD11  | 1:G:222:VAL:HA  | 1.32                     | 1.09              |
| 1:A:82:ILE:HD11  | 1:A:222:VAL:HA  | 1.34                     | 1.08              |
| 1:C:367:VAL:HG13 | 1:E:1:MET:HG3   | 1.29                     | 1.08              |
| 1:E:82:ILE:HD11  | 1:E:222:VAL:HA  | 1.36                     | 1.06              |
| 1:B:82:ILE:HD11  | 1:B:222:VAL:HA  | 1.35                     | 1.05              |
| 1:C:82:ILE:HD11  | 1:C:222:VAL:HA  | 1.37                     | 1.05              |
| 1:D:82:ILE:HD11  | 1:D:222:VAL:HA  | 1.35                     | 1.02              |
| 1:I:361:GLY:HA3  | 1:J:274:HIS:NE2 | 1.75                     | 1.01              |
| 1:I:82:ILE:HD11  | 1:I:222:VAL:HA  | 1.37                     | 1.01              |
| 1:F:42:LYS:HD2   | 1:G:28:SER:HB3  | 1.40                     | 1.00              |
| 1:C:367:VAL:O    | 1:E:1:MET:N     | 1.96                     | 0.98              |
| 2:K:1:C:P        | 2:K:70:C:H3'    | 2.04                     | 0.97              |
| 1:C:367:VAL:HA   | 1:E:1:MET:HG2   | 1.45                     | 0.96              |
| 1:C:367:VAL:CG1  | 1:E:1:MET:HG3   | 1.99                     | 0.93              |
| 1:H:75:GLY:O     | 1:H:79:THR:HG22 | 1.71                     | 0.90              |
| 1:E:361:GLY:HA3  | 1:F:274:HIS:NE2 | 1.88                     | 0.88              |
| 1:H:256:VAL:HG12 | 2:K:53:C:OP1    | 1.72                     | 0.88              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:361:GLY:HA3  | 1:C:274:HIS:NE2  | 1.90                     | 0.87              |
| 1:C:236:GLY:O    | 1:D:305:ASN:HB2  | 1.76                     | 0.86              |
| 1:F:42:LYS:HD2   | 1:G:28:SER:CB    | 2.05                     | 0.86              |
| 1:F:75:GLY:O     | 1:F:79:THR:HG22  | 1.76                     | 0.85              |
| 1:C:366:SER:O    | 1:E:1:MET:HE3    | 1.76                     | 0.85              |
| 1:G:75:GLY:O     | 1:G:79:THR:HG22  | 1.77                     | 0.85              |
| 1:I:75:GLY:O     | 1:I:79:THR:HG22  | 1.76                     | 0.85              |
| 1:E:75:GLY:O     | 1:E:79:THR:HG22  | 1.77                     | 0.84              |
| 1:D:75:GLY:O     | 1:D:79:THR:HG22  | 1.77                     | 0.84              |
| 1:A:75:GLY:O     | 1:A:79:THR:HG22  | 1.77                     | 0.84              |
| 1:J:75:GLY:O     | 1:J:79:THR:HG22  | 1.78                     | 0.83              |
| 1:F:361:GLY:HA3  | 1:G:274:HIS:NE2  | 1.93                     | 0.83              |
| 1:A:28:SER:HB3   | 1:J:42:LYS:HD2   | 1.62                     | 0.81              |
| 1:C:75:GLY:O     | 1:C:79:THR:HG22  | 1.80                     | 0.81              |
| 1:D:256:VAL:HG12 | 2:K:25:C:OP1     | 1.81                     | 0.80              |
| 1:C:367:VAL:HG13 | 1:E:1:MET:CG     | 2.11                     | 0.80              |
| 1:B:75:GLY:O     | 1:B:79:THR:HG22  | 1.81                     | 0.79              |
| 1:H:3:LEU:O      | 1:H:6:VAL:HG13   | 1.83                     | 0.79              |
| 1:I:3:LEU:O      | 1:I:6:VAL:HG13   | 1.85                     | 0.77              |
| 1:G:368:LEU:HG   | 1:I:3:LEU:HD11   | 1.67                     | 0.77              |
| 1:C:3:LEU:O      | 1:C:6:VAL:HG13   | 1.85                     | 0.76              |
| 1:B:3:LEU:O      | 1:B:6:VAL:HG13   | 1.86                     | 0.76              |
| 1:D:3:LEU:O      | 1:D:6:VAL:HG13   | 1.85                     | 0.76              |
| 1:J:3:LEU:O      | 1:J:6:VAL:HG13   | 1.86                     | 0.76              |
| 1:D:367:VAL:HG12 | 1:F:3:LEU:HD13   | 1.68                     | 0.75              |
| 1:E:42:LYS:NZ    | 1:F:30:GLY:C     | 2.45                     | 0.75              |
| 1:F:3:LEU:O      | 1:F:6:VAL:HG13   | 1.86                     | 0.75              |
| 1:I:256:VAL:HG12 | 2:K:60:C:OP1     | 1.87                     | 0.74              |
| 1:A:3:LEU:O      | 1:A:6:VAL:HG13   | 1.87                     | 0.74              |
| 1:E:42:LYS:HZ2   | 1:F:30:GLY:C     | 1.96                     | 0.74              |
| 1:H:331:LEU:HD13 | 1:H:354:ALA:HB1  | 1.70                     | 0.74              |
| 1:A:28:SER:CB    | 1:J:42:LYS:HD2   | 2.18                     | 0.73              |
| 1:I:331:LEU:HD13 | 1:I:354:ALA:HB1  | 1.69                     | 0.73              |
| 1:D:331:LEU:HD13 | 1:D:354:ALA:HB1  | 1.69                     | 0.72              |
| 1:C:331:LEU:HD13 | 1:C:354:ALA:HB1  | 1.70                     | 0.72              |
| 1:A:331:LEU:HD13 | 1:A:354:ALA:HB1  | 1.72                     | 0.72              |
| 1:E:3:LEU:O      | 1:E:6:VAL:HG13   | 1.88                     | 0.72              |
| 1:G:3:LEU:O      | 1:G:6:VAL:HG13   | 1.88                     | 0.71              |
| 1:H:253:ALA:HB3  | 1:H:303:ILE:HD11 | 1.72                     | 0.71              |
| 1:B:253:ALA:HB3  | 1:B:303:ILE:HD11 | 1.72                     | 0.71              |
| 1:E:331:LEU:HD13 | 1:E:354:ALA:HB1  | 1.73                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:331:LEU:HD13 | 1:B:354:ALA:HB1  | 1.72                     | 0.71              |
| 1:F:253:ALA:HB3  | 1:F:303:ILE:HD11 | 1.72                     | 0.70              |
| 1:F:331:LEU:HD13 | 1:F:354:ALA:HB1  | 1.71                     | 0.70              |
| 1:D:236:GLY:O    | 1:E:305:ASN:HB2  | 1.90                     | 0.70              |
| 1:G:331:LEU:HD13 | 1:G:354:ALA:HB1  | 1.73                     | 0.70              |
| 1:I:253:ALA:HB3  | 1:I:303:ILE:HD11 | 1.74                     | 0.70              |
| 1:E:29:THR:CG2   | 1:E:88:TYR:HB3   | 2.22                     | 0.70              |
| 1:E:361:GLY:HA3  | 1:F:274:HIS:HE2  | 1.55                     | 0.69              |
| 1:F:29:THR:CG2   | 1:F:88:TYR:HB3   | 2.22                     | 0.69              |
| 1:H:236:GLY:O    | 1:I:305:ASN:HB2  | 1.92                     | 0.69              |
| 1:A:29:THR:CG2   | 1:A:88:TYR:HB3   | 2.23                     | 0.69              |
| 1:G:253:ALA:HB3  | 1:G:303:ILE:HD11 | 1.74                     | 0.69              |
| 1:J:29:THR:CG2   | 1:J:88:TYR:HB3   | 2.23                     | 0.69              |
| 1:D:29:THR:CG2   | 1:D:88:TYR:HB3   | 2.23                     | 0.69              |
| 1:G:256:VAL:HG12 | 2:K:46:C:OP1     | 1.93                     | 0.69              |
| 1:C:29:THR:CG2   | 1:C:88:TYR:HB3   | 2.22                     | 0.69              |
| 1:C:367:VAL:HA   | 1:E:1:MET:CG     | 2.22                     | 0.68              |
| 1:I:29:THR:CG2   | 1:I:88:TYR:HB3   | 2.23                     | 0.68              |
| 1:J:331:LEU:HD13 | 1:J:354:ALA:HB1  | 1.74                     | 0.68              |
| 1:F:240:GLU:OE2  | 1:G:27:ARG:HD3   | 1.94                     | 0.68              |
| 1:B:29:THR:CG2   | 1:B:88:TYR:HB3   | 2.24                     | 0.67              |
| 1:J:253:ALA:HB3  | 1:J:303:ILE:HD11 | 1.76                     | 0.67              |
| 1:H:29:THR:CG2   | 1:H:88:TYR:HB3   | 2.23                     | 0.67              |
| 1:A:361:GLY:HA3  | 1:B:274:HIS:NE2  | 2.10                     | 0.67              |
| 1:G:367:VAL:CG1  | 1:I:2:ALA:HB3    | 2.25                     | 0.67              |
| 1:G:236:GLY:O    | 1:H:305:ASN:HB2  | 1.95                     | 0.66              |
| 1:D:253:ALA:HB3  | 1:D:303:ILE:HD11 | 1.77                     | 0.66              |
| 1:G:29:THR:CG2   | 1:G:88:TYR:HB3   | 2.25                     | 0.66              |
| 1:G:361:GLY:HA3  | 1:H:274:HIS:NE2  | 2.11                     | 0.66              |
| 1:G:146:ALA:HB3  | 1:G:149:TYR:HD2  | 1.60                     | 0.66              |
| 1:B:236:GLY:O    | 1:C:305:ASN:HB2  | 1.96                     | 0.65              |
| 1:E:253:ALA:HB3  | 1:E:303:ILE:HD11 | 1.79                     | 0.65              |
| 1:A:146:ALA:HB3  | 1:A:149:TYR:HD2  | 1.61                     | 0.65              |
| 1:A:253:ALA:HB3  | 1:A:303:ILE:HD11 | 1.78                     | 0.64              |
| 1:D:367:VAL:HG12 | 1:F:3:LEU:CD1    | 2.26                     | 0.64              |
| 1:C:146:ALA:HB3  | 1:C:149:TYR:HD2  | 1.62                     | 0.64              |
| 1:J:146:ALA:HB3  | 1:J:149:TYR:HD2  | 1.63                     | 0.64              |
| 1:E:146:ALA:HB3  | 1:E:149:TYR:HD2  | 1.63                     | 0.63              |
| 1:A:274:HIS:NE2  | 1:J:361:GLY:HA3  | 2.13                     | 0.63              |
| 1:F:256:VAL:HG12 | 2:K:39:C:OP1     | 1.98                     | 0.63              |
| 1:B:146:ALA:HB3  | 1:B:149:TYR:HD2  | 1.63                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:368:LEU:H    | 1:C:368:LEU:HD12 | 1.64                     | 0.63              |
| 1:D:146:ALA:HB3  | 1:D:149:TYR:HD2  | 1.63                     | 0.62              |
| 1:H:146:ALA:HB3  | 1:H:149:TYR:HD2  | 1.64                     | 0.62              |
| 1:C:1:MET:HG3    | 1:C:2:ALA:H      | 1.65                     | 0.62              |
| 1:B:1:MET:HG3    | 1:B:2:ALA:H      | 1.65                     | 0.62              |
| 1:F:146:ALA:HB3  | 1:F:149:TYR:HD2  | 1.65                     | 0.62              |
| 1:A:236:GLY:O    | 1:B:305:ASN:HB2  | 2.00                     | 0.61              |
| 1:I:146:ALA:HB3  | 1:I:149:TYR:HD2  | 1.64                     | 0.61              |
| 1:H:234:ARG:NH2  | 1:I:86:ALA:HB2   | 2.14                     | 0.61              |
| 1:D:368:LEU:HD12 | 1:D:368:LEU:H    | 1.65                     | 0.61              |
| 1:F:1:MET:HG3    | 1:F:2:ALA:H      | 1.66                     | 0.61              |
| 1:D:215:LYS:HE3  | 1:D:216:HIS:HE1  | 1.66                     | 0.61              |
| 1:E:1:MET:HG3    | 1:E:2:ALA:H      | 1.67                     | 0.60              |
| 1:I:1:MET:HG3    | 1:I:2:ALA:H      | 1.66                     | 0.60              |
| 1:C:253:ALA:HB3  | 1:C:303:ILE:HD11 | 1.83                     | 0.60              |
| 1:G:366:SER:O    | 1:I:1:MET:HE3    | 2.02                     | 0.60              |
| 1:J:301:TYR:HB3  | 1:J:309:ALA:HB2  | 1.83                     | 0.60              |
| 1:J:368:LEU:H    | 1:J:368:LEU:HD12 | 1.67                     | 0.60              |
| 1:E:215:LYS:HE3  | 1:E:216:HIS:HE1  | 1.67                     | 0.60              |
| 1:A:368:LEU:HD12 | 1:A:368:LEU:H    | 1.67                     | 0.60              |
| 1:G:1:MET:HG3    | 1:G:2:ALA:H      | 1.66                     | 0.60              |
| 1:C:301:TYR:HB3  | 1:C:309:ALA:HB2  | 1.83                     | 0.59              |
| 1:E:301:TYR:HB3  | 1:E:309:ALA:HB2  | 1.82                     | 0.59              |
| 1:A:215:LYS:HE3  | 1:A:216:HIS:HE1  | 1.67                     | 0.59              |
| 1:D:361:GLY:HA3  | 1:E:274:HIS:NE2  | 2.18                     | 0.59              |
| 1:J:29:THR:HG22  | 1:J:88:TYR:HB3   | 1.84                     | 0.59              |
| 1:A:301:TYR:HB3  | 1:A:309:ALA:HB2  | 1.85                     | 0.59              |
| 1:E:361:GLY:HA3  | 1:F:274:HIS:CE1  | 2.37                     | 0.59              |
| 1:B:368:LEU:HG   | 1:D:3:LEU:HD11   | 1.85                     | 0.59              |
| 1:D:367:VAL:CG1  | 1:F:3:LEU:CD1    | 2.81                     | 0.59              |
| 1:J:256:VAL:HG12 | 2:K:67:C:OP1     | 2.03                     | 0.59              |
| 1:C:335:GLY:CA   | 1:C:337:TYR:H    | 2.16                     | 0.59              |
| 1:F:29:THR:HG22  | 1:F:88:TYR:HB3   | 1.85                     | 0.59              |
| 1:C:29:THR:HG22  | 1:C:88:TYR:HB3   | 1.84                     | 0.58              |
| 1:F:231:SER:HB2  | 1:G:18:LEU:HD22  | 1.85                     | 0.58              |
| 1:C:217:PRO:O    | 1:C:220:ILE:HG23 | 2.02                     | 0.58              |
| 1:E:29:THR:HG22  | 1:E:88:TYR:HB3   | 1.85                     | 0.58              |
| 1:D:29:THR:HG22  | 1:D:88:TYR:HB3   | 1.85                     | 0.58              |
| 1:A:256:VAL:HG12 | 2:K:4:C:OP1      | 2.04                     | 0.58              |
| 1:B:368:LEU:HD12 | 1:B:368:LEU:H    | 1.67                     | 0.58              |
| 1:D:1:MET:HG3    | 1:D:2:ALA:H      | 1.69                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:335:GLY:CA   | 1:D:337:TYR:H    | 2.17                     | 0.58              |
| 1:F:301:TYR:HB3  | 1:F:309:ALA:HB2  | 1.86                     | 0.58              |
| 1:F:335:GLY:CA   | 1:F:337:TYR:H    | 2.17                     | 0.58              |
| 1:C:256:VAL:HG12 | 2:K:18:C:OP1     | 2.04                     | 0.58              |
| 1:H:234:ARG:HH21 | 1:I:86:ALA:HB2   | 1.68                     | 0.58              |
| 1:F:368:LEU:HD12 | 1:F:368:LEU:H    | 1.67                     | 0.58              |
| 1:E:335:GLY:CA   | 1:E:337:TYR:H    | 2.16                     | 0.58              |
| 1:H:335:GLY:CA   | 1:H:337:TYR:H    | 2.17                     | 0.58              |
| 1:J:1:MET:HG3    | 1:J:2:ALA:H      | 1.68                     | 0.58              |
| 1:B:335:GLY:CA   | 1:B:337:TYR:H    | 2.17                     | 0.58              |
| 1:H:1:MET:HG3    | 1:H:2:ALA:H      | 1.67                     | 0.58              |
| 1:D:301:TYR:HB3  | 1:D:309:ALA:HB2  | 1.86                     | 0.57              |
| 1:E:368:LEU:H    | 1:E:368:LEU:HD12 | 1.68                     | 0.57              |
| 1:G:368:LEU:HD12 | 1:G:368:LEU:H    | 1.67                     | 0.57              |
| 1:E:217:PRO:O    | 1:E:220:ILE:HG23 | 2.04                     | 0.57              |
| 1:J:335:GLY:CA   | 1:J:337:TYR:H    | 2.18                     | 0.57              |
| 1:A:1:MET:HG3    | 1:A:2:ALA:H      | 1.67                     | 0.57              |
| 1:F:289:GLU:OE2  | 1:G:5:LYS:HD2    | 2.04                     | 0.57              |
| 1:I:335:GLY:CA   | 1:I:337:TYR:H    | 2.17                     | 0.57              |
| 2:K:69:C:H2'     | 2:K:70:C:O4'     | 2.04                     | 0.57              |
| 1:G:301:TYR:HB3  | 1:G:309:ALA:HB2  | 1.87                     | 0.57              |
| 1:A:27:ARG:HD3   | 1:J:240:GLU:OE2  | 2.04                     | 0.57              |
| 1:C:244:ALA:HB1  | 1:D:307:PRO:HB3  | 1.86                     | 0.57              |
| 1:H:29:THR:HG22  | 1:H:88:TYR:HB3   | 1.85                     | 0.57              |
| 1:I:29:THR:HG22  | 1:I:88:TYR:HB3   | 1.85                     | 0.57              |
| 1:B:301:TYR:HB3  | 1:B:309:ALA:HB2  | 1.87                     | 0.57              |
| 1:H:217:PRO:O    | 1:H:220:ILE:HG23 | 2.04                     | 0.57              |
| 1:E:42:LYS:NZ    | 1:F:30:GLY:O     | 2.33                     | 0.57              |
| 1:H:368:LEU:H    | 1:H:368:LEU:HD12 | 1.70                     | 0.57              |
| 1:J:217:PRO:O    | 1:J:220:ILE:HG23 | 2.04                     | 0.57              |
| 1:C:367:VAL:CG1  | 1:E:2:ALA:H      | 2.18                     | 0.56              |
| 1:G:335:GLY:CA   | 1:G:337:TYR:H    | 2.17                     | 0.56              |
| 1:A:29:THR:HG22  | 1:A:88:TYR:HB3   | 1.86                     | 0.56              |
| 1:B:29:THR:HG22  | 1:B:88:TYR:HB3   | 1.86                     | 0.56              |
| 1:I:301:TYR:HB3  | 1:I:309:ALA:HB2  | 1.87                     | 0.56              |
| 1:H:367:VAL:O    | 1:J:1:MET:N      | 2.39                     | 0.56              |
| 1:B:217:PRO:O    | 1:B:220:ILE:HG23 | 2.06                     | 0.56              |
| 1:G:29:THR:HG22  | 1:G:88:TYR:HB3   | 1.88                     | 0.56              |
| 1:I:361:GLY:HA3  | 1:J:274:HIS:CE1  | 2.41                     | 0.56              |
| 1:B:244:ALA:HB1  | 1:C:307:PRO:HB3  | 1.88                     | 0.56              |
| 1:I:215:LYS:HE3  | 1:I:216:HIS:HE1  | 1.70                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:236:GLY:O    | 1:J:305:ASN:HB2  | 2.05                     | 0.56              |
| 1:C:335:GLY:HA2  | 1:C:337:TYR:H    | 1.70                     | 0.56              |
| 1:I:368:LEU:HD12 | 1:I:368:LEU:H    | 1.69                     | 0.56              |
| 1:E:244:ALA:HB1  | 1:F:307:PRO:HB3  | 1.87                     | 0.55              |
| 1:A:82:ILE:HD12  | 1:A:225:HIS:HB2  | 1.89                     | 0.55              |
| 1:A:335:GLY:CA   | 1:A:337:TYR:H    | 2.19                     | 0.55              |
| 1:F:82:ILE:HD12  | 1:F:225:HIS:HB2  | 1.88                     | 0.55              |
| 1:F:184:ARG:NH1  | 2:K:42:C:OP2     | 2.38                     | 0.55              |
| 1:G:215:LYS:HE3  | 1:G:216:HIS:HE1  | 1.70                     | 0.55              |
| 2:K:16:C:H2'     | 2:K:17:C:O4'     | 2.07                     | 0.55              |
| 1:A:217:PRO:O    | 1:A:220:ILE:HG23 | 2.07                     | 0.55              |
| 1:C:368:LEU:HD12 | 1:C:368:LEU:N    | 2.21                     | 0.55              |
| 1:H:215:LYS:HE3  | 1:H:216:HIS:HE1  | 1.71                     | 0.55              |
| 1:D:82:ILE:HD12  | 1:D:225:HIS:HB2  | 1.89                     | 0.55              |
| 1:G:146:ALA:HB3  | 1:G:149:TYR:CD2  | 2.41                     | 0.55              |
| 1:I:335:GLY:HA2  | 1:I:337:TYR:H    | 1.72                     | 0.55              |
| 1:C:215:LYS:HE3  | 1:C:216:HIS:HE1  | 1.71                     | 0.55              |
| 1:G:335:GLY:HA2  | 1:G:337:TYR:H    | 1.72                     | 0.55              |
| 1:A:18:LEU:HD22  | 1:J:231:SER:HB2  | 1.89                     | 0.54              |
| 1:B:335:GLY:HA2  | 1:B:337:TYR:H    | 1.73                     | 0.54              |
| 1:D:335:GLY:HA2  | 1:D:337:TYR:H    | 1.72                     | 0.54              |
| 1:E:82:ILE:HD12  | 1:E:225:HIS:HB2  | 1.89                     | 0.54              |
| 1:F:236:GLY:O    | 1:G:305:ASN:HB2  | 2.07                     | 0.54              |
| 1:G:368:LEU:HD12 | 1:G:368:LEU:N    | 2.23                     | 0.54              |
| 1:F:335:GLY:HA2  | 1:F:337:TYR:H    | 1.72                     | 0.54              |
| 1:C:368:LEU:HG   | 1:E:3:LEU:HD11   | 1.90                     | 0.54              |
| 1:D:217:PRO:O    | 1:D:220:ILE:HG23 | 2.08                     | 0.54              |
| 1:D:368:LEU:HD12 | 1:D:368:LEU:N    | 2.22                     | 0.54              |
| 1:F:215:LYS:HE3  | 1:F:216:HIS:HE1  | 1.72                     | 0.54              |
| 1:F:240:GLU:CD   | 1:G:27:ARG:HH11  | 2.16                     | 0.54              |
| 1:H:301:TYR:HB3  | 1:H:309:ALA:HB2  | 1.90                     | 0.54              |
| 1:I:82:ILE:HD12  | 1:I:225:HIS:HB2  | 1.90                     | 0.54              |
| 1:A:278:GLN:OE1  | 1:J:367:VAL:HG11 | 2.08                     | 0.54              |
| 1:E:335:GLY:HA2  | 1:E:337:TYR:H    | 1.71                     | 0.54              |
| 1:B:215:LYS:HE3  | 1:B:216:HIS:HE1  | 1.73                     | 0.54              |
| 1:B:368:LEU:HD12 | 1:B:368:LEU:N    | 2.23                     | 0.54              |
| 1:E:38:TYR:CE1   | 1:F:26:GLN:HB2   | 2.43                     | 0.54              |
| 1:D:172:ALA:HB2  | 1:D:253:ALA:HB1  | 1.90                     | 0.54              |
| 1:A:368:LEU:HD12 | 1:A:368:LEU:N    | 2.23                     | 0.53              |
| 1:E:240:GLU:OE2  | 1:F:27:ARG:HD3   | 2.08                     | 0.53              |
| 1:F:244:ALA:HB1  | 1:G:307:PRO:HB3  | 1.89                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:281:MET:HA   | 1:G:284:VAL:HG22 | 1.90                     | 0.53              |
| 1:H:86:ALA:HB1   | 1:H:88:TYR:HE1   | 1.73                     | 0.53              |
| 1:B:82:ILE:HD12  | 1:B:225:HIS:HB2  | 1.89                     | 0.53              |
| 1:F:329:ALA:HA   | 1:F:334:MET:HG2  | 1.91                     | 0.53              |
| 1:G:38:TYR:CE1   | 1:H:26:GLN:HB2   | 2.43                     | 0.53              |
| 1:H:335:GLY:HA2  | 1:H:337:TYR:H    | 1.74                     | 0.53              |
| 1:J:368:LEU:HD12 | 1:J:368:LEU:N    | 2.24                     | 0.53              |
| 1:J:82:ILE:HD12  | 1:J:225:HIS:HB2  | 1.89                     | 0.53              |
| 1:J:86:ALA:HB1   | 1:J:88:TYR:HE1   | 1.74                     | 0.53              |
| 1:J:335:GLY:HA2  | 1:J:337:TYR:H    | 1.74                     | 0.53              |
| 1:H:281:MET:HA   | 1:H:284:VAL:HG22 | 1.91                     | 0.53              |
| 1:C:172:ALA:HB2  | 1:C:253:ALA:HB1  | 1.91                     | 0.53              |
| 1:E:172:ALA:HB2  | 1:E:253:ALA:HB1  | 1.91                     | 0.53              |
| 1:F:368:LEU:HD12 | 1:F:368:LEU:N    | 2.24                     | 0.53              |
| 1:B:86:ALA:HB1   | 1:B:88:TYR:HE1   | 1.74                     | 0.52              |
| 1:E:86:ALA:HB1   | 1:E:88:TYR:HE1   | 1.73                     | 0.52              |
| 1:D:281:MET:HA   | 1:D:284:VAL:HG22 | 1.91                     | 0.52              |
| 1:F:367:VAL:HG11 | 1:G:278:GLN:OE1  | 2.09                     | 0.52              |
| 1:E:78:ASP:O     | 1:E:82:ILE:HG23  | 2.10                     | 0.52              |
| 1:E:146:ALA:HB3  | 1:E:149:TYR:CD2  | 2.45                     | 0.52              |
| 1:I:172:ALA:HB2  | 1:I:253:ALA:HB1  | 1.92                     | 0.52              |
| 1:J:215:LYS:HE3  | 1:J:216:HIS:HE1  | 1.74                     | 0.52              |
| 1:D:146:ALA:HB3  | 1:D:149:TYR:CD2  | 2.44                     | 0.52              |
| 1:G:217:PRO:O    | 1:G:220:ILE:HG23 | 2.09                     | 0.52              |
| 1:J:172:ALA:HB2  | 1:J:253:ALA:HB1  | 1.91                     | 0.52              |
| 1:G:367:VAL:HG11 | 1:I:2:ALA:HB3    | 1.91                     | 0.52              |
| 1:I:74:LEU:HD21  | 1:I:226:PHE:HA   | 1.90                     | 0.52              |
| 1:I:86:ALA:HB1   | 1:I:88:TYR:HE1   | 1.73                     | 0.52              |
| 1:F:217:PRO:O    | 1:F:220:ILE:HG23 | 2.09                     | 0.52              |
| 1:G:86:ALA:HB1   | 1:G:88:TYR:HE1   | 1.73                     | 0.52              |
| 1:I:368:LEU:HD12 | 1:I:368:LEU:N    | 2.25                     | 0.52              |
| 1:G:74:LEU:HD21  | 1:G:226:PHE:HA   | 1.92                     | 0.52              |
| 1:H:82:ILE:HD12  | 1:H:225:HIS:HB2  | 1.92                     | 0.52              |
| 1:D:244:ALA:HB1  | 1:E:307:PRO:HB3  | 1.92                     | 0.51              |
| 1:G:303:ILE:HD12 | 1:G:303:ILE:H    | 1.75                     | 0.51              |
| 1:I:217:PRO:O    | 1:I:220:ILE:HG23 | 2.11                     | 0.51              |
| 1:C:82:ILE:HD12  | 1:C:225:HIS:HB2  | 1.91                     | 0.51              |
| 1:F:86:ALA:HB1   | 1:F:88:TYR:HE1   | 1.75                     | 0.51              |
| 1:H:368:LEU:HG   | 1:J:3:LEU:HD11   | 1.92                     | 0.51              |
| 1:J:146:ALA:HB3  | 1:J:149:TYR:CD2  | 2.45                     | 0.51              |
| 1:B:172:ALA:HB2  | 1:B:253:ALA:HB1  | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:236:GLY:O    | 1:F:305:ASN:HB2  | 2.09                     | 0.51              |
| 1:E:368:LEU:HD12 | 1:E:368:LEU:N    | 2.24                     | 0.51              |
| 1:A:305:ASN:HB2  | 1:J:236:GLY:O    | 2.09                     | 0.51              |
| 1:G:82:ILE:HD12  | 1:G:225:HIS:HB2  | 1.91                     | 0.51              |
| 1:G:329:ALA:HA   | 1:G:334:MET:HG2  | 1.93                     | 0.51              |
| 1:A:329:ALA:HA   | 1:A:334:MET:HG2  | 1.93                     | 0.51              |
| 1:C:86:ALA:HB1   | 1:C:88:TYR:HE1   | 1.76                     | 0.51              |
| 1:H:67:MET:HE2   | 1:H:67:MET:HA    | 1.91                     | 0.51              |
| 1:A:86:ALA:HB1   | 1:A:88:TYR:HE1   | 1.75                     | 0.51              |
| 1:B:329:ALA:HA   | 1:B:334:MET:HG2  | 1.93                     | 0.51              |
| 1:E:367:VAL:HG12 | 1:G:3:LEU:CD1    | 2.39                     | 0.51              |
| 1:G:172:ALA:HB2  | 1:G:253:ALA:HB1  | 1.91                     | 0.51              |
| 1:D:329:ALA:HA   | 1:D:334:MET:HG2  | 1.92                     | 0.51              |
| 1:C:146:ALA:HB3  | 1:C:149:TYR:CD2  | 2.45                     | 0.51              |
| 1:C:329:ALA:HA   | 1:C:334:MET:HG2  | 1.93                     | 0.51              |
| 1:C:367:VAL:HG11 | 1:E:2:ALA:HB3    | 1.92                     | 0.51              |
| 1:F:146:ALA:HB3  | 1:F:149:TYR:CD2  | 2.46                     | 0.51              |
| 2:K:3:C:H6       | 2:K:3:C:O5'      | 1.93                     | 0.51              |
| 1:B:281:MET:HA   | 1:B:284:VAL:HG22 | 1.93                     | 0.51              |
| 1:H:172:ALA:HB2  | 1:H:253:ALA:HB1  | 1.93                     | 0.50              |
| 1:C:361:GLY:HA3  | 1:D:274:HIS:NE2  | 2.27                     | 0.50              |
| 1:D:74:LEU:HD21  | 1:D:226:PHE:HA   | 1.93                     | 0.50              |
| 1:D:367:VAL:CG1  | 1:F:3:LEU:HD12   | 2.41                     | 0.50              |
| 1:H:368:LEU:HD12 | 1:H:368:LEU:N    | 2.26                     | 0.50              |
| 1:D:303:ILE:HD12 | 1:D:303:ILE:H    | 1.75                     | 0.50              |
| 1:H:78:ASP:O     | 1:H:82:ILE:HG23  | 2.11                     | 0.50              |
| 1:H:303:ILE:HD12 | 1:H:303:ILE:H    | 1.76                     | 0.50              |
| 2:K:64:C:H2'     | 2:K:65:C:O4'     | 2.11                     | 0.50              |
| 1:A:74:LEU:HD21  | 1:A:226:PHE:HA   | 1.94                     | 0.50              |
| 1:A:172:ALA:HB2  | 1:A:253:ALA:HB1  | 1.92                     | 0.50              |
| 1:A:146:ALA:HB3  | 1:A:149:TYR:CD2  | 2.43                     | 0.50              |
| 1:C:281:MET:HA   | 1:C:284:VAL:HG22 | 1.94                     | 0.50              |
| 1:F:367:VAL:HG12 | 1:H:3:LEU:CD1    | 2.40                     | 0.50              |
| 1:C:166:LEU:O    | 1:C:169:THR:HB   | 2.11                     | 0.50              |
| 1:D:86:ALA:HB1   | 1:D:88:TYR:HE1   | 1.75                     | 0.50              |
| 1:F:82:ILE:HG22  | 1:G:23:TYR:CE1   | 2.46                     | 0.50              |
| 1:F:281:MET:HA   | 1:F:284:VAL:HG22 | 1.94                     | 0.50              |
| 1:H:159:ILE:O    | 1:H:162:CYS:HB2  | 2.12                     | 0.50              |
| 1:J:74:LEU:HD21  | 1:J:226:PHE:HA   | 1.93                     | 0.50              |
| 1:A:166:LEU:O    | 1:A:169:THR:HB   | 2.12                     | 0.50              |
| 1:C:303:ILE:HD12 | 1:C:303:ILE:H    | 1.76                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:146:ALA:HB3  | 1:I:149:TYR:CD2  | 2.45                     | 0.50              |
| 1:H:329:ALA:HA   | 1:H:334:MET:HG2  | 1.93                     | 0.50              |
| 1:E:329:ALA:HA   | 1:E:334:MET:HG2  | 1.94                     | 0.49              |
| 1:A:67:MET:HE1   | 1:A:223:PHE:CD1  | 2.47                     | 0.49              |
| 1:J:281:MET:HA   | 1:J:284:VAL:HG22 | 1.94                     | 0.49              |
| 1:F:74:LEU:HD21  | 1:F:226:PHE:HA   | 1.94                     | 0.49              |
| 1:I:329:ALA:HA   | 1:I:334:MET:HG2  | 1.93                     | 0.49              |
| 1:J:166:LEU:O    | 1:J:169:THR:HB   | 2.13                     | 0.49              |
| 1:A:335:GLY:HA2  | 1:A:337:TYR:H    | 1.75                     | 0.49              |
| 1:F:78:ASP:O     | 1:F:82:ILE:HG23  | 2.13                     | 0.49              |
| 1:E:166:LEU:O    | 1:E:169:THR:HB   | 2.13                     | 0.49              |
| 1:A:281:MET:HA   | 1:A:284:VAL:HG22 | 1.95                     | 0.49              |
| 1:E:36:PRO:HD2   | 1:E:71:MET:HB3   | 1.95                     | 0.49              |
| 1:J:67:MET:HE2   | 1:J:67:MET:HA    | 1.94                     | 0.49              |
| 1:B:146:ALA:HB3  | 1:B:149:TYR:CD2  | 2.44                     | 0.49              |
| 1:B:366:SER:O    | 1:D:1:MET:HE3    | 2.13                     | 0.49              |
| 1:F:64:LEU:HD12  | 1:F:119:LEU:HD13 | 1.95                     | 0.48              |
| 1:D:67:MET:HA    | 1:D:67:MET:HE2   | 1.95                     | 0.48              |
| 1:H:262:VAL:HG13 | 1:I:7:LYS:HA     | 1.95                     | 0.48              |
| 1:I:64:LEU:HD12  | 1:I:119:LEU:HD13 | 1.94                     | 0.48              |
| 1:B:166:LEU:O    | 1:B:169:THR:HB   | 2.13                     | 0.48              |
| 1:D:38:TYR:CE1   | 1:E:26:GLN:HB2   | 2.48                     | 0.48              |
| 1:E:42:LYS:HZ1   | 1:F:30:GLY:C     | 2.18                     | 0.48              |
| 1:E:78:ASP:O     | 1:E:82:ILE:CG2   | 2.62                     | 0.48              |
| 1:F:172:ALA:HB2  | 1:F:253:ALA:HB1  | 1.95                     | 0.48              |
| 1:H:74:LEU:HD21  | 1:H:226:PHE:HA   | 1.94                     | 0.48              |
| 1:B:361:GLY:HA3  | 1:C:274:HIS:HE2  | 1.74                     | 0.48              |
| 1:E:255:GLN:HB2  | 1:E:259:ARG:NH1  | 2.29                     | 0.48              |
| 1:B:74:LEU:HD21  | 1:B:226:PHE:HA   | 1.95                     | 0.48              |
| 1:E:281:MET:HA   | 1:E:284:VAL:HG22 | 1.94                     | 0.48              |
| 1:C:88:TYR:CD1   | 1:C:88:TYR:N     | 2.82                     | 0.48              |
| 1:G:78:ASP:O     | 1:G:82:ILE:HG23  | 2.14                     | 0.48              |
| 1:G:34:ASP:HA    | 1:G:93:ASN:HB3   | 1.96                     | 0.48              |
| 1:H:166:LEU:O    | 1:H:169:THR:HB   | 2.14                     | 0.48              |
| 1:A:23:TYR:CE1   | 1:J:82:ILE:HG22  | 2.49                     | 0.47              |
| 1:A:78:ASP:O     | 1:A:82:ILE:HG23  | 2.13                     | 0.47              |
| 1:C:74:LEU:HD21  | 1:C:226:PHE:HA   | 1.95                     | 0.47              |
| 1:J:329:ALA:HA   | 1:J:334:MET:HG2  | 1.95                     | 0.47              |
| 1:D:64:LEU:HD12  | 1:D:119:LEU:HD13 | 1.95                     | 0.47              |
| 1:H:366:SER:O    | 1:J:1:MET:HE3    | 2.14                     | 0.47              |
| 1:A:23:TYR:CZ    | 1:J:82:ILE:HB    | 2.48                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:78:ASP:O     | 1:D:82:ILE:HG23  | 2.15                     | 0.47              |
| 1:E:303:ILE:H    | 1:E:303:ILE:HD12 | 1.80                     | 0.47              |
| 1:B:67:MET:HE2   | 1:B:67:MET:HA    | 1.96                     | 0.47              |
| 1:I:88:TYR:CD1   | 1:I:88:TYR:N     | 2.82                     | 0.47              |
| 2:K:30:C:H2'     | 2:K:31:C:O4'     | 2.15                     | 0.47              |
| 1:B:34:ASP:HA    | 1:B:93:ASN:HB3   | 1.96                     | 0.47              |
| 1:G:67:MET:HE1   | 1:G:223:PHE:CD1  | 2.49                     | 0.47              |
| 1:H:78:ASP:O     | 1:H:82:ILE:CG2   | 2.62                     | 0.47              |
| 1:B:3:LEU:CD1    | 1:J:367:VAL:HG12 | 2.44                     | 0.47              |
| 1:B:64:LEU:HD12  | 1:B:119:LEU:HD13 | 1.96                     | 0.47              |
| 1:E:42:LYS:HD2   | 1:F:28:SER:HB3   | 1.97                     | 0.47              |
| 1:H:88:TYR:CD1   | 1:H:88:TYR:N     | 2.83                     | 0.47              |
| 1:I:234:ARG:HH21 | 1:J:86:ALA:HB2   | 1.79                     | 0.47              |
| 1:F:78:ASP:O     | 1:F:82:ILE:CG2   | 2.63                     | 0.47              |
| 1:F:107:LYS:H    | 1:F:107:LYS:HG3  | 1.58                     | 0.47              |
| 1:H:34:ASP:HA    | 1:H:93:ASN:HB3   | 1.96                     | 0.47              |
| 1:I:187:ASN:O    | 1:I:191:LYS:HB3  | 2.15                     | 0.47              |
| 1:I:281:MET:HA   | 1:I:284:VAL:HG22 | 1.96                     | 0.47              |
| 1:I:303:ILE:HD12 | 1:I:303:ILE:H    | 1.80                     | 0.47              |
| 1:J:34:ASP:HA    | 1:J:93:ASN:HB3   | 1.97                     | 0.47              |
| 1:J:64:LEU:HD12  | 1:J:119:LEU:HD13 | 1.96                     | 0.47              |
| 1:E:34:ASP:HA    | 1:E:93:ASN:HB3   | 1.97                     | 0.47              |
| 1:E:74:LEU:HD21  | 1:E:226:PHE:HA   | 1.97                     | 0.47              |
| 1:G:166:LEU:O    | 1:G:169:THR:HB   | 2.15                     | 0.47              |
| 1:J:67:MET:HE1   | 1:J:223:PHE:CD1  | 2.50                     | 0.47              |
| 1:C:367:VAL:CG1  | 1:E:1:MET:CG     | 2.80                     | 0.47              |
| 1:B:361:GLY:HA3  | 1:C:274:HIS:CE1  | 2.50                     | 0.47              |
| 1:E:337:TYR:CE1  | 2:K:32:C:H2'     | 2.50                     | 0.47              |
| 1:B:303:ILE:HD12 | 1:B:303:ILE:H    | 1.80                     | 0.46              |
| 1:C:67:MET:HE2   | 1:C:67:MET:HA    | 1.96                     | 0.46              |
| 1:C:42:LYS:NZ    | 1:D:30:GLY:C     | 2.74                     | 0.46              |
| 1:E:135:TYR:OH   | 1:E:145:VAL:HG21 | 2.16                     | 0.46              |
| 1:A:34:ASP:HA    | 1:A:93:ASN:HB3   | 1.96                     | 0.46              |
| 1:A:67:MET:HE2   | 1:A:67:MET:HA    | 1.96                     | 0.46              |
| 1:A:303:ILE:HD12 | 1:A:303:ILE:H    | 1.80                     | 0.46              |
| 1:B:256:VAL:HG12 | 2:K:11:C:OP1     | 2.14                     | 0.46              |
| 1:C:34:ASP:HA    | 1:C:93:ASN:HB3   | 1.96                     | 0.46              |
| 1:E:88:TYR:N     | 1:E:88:TYR:CD1   | 2.83                     | 0.46              |
| 1:I:34:ASP:HA    | 1:I:93:ASN:HB3   | 1.96                     | 0.46              |
| 1:G:64:LEU:HD12  | 1:G:119:LEU:HD13 | 1.96                     | 0.46              |
| 1:A:28:SER:HB2   | 1:J:42:LYS:HD2   | 1.96                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:78:ASP:O     | 1:A:82:ILE:CG2   | 2.64                     | 0.46              |
| 1:B:88:TYR:CD1   | 1:B:88:TYR:N     | 2.83                     | 0.46              |
| 1:C:107:LYS:H    | 1:C:107:LYS:HG3  | 1.53                     | 0.46              |
| 1:F:34:ASP:HA    | 1:F:93:ASN:HB3   | 1.97                     | 0.46              |
| 1:H:146:ALA:HB3  | 1:H:149:TYR:CD2  | 2.46                     | 0.46              |
| 1:A:135:TYR:OH   | 1:A:145:VAL:HG21 | 2.16                     | 0.46              |
| 1:B:231:SER:HB2  | 1:C:18:LEU:HD22  | 1.97                     | 0.46              |
| 1:I:67:MET:HE1   | 1:I:223:PHE:CD1  | 2.51                     | 0.46              |
| 1:I:78:ASP:O     | 1:I:82:ILE:HG23  | 2.15                     | 0.46              |
| 1:J:88:TYR:CD1   | 1:J:88:TYR:N     | 2.83                     | 0.46              |
| 1:F:303:ILE:HD12 | 1:F:303:ILE:H    | 1.80                     | 0.46              |
| 1:B:78:ASP:O     | 1:B:82:ILE:HG23  | 2.15                     | 0.46              |
| 1:D:88:TYR:N     | 1:D:88:TYR:CD1   | 2.83                     | 0.46              |
| 2:K:54:C:N4      | 2:K:55:C:N4      | 2.63                     | 0.46              |
| 1:C:64:LEU:HD12  | 1:C:119:LEU:HD13 | 1.97                     | 0.46              |
| 1:D:215:LYS:HE3  | 1:D:216:HIS:CE1  | 2.50                     | 0.46              |
| 1:D:255:GLN:HB2  | 1:D:259:ARG:NH1  | 2.31                     | 0.46              |
| 1:I:166:LEU:O    | 1:I:169:THR:HB   | 2.16                     | 0.46              |
| 1:C:255:GLN:HB2  | 1:C:259:ARG:NH1  | 2.31                     | 0.46              |
| 1:C:265:LYS:HE3  | 1:D:4:SER:HA     | 1.97                     | 0.46              |
| 1:D:166:LEU:O    | 1:D:169:THR:HB   | 2.17                     | 0.46              |
| 1:G:78:ASP:O     | 1:G:82:ILE:CG2   | 2.64                     | 0.46              |
| 1:H:361:GLY:HA3  | 1:I:274:HIS:NE2  | 2.31                     | 0.46              |
| 1:I:120:THR:CG2  | 1:I:122:GLU:HG2  | 2.46                     | 0.46              |
| 1:J:36:PRO:HD2   | 1:J:71:MET:HB3   | 1.98                     | 0.46              |
| 1:B:187:ASN:O    | 1:B:191:LYS:HB3  | 2.16                     | 0.45              |
| 1:F:42:LYS:CD    | 1:G:28:SER:HB3   | 2.28                     | 0.45              |
| 1:E:231:SER:HA   | 1:F:307:PRO:HG2  | 1.97                     | 0.45              |
| 1:E:367:VAL:HG21 | 1:F:278:GLN:CD   | 2.41                     | 0.45              |
| 1:H:64:LEU:HD12  | 1:H:119:LEU:HD13 | 1.96                     | 0.45              |
| 1:C:78:ASP:O     | 1:C:82:ILE:HG23  | 2.16                     | 0.45              |
| 1:H:120:THR:CG2  | 1:H:122:GLU:HG2  | 2.47                     | 0.45              |
| 1:D:319:HIS:O    | 1:D:323:VAL:HG12 | 2.17                     | 0.45              |
| 1:F:88:TYR:N     | 1:F:88:TYR:CD1   | 2.85                     | 0.45              |
| 1:H:107:LYS:H    | 1:H:107:LYS:HG3  | 1.56                     | 0.45              |
| 1:B:67:MET:HE1   | 1:B:223:PHE:CD1  | 2.51                     | 0.45              |
| 1:F:166:LEU:O    | 1:F:169:THR:HB   | 2.16                     | 0.45              |
| 1:H:67:MET:HE1   | 1:H:223:PHE:CD1  | 2.51                     | 0.45              |
| 1:H:303:ILE:HD12 | 1:H:303:ILE:N    | 2.31                     | 0.45              |
| 1:D:34:ASP:HA    | 1:D:93:ASN:HB3   | 1.98                     | 0.45              |
| 1:H:187:ASN:O    | 1:H:191:LYS:HB3  | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:36:PRO:HD2   | 1:I:71:MET:HB3   | 1.99                     | 0.45              |
| 1:E:187:ASN:O    | 1:E:191:LYS:HB3  | 2.16                     | 0.45              |
| 1:A:323:VAL:HG23 | 1:A:350:ALA:HB2  | 1.98                     | 0.45              |
| 1:J:78:ASP:O     | 1:J:82:ILE:CG2   | 2.65                     | 0.45              |
| 1:J:255:GLN:HB2  | 1:J:259:ARG:NH1  | 2.32                     | 0.45              |
| 2:K:54:C:H2'     | 2:K:55:C:O4'     | 2.17                     | 0.45              |
| 1:A:64:LEU:HD12  | 1:A:119:LEU:HD13 | 1.98                     | 0.45              |
| 1:B:159:ILE:O    | 1:B:162:CYS:HB2  | 2.17                     | 0.45              |
| 1:I:42:LYS:HD2   | 1:J:28:SER:HB3   | 1.99                     | 0.45              |
| 2:K:23:C:H2'     | 2:K:24:C:O4'     | 2.17                     | 0.45              |
| 1:A:88:TYR:CD1   | 1:A:88:TYR:N     | 2.84                     | 0.45              |
| 1:A:3:LEU:CD1    | 1:I:367:VAL:HG12 | 2.47                     | 0.44              |
| 1:C:135:TYR:OH   | 1:C:145:VAL:HG21 | 2.17                     | 0.44              |
| 1:F:159:ILE:O    | 1:F:162:CYS:HB2  | 2.17                     | 0.44              |
| 1:G:120:THR:CG2  | 1:G:122:GLU:HG2  | 2.47                     | 0.44              |
| 1:J:323:VAL:HG23 | 1:J:350:ALA:HB2  | 1.99                     | 0.44              |
| 1:D:303:ILE:HD12 | 1:D:303:ILE:N    | 2.31                     | 0.44              |
| 1:F:120:THR:CG2  | 1:F:122:GLU:HG2  | 2.47                     | 0.44              |
| 1:F:135:TYR:OH   | 1:F:145:VAL:HG21 | 2.18                     | 0.44              |
| 1:D:78:ASP:O     | 1:D:82:ILE:CG2   | 2.66                     | 0.44              |
| 1:I:240:GLU:OE2  | 1:J:27:ARG:HD3   | 2.16                     | 0.44              |
| 1:G:88:TYR:CD1   | 1:G:88:TYR:N     | 2.85                     | 0.44              |
| 1:C:230:GLN:O    | 1:C:233:THR:HG22 | 2.18                     | 0.44              |
| 1:D:135:TYR:OH   | 1:D:145:VAL:HG21 | 2.17                     | 0.44              |
| 1:E:67:MET:HE1   | 1:E:223:PHE:CD1  | 2.52                     | 0.44              |
| 1:F:67:MET:HA    | 1:F:67:MET:HE2   | 1.99                     | 0.44              |
| 1:F:255:GLN:HB2  | 1:F:259:ARG:NH1  | 2.33                     | 0.44              |
| 1:G:42:LYS:NZ    | 1:H:30:GLY:C     | 2.76                     | 0.44              |
| 1:G:153:SER:HA   | 1:G:154:PRO:HD2  | 1.82                     | 0.44              |
| 1:G:159:ILE:O    | 1:G:162:CYS:HB2  | 2.18                     | 0.44              |
| 1:J:270:ILE:HD13 | 1:J:270:ILE:HA   | 1.76                     | 0.44              |
| 1:C:36:PRO:HD2   | 1:C:71:MET:HB3   | 1.99                     | 0.44              |
| 1:C:187:ASN:O    | 1:C:191:LYS:HB3  | 2.17                     | 0.44              |
| 1:D:251:TYR:OH   | 1:E:13:ASN:HB3   | 2.18                     | 0.44              |
| 1:E:67:MET:HE2   | 1:E:67:MET:HA    | 1.99                     | 0.44              |
| 1:E:73:ARG:CZ    | 1:F:27:ARG:HG2   | 2.48                     | 0.44              |
| 1:G:303:ILE:HD12 | 1:G:303:ILE:N    | 2.33                     | 0.44              |
| 1:F:323:VAL:HG23 | 1:F:350:ALA:HB2  | 1.99                     | 0.44              |
| 1:I:78:ASP:O     | 1:I:82:ILE:CG2   | 2.66                     | 0.44              |
| 1:I:159:ILE:O    | 1:I:162:CYS:HB2  | 2.18                     | 0.44              |
| 1:A:120:THR:CG2  | 1:A:122:GLU:HG2  | 2.47                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:78:ASP:O     | 1:B:82:ILE:CG2   | 2.66                     | 0.44              |
| 1:E:184:ARG:NH1  | 2:K:35:C:OP2     | 2.50                     | 0.44              |
| 1:E:120:THR:CG2  | 1:E:122:GLU:HG2  | 2.47                     | 0.43              |
| 1:G:255:GLN:HB2  | 1:G:259:ARG:NH1  | 2.33                     | 0.43              |
| 1:J:187:ASN:O    | 1:J:191:LYS:HB3  | 2.18                     | 0.43              |
| 1:A:234:ARG:HH21 | 1:B:86:ALA:HB2   | 1.83                     | 0.43              |
| 1:B:255:GLN:HB2  | 1:B:259:ARG:NH1  | 2.33                     | 0.43              |
| 1:C:367:VAL:CA   | 1:E:1:MET:HG2    | 2.32                     | 0.43              |
| 1:A:159:ILE:O    | 1:A:162:CYS:HB2  | 2.18                     | 0.43              |
| 1:A:270:ILE:HD13 | 1:A:270:ILE:HA   | 1.78                     | 0.43              |
| 1:D:120:THR:CG2  | 1:D:122:GLU:HG2  | 2.48                     | 0.43              |
| 1:F:29:THR:HG22  | 1:F:88:TYR:HD2   | 1.83                     | 0.43              |
| 1:F:67:MET:HE1   | 1:F:223:PHE:CD1  | 2.53                     | 0.43              |
| 1:H:36:PRO:HD2   | 1:H:71:MET:HB3   | 2.00                     | 0.43              |
| 1:H:135:TYR:OH   | 1:H:145:VAL:HG21 | 2.18                     | 0.43              |
| 1:A:187:ASN:O    | 1:A:191:LYS:HB3  | 2.18                     | 0.43              |
| 1:B:270:ILE:HD13 | 1:B:270:ILE:HA   | 1.78                     | 0.43              |
| 1:B:303:ILE:HD12 | 1:B:303:ILE:N    | 2.34                     | 0.43              |
| 1:D:230:GLN:O    | 1:D:233:THR:HG22 | 2.18                     | 0.43              |
| 1:G:135:TYR:OH   | 1:G:145:VAL:HG21 | 2.18                     | 0.43              |
| 1:H:255:GLN:HB2  | 1:H:259:ARG:NH1  | 2.33                     | 0.43              |
| 1:J:319:HIS:O    | 1:J:323:VAL:HG12 | 2.18                     | 0.43              |
| 1:B:120:THR:CG2  | 1:B:122:GLU:HG2  | 2.49                     | 0.43              |
| 1:H:6:VAL:O      | 1:H:6:VAL:HG22   | 2.18                     | 0.43              |
| 1:F:187:ASN:O    | 1:F:191:LYS:HB3  | 2.19                     | 0.43              |
| 1:G:6:VAL:O      | 1:G:6:VAL:HG22   | 2.17                     | 0.43              |
| 1:H:265:LYS:HG3  | 1:I:3:LEU:O      | 2.18                     | 0.43              |
| 1:E:159:ILE:O    | 1:E:162:CYS:HB2  | 2.18                     | 0.43              |
| 1:E:257:MET:HE1  | 1:E:325:LEU:HD23 | 2.00                     | 0.43              |
| 1:F:230:GLN:O    | 1:F:233:THR:HG22 | 2.19                     | 0.43              |
| 1:I:333:ILE:H    | 1:I:333:ILE:HG13 | 1.68                     | 0.43              |
| 1:A:294:LEU:HB3  | 1:A:298:ALA:HB2  | 2.01                     | 0.43              |
| 1:C:38:TYR:CE1   | 1:D:26:GLN:HB2   | 2.53                     | 0.43              |
| 1:D:270:ILE:HD13 | 1:D:270:ILE:HA   | 1.79                     | 0.43              |
| 1:F:319:HIS:O    | 1:F:323:VAL:HG12 | 2.19                     | 0.43              |
| 1:I:319:HIS:O    | 1:I:323:VAL:HG12 | 2.19                     | 0.43              |
| 1:C:257:MET:HE1  | 1:C:325:LEU:HD23 | 2.01                     | 0.43              |
| 1:G:319:HIS:O    | 1:G:323:VAL:HG12 | 2.18                     | 0.43              |
| 1:I:67:MET:HA    | 1:I:67:MET:HE2   | 2.01                     | 0.43              |
| 1:A:36:PRO:HD2   | 1:A:71:MET:HB3   | 2.01                     | 0.43              |
| 1:F:36:PRO:HD2   | 1:F:71:MET:HB3   | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:29:THR:HG22  | 1:G:88:TYR:HD2   | 1.84                     | 0.43              |
| 1:J:135:TYR:OH   | 1:J:145:VAL:HG21 | 2.19                     | 0.43              |
| 1:E:303:ILE:HD12 | 1:E:303:ILE:N    | 2.34                     | 0.42              |
| 1:F:294:LEU:HB3  | 1:F:298:ALA:HB2  | 2.01                     | 0.42              |
| 1:I:244:ALA:HB1  | 1:J:307:PRO:HB3  | 2.01                     | 0.42              |
| 1:E:103:ASP:HA   | 1:E:108:GLU:HA   | 2.01                     | 0.42              |
| 1:H:301:TYR:O    | 1:H:304:LEU:O    | 2.37                     | 0.42              |
| 1:I:215:LYS:HE3  | 1:I:216:HIS:CE1  | 2.54                     | 0.42              |
| 1:I:370:LEU:HG   | 1:J:268:LYS:HD3  | 2.01                     | 0.42              |
| 1:B:36:PRO:HD2   | 1:B:71:MET:HB3   | 2.00                     | 0.42              |
| 1:I:29:THR:HG22  | 1:I:88:TYR:HD2   | 1.83                     | 0.42              |
| 1:I:270:ILE:HA   | 1:I:270:ILE:HD13 | 1.80                     | 0.42              |
| 1:A:319:HIS:O    | 1:A:323:VAL:HG12 | 2.19                     | 0.42              |
| 1:C:120:THR:CG2  | 1:C:122:GLU:HG2  | 2.49                     | 0.42              |
| 1:J:230:GLN:O    | 1:J:233:THR:HG22 | 2.19                     | 0.42              |
| 1:J:303:ILE:H    | 1:J:303:ILE:HD12 | 1.84                     | 0.42              |
| 1:A:3:LEU:HD13   | 1:I:367:VAL:HG12 | 2.01                     | 0.42              |
| 1:A:25:ILE:HA    | 1:J:73:ARG:O     | 2.19                     | 0.42              |
| 1:A:335:GLY:HA2  | 1:A:336:GLU:HA   | 1.87                     | 0.42              |
| 1:C:294:LEU:HB3  | 1:C:298:ALA:HB2  | 2.02                     | 0.42              |
| 1:D:184:ARG:NH1  | 2:K:28:C:OP2     | 2.52                     | 0.42              |
| 1:D:187:ASN:O    | 1:D:191:LYS:HB3  | 2.19                     | 0.42              |
| 1:D:258:LEU:HD12 | 1:D:258:LEU:HA   | 1.93                     | 0.42              |
| 1:G:187:ASN:O    | 1:G:191:LYS:HB3  | 2.19                     | 0.42              |
| 1:G:323:VAL:HG23 | 1:G:350:ALA:HB2  | 2.01                     | 0.42              |
| 1:A:209:PHE:HA   | 1:A:212:VAL:HG12 | 2.00                     | 0.42              |
| 1:B:240:GLU:OE2  | 1:C:27:ARG:HD3   | 2.18                     | 0.42              |
| 1:D:257:MET:HE1  | 1:D:325:LEU:HD23 | 2.01                     | 0.42              |
| 1:F:73:ARG:O     | 1:G:25:ILE:HA    | 2.20                     | 0.42              |
| 1:I:361:GLY:HA3  | 1:J:274:HIS:CD2  | 2.51                     | 0.42              |
| 1:J:34:ASP:OD2   | 1:J:117:ALA:N    | 2.46                     | 0.42              |
| 2:K:6:C:H2'      | 2:K:7:C:O4'      | 2.20                     | 0.42              |
| 1:A:234:ARG:NH2  | 1:B:86:ALA:HB2   | 2.35                     | 0.42              |
| 1:C:6:VAL:O      | 1:C:6:VAL:HG22   | 2.20                     | 0.42              |
| 1:D:262:VAL:HG13 | 1:E:7:LYS:HA     | 2.02                     | 0.42              |
| 1:E:335:GLY:HA2  | 1:E:337:TYR:N    | 2.35                     | 0.42              |
| 1:F:153:SER:HA   | 1:F:154:PRO:HD2  | 1.80                     | 0.42              |
| 1:F:364:ASN:HB3  | 1:G:273:GLY:O    | 2.19                     | 0.42              |
| 1:I:255:GLN:HB2  | 1:I:259:ARG:NH1  | 2.34                     | 0.42              |
| 1:I:283:GLN:O    | 1:I:286:GLU:HB2  | 2.19                     | 0.42              |
| 2:K:19:C:H2'     | 2:K:20:C:O4'     | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:29:THR:HG22  | 1:A:88:TYR:HD2   | 1.85                     | 0.42              |
| 1:A:255:GLN:HB2  | 1:A:259:ARG:NH1  | 2.35                     | 0.42              |
| 1:B:209:PHE:HA   | 1:B:212:VAL:HG12 | 2.01                     | 0.42              |
| 1:C:159:ILE:O    | 1:C:162:CYS:HB2  | 2.20                     | 0.42              |
| 1:E:64:LEU:HD12  | 1:E:119:LEU:HD13 | 2.00                     | 0.42              |
| 1:G:36:PRO:HD2   | 1:G:71:MET:HB3   | 2.00                     | 0.42              |
| 1:H:270:ILE:HD13 | 1:H:270:ILE:HA   | 1.78                     | 0.42              |
| 1:J:209:PHE:HA   | 1:J:212:VAL:HG12 | 2.01                     | 0.42              |
| 1:B:42:LYS:HD2   | 1:C:28:SER:HB3   | 2.00                     | 0.42              |
| 1:D:36:PRO:HD2   | 1:D:71:MET:HB3   | 2.01                     | 0.42              |
| 1:D:234:ARG:NH2  | 1:E:86:ALA:HB2   | 2.34                     | 0.42              |
| 1:C:303:ILE:HD12 | 1:C:303:ILE:N    | 2.33                     | 0.42              |
| 1:D:159:ILE:O    | 1:D:162:CYS:HB2  | 2.19                     | 0.42              |
| 1:D:323:VAL:HG23 | 1:D:350:ALA:HB2  | 2.02                     | 0.42              |
| 1:E:333:ILE:H    | 1:E:333:ILE:HG13 | 1.69                     | 0.42              |
| 1:G:67:MET:HE2   | 1:G:67:MET:HA    | 2.01                     | 0.42              |
| 1:G:244:ALA:HB1  | 1:H:307:PRO:HB3  | 2.01                     | 0.42              |
| 1:H:29:THR:HG22  | 1:H:88:TYR:HD2   | 1.84                     | 0.42              |
| 1:I:301:TYR:O    | 1:I:304:LEU:O    | 2.38                     | 0.42              |
| 1:J:78:ASP:O     | 1:J:82:ILE:HG23  | 2.19                     | 0.42              |
| 1:B:135:TYR:OH   | 1:B:145:VAL:HG21 | 2.20                     | 0.41              |
| 1:C:29:THR:HG22  | 1:C:88:TYR:HD2   | 1.84                     | 0.41              |
| 1:C:78:ASP:O     | 1:C:82:ILE:CG2   | 2.68                     | 0.41              |
| 1:C:153:SER:HA   | 1:C:154:PRO:HD2  | 1.81                     | 0.41              |
| 1:C:323:VAL:HG23 | 1:C:350:ALA:HB2  | 2.00                     | 0.41              |
| 1:H:153:SER:HA   | 1:H:154:PRO:HD2  | 1.80                     | 0.41              |
| 1:J:153:SER:HA   | 1:J:154:PRO:HD2  | 1.83                     | 0.41              |
| 1:J:294:LEU:HB3  | 1:J:298:ALA:HB2  | 2.02                     | 0.41              |
| 1:D:234:ARG:NH2  | 1:E:221:ASP:OD1  | 2.52                     | 0.41              |
| 1:E:107:LYS:H    | 1:E:107:LYS:HG3  | 1.56                     | 0.41              |
| 1:G:257:MET:HE1  | 1:G:325:LEU:HD23 | 2.02                     | 0.41              |
| 1:H:294:LEU:HB3  | 1:H:298:ALA:HB2  | 2.03                     | 0.41              |
| 1:C:103:ASP:HA   | 1:C:108:GLU:HA   | 2.02                     | 0.41              |
| 1:H:215:LYS:HE3  | 1:H:216:HIS:CE1  | 2.54                     | 0.41              |
| 1:I:294:LEU:HB3  | 1:I:298:ALA:HB2  | 2.03                     | 0.41              |
| 1:J:120:THR:CG2  | 1:J:122:GLU:HG2  | 2.50                     | 0.41              |
| 1:C:67:MET:HE1   | 1:C:223:PHE:CD1  | 2.55                     | 0.41              |
| 1:C:231:SER:HB2  | 1:D:18:LEU:HD22  | 2.03                     | 0.41              |
| 1:F:166:LEU:HD21 | 1:F:246:LEU:HD22 | 2.02                     | 0.41              |
| 1:J:159:ILE:O    | 1:J:162:CYS:HB2  | 2.19                     | 0.41              |
| 1:B:6:VAL:O      | 1:B:6:VAL:HG22   | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:323:VAL:HG23 | 1:B:350:ALA:HB2  | 2.03                     | 0.41              |
| 1:G:103:ASP:HA   | 1:G:108:GLU:HA   | 2.02                     | 0.41              |
| 1:J:29:THR:HG22  | 1:J:88:TYR:HD2   | 1.85                     | 0.41              |
| 1:J:184:ARG:NH2  | 2:K:69:C:OP1     | 2.50                     | 0.41              |
| 1:C:335:GLY:HA2  | 1:C:337:TYR:N    | 2.35                     | 0.41              |
| 1:E:319:HIS:O    | 1:E:323:VAL:HG12 | 2.19                     | 0.41              |
| 1:I:303:ILE:HD12 | 1:I:303:ILE:N    | 2.35                     | 0.41              |
| 2:K:26:C:H2'     | 2:K:27:C:O4'     | 2.21                     | 0.41              |
| 1:B:301:TYR:O    | 1:B:304:LEU:O    | 2.39                     | 0.41              |
| 1:B:319:HIS:O    | 1:B:323:VAL:HG12 | 2.20                     | 0.41              |
| 1:D:67:MET:HE1   | 1:D:223:PHE:CD1  | 2.55                     | 0.41              |
| 1:I:88:TYR:HD1   | 1:I:88:TYR:H     | 1.69                     | 0.41              |
| 1:A:307:PRO:HB3  | 1:J:244:ALA:HB1  | 2.01                     | 0.41              |
| 1:E:125:ILE:HG13 | 1:E:126:ASN:N    | 2.35                     | 0.41              |
| 1:F:283:GLN:O    | 1:F:286:GLU:HB2  | 2.21                     | 0.41              |
| 1:I:29:THR:HG22  | 1:I:88:TYR:CD2   | 2.56                     | 0.41              |
| 1:A:23:TYR:CD1   | 1:J:82:ILE:HG22  | 2.56                     | 0.41              |
| 1:C:209:PHE:HA   | 1:C:212:VAL:HG12 | 2.02                     | 0.41              |
| 1:D:6:VAL:O      | 1:D:6:VAL:HG22   | 2.20                     | 0.41              |
| 1:E:270:ILE:HA   | 1:E:270:ILE:HD13 | 1.77                     | 0.41              |
| 1:E:283:GLN:O    | 1:E:286:GLU:HB2  | 2.21                     | 0.41              |
| 1:E:323:VAL:HG23 | 1:E:350:ALA:HB2  | 2.03                     | 0.41              |
| 1:F:29:THR:HG22  | 1:F:88:TYR:CD2   | 2.56                     | 0.41              |
| 1:F:45:ASN:HB2   | 1:F:69:TYR:CE1   | 2.56                     | 0.41              |
| 1:F:335:GLY:HA2  | 1:F:336:GLU:HA   | 1.88                     | 0.41              |
| 1:G:209:PHE:HA   | 1:G:212:VAL:HG12 | 2.02                     | 0.41              |
| 1:H:29:THR:HG22  | 1:H:88:TYR:CD2   | 2.56                     | 0.41              |
| 2:K:33:C:H2'     | 2:K:34:C:O4'     | 2.20                     | 0.41              |
| 1:A:103:ASP:HA   | 1:A:108:GLU:HA   | 2.03                     | 0.41              |
| 1:A:303:ILE:HD12 | 1:A:303:ILE:N    | 2.36                     | 0.41              |
| 1:B:283:GLN:O    | 1:B:286:GLU:HB2  | 2.21                     | 0.41              |
| 1:E:209:PHE:HA   | 1:E:212:VAL:HG12 | 2.02                     | 0.41              |
| 1:F:303:ILE:HD12 | 1:F:303:ILE:N    | 2.35                     | 0.41              |
| 1:I:42:LYS:HD2   | 1:J:28:SER:CB    | 2.50                     | 0.41              |
| 1:A:301:TYR:O    | 1:A:304:LEU:O    | 2.39                     | 0.40              |
| 1:B:294:LEU:HB3  | 1:B:298:ALA:HB2  | 2.02                     | 0.40              |
| 1:E:29:THR:HG22  | 1:E:88:TYR:HD2   | 1.84                     | 0.40              |
| 1:H:125:ILE:HG13 | 1:H:126:ASN:N    | 2.36                     | 0.40              |
| 2:K:37:C:H2'     | 2:K:38:C:O4'     | 2.21                     | 0.40              |
| 1:B:335:GLY:HA2  | 1:B:337:TYR:N    | 2.37                     | 0.40              |
| 1:C:319:HIS:O    | 1:C:323:VAL:HG12 | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:29:THR:HG22  | 1:D:88:TYR:HD2   | 1.85                     | 0.40              |
| 1:D:231:SER:HA   | 1:E:307:PRO:HG2  | 2.03                     | 0.40              |
| 1:I:135:TYR:OH   | 1:I:145:VAL:HG21 | 2.20                     | 0.40              |
| 1:B:29:THR:HG22  | 1:B:88:TYR:HD2   | 1.86                     | 0.40              |
| 1:B:41:GLN:NE2   | 1:B:73:ARG:HA    | 2.37                     | 0.40              |
| 1:B:230:GLN:O    | 1:B:233:THR:HG22 | 2.21                     | 0.40              |
| 1:D:294:LEU:HB3  | 1:D:298:ALA:HB2  | 2.03                     | 0.40              |
| 1:I:257:MET:HE1  | 1:I:325:LEU:HD23 | 2.02                     | 0.40              |
| 1:J:283:GLN:O    | 1:J:286:GLU:HB2  | 2.22                     | 0.40              |
| 1:B:42:LYS:HD2   | 1:C:28:SER:CB    | 2.51                     | 0.40              |
| 1:B:107:LYS:H    | 1:B:107:LYS:HG3  | 1.51                     | 0.40              |
| 1:C:125:ILE:HG13 | 1:C:126:ASN:N    | 2.37                     | 0.40              |
| 1:F:209:PHE:HA   | 1:F:212:VAL:HG12 | 2.03                     | 0.40              |
| 1:G:301:TYR:O    | 1:G:304:LEU:O    | 2.40                     | 0.40              |
| 1:J:103:ASP:HA   | 1:J:108:GLU:HA   | 2.02                     | 0.40              |
| 1:C:270:ILE:HD13 | 1:C:270:ILE:HA   | 1.78                     | 0.40              |
| 1:D:103:ASP:HA   | 1:D:108:GLU:HA   | 2.02                     | 0.40              |
| 1:D:125:ILE:HG13 | 1:D:126:ASN:N    | 2.36                     | 0.40              |
| 1:E:6:VAL:O      | 1:E:6:VAL:HG22   | 2.22                     | 0.40              |
| 1:E:170:LYS:HB3  | 1:E:178:GLY:HA3  | 2.03                     | 0.40              |
| 1:F:168:ILE:HG22 | 1:F:250:ALA:CB   | 2.52                     | 0.40              |
| 1:H:41:GLN:NE2   | 1:H:73:ARG:HA    | 2.37                     | 0.40              |
| 1:H:283:GLN:O    | 1:H:286:GLU:HB2  | 2.21                     | 0.40              |

All (18) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1         | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 1:E:96:ASP:OD2 | 1:I:374:GLU:CA[4_555]  | 1.20                     | 1.00              |
| 1:E:359:GLU:CG | 1:J:77:GLU:OE1[4_455]  | 1.36                     | 0.84              |
| 1:E:96:ASP:OD2 | 1:I:374:GLU:CB[4_555]  | 1.42                     | 0.78              |
| 1:E:359:GLU:CD | 1:J:77:GLU:OE1[4_455]  | 1.46                     | 0.74              |
| 1:E:96:ASP:CG  | 1:I:374:GLU:CG[4_555]  | 1.49                     | 0.71              |
| 1:F:91:LYS:CE  | 1:J:374:GLU:O[4_555]   | 1.53                     | 0.67              |
| 1:E:96:ASP:CB  | 1:I:374:GLU:CG[4_555]  | 1.65                     | 0.55              |
| 1:E:96:ASP:OD2 | 1:I:374:GLU:CG[4_555]  | 1.77                     | 0.43              |
| 1:F:91:LYS:NZ  | 1:J:375:LEU:C[4_555]   | 1.84                     | 0.36              |
| 1:D:359:GLU:O  | 1:I:77:GLU:OE2[4_455]  | 1.86                     | 0.34              |
| 1:E:136:LYS:NZ | 1:I:148:GLU:OE1[1_565] | 1.91                     | 0.29              |
| 1:F:91:LYS:NZ  | 1:J:374:GLU:O[4_555]   | 2.05                     | 0.15              |

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| Atom-1          | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------------|--------------------------|-------------------|
| 1:F:91:LYS:NZ   | 1:J:375:LEU:CA[4_555] | 2.06                     | 0.14              |
| 1:E:359:GLU:CD  | 1:J:77:GLU:CD[4_455]  | 2.13                     | 0.07              |
| 1:E:359:GLU:OE2 | 1:J:77:GLU:OE1[4_455] | 2.14                     | 0.06              |
| 1:E:359:GLU:OE1 | 1:J:77:GLU:CD[4_455]  | 2.18                     | 0.02              |
| 1:E:96:ASP:CG   | 1:I:374:GLU:CB[4_555] | 2.19                     | 0.01              |
| 1:E:359:GLU:OE1 | 1:J:77:GLU:OE1[4_455] | 2.19                     | 0.01              |

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed         | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|------------------|------------|---------|----------|-------------|-----|
| 1   | A     | 373/375 (100%)   | 370 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 1   | B     | 373/375 (100%)   | 370 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 1   | C     | 373/375 (100%)   | 369 (99%)  | 4 (1%)  | 0        | 100         | 100 |
| 1   | D     | 373/375 (100%)   | 368 (99%)  | 5 (1%)  | 0        | 100         | 100 |
| 1   | E     | 373/375 (100%)   | 369 (99%)  | 4 (1%)  | 0        | 100         | 100 |
| 1   | F     | 373/375 (100%)   | 370 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 1   | G     | 373/375 (100%)   | 368 (99%)  | 5 (1%)  | 0        | 100         | 100 |
| 1   | H     | 373/375 (100%)   | 369 (99%)  | 4 (1%)  | 0        | 100         | 100 |
| 1   | I     | 373/375 (100%)   | 370 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 1   | J     | 373/375 (100%)   | 369 (99%)  | 4 (1%)  | 0        | 100         | 100 |
| All | All   | 3730/3750 (100%) | 3692 (99%) | 38 (1%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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     | 313/313 (100%)   | 267 (85%)  | 46 (15%)  | 3           | 17 |
| 1   | B     | 313/313 (100%)   | 268 (86%)  | 45 (14%)  | 3           | 18 |
| 1   | C     | 313/313 (100%)   | 268 (86%)  | 45 (14%)  | 3           | 18 |
| 1   | D     | 313/313 (100%)   | 269 (86%)  | 44 (14%)  | 3           | 19 |
| 1   | E     | 313/313 (100%)   | 268 (86%)  | 45 (14%)  | 3           | 18 |
| 1   | F     | 313/313 (100%)   | 268 (86%)  | 45 (14%)  | 3           | 18 |
| 1   | G     | 313/313 (100%)   | 268 (86%)  | 45 (14%)  | 3           | 18 |
| 1   | H     | 313/313 (100%)   | 269 (86%)  | 44 (14%)  | 3           | 19 |
| 1   | I     | 313/313 (100%)   | 268 (86%)  | 45 (14%)  | 3           | 18 |
| 1   | J     | 313/313 (100%)   | 267 (85%)  | 46 (15%)  | 3           | 17 |
| All | All   | 3130/3130 (100%) | 2680 (86%) | 450 (14%) | 3           | 18 |

All (450) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 3   | LEU  |
| 1   | A     | 5   | LYS  |
| 1   | A     | 6   | VAL  |
| 1   | A     | 8   | LEU  |
| 1   | A     | 11  | THR  |
| 1   | A     | 12  | LEU  |
| 1   | A     | 22  | LYS  |
| 1   | A     | 24  | THR  |
| 1   | A     | 33  | ILE  |
| 1   | A     | 47  | LEU  |
| 1   | A     | 64  | LEU  |
| 1   | A     | 82  | ILE  |
| 1   | A     | 83  | LEU  |
| 1   | A     | 88  | TYR  |
| 1   | A     | 90  | VAL  |
| 1   | A     | 103 | ASP  |
| 1   | A     | 104 | ILE  |
| 1   | A     | 107 | LYS  |
| 1   | A     | 120 | THR  |
| 1   | A     | 123 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 145 | VAL  |
| 1   | A     | 163 | ILE  |
| 1   | A     | 168 | ILE  |
| 1   | A     | 170 | LYS  |
| 1   | A     | 196 | ARG  |
| 1   | A     | 220 | ILE  |
| 1   | A     | 255 | GLN  |
| 1   | A     | 270 | ILE  |
| 1   | A     | 272 | LEU  |
| 1   | A     | 284 | VAL  |
| 1   | A     | 287 | VAL  |
| 1   | A     | 293 | LYS  |
| 1   | A     | 304 | LEU  |
| 1   | A     | 313 | SER  |
| 1   | A     | 323 | VAL  |
| 1   | A     | 325 | LEU  |
| 1   | A     | 331 | LEU  |
| 1   | A     | 333 | ILE  |
| 1   | A     | 359 | GLU  |
| 1   | A     | 360 | ASN  |
| 1   | A     | 367 | VAL  |
| 1   | A     | 368 | LEU  |
| 1   | A     | 370 | LEU  |
| 1   | A     | 371 | THR  |
| 1   | A     | 373 | GLU  |
| 1   | A     | 375 | LEU  |
| 1   | B     | 3   | LEU  |
| 1   | B     | 5   | LYS  |
| 1   | B     | 6   | VAL  |
| 1   | B     | 8   | LEU  |
| 1   | B     | 11  | THR  |
| 1   | B     | 12  | LEU  |
| 1   | B     | 22  | LYS  |
| 1   | B     | 24  | THR  |
| 1   | B     | 33  | ILE  |
| 1   | B     | 47  | LEU  |
| 1   | B     | 64  | LEU  |
| 1   | B     | 82  | ILE  |
| 1   | B     | 83  | LEU  |
| 1   | B     | 88  | TYR  |
| 1   | B     | 90  | VAL  |
| 1   | B     | 103 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 104 | ILE  |
| 1   | B     | 107 | LYS  |
| 1   | B     | 120 | THR  |
| 1   | B     | 123 | ILE  |
| 1   | B     | 145 | VAL  |
| 1   | B     | 163 | ILE  |
| 1   | B     | 168 | ILE  |
| 1   | B     | 170 | LYS  |
| 1   | B     | 220 | ILE  |
| 1   | B     | 255 | GLN  |
| 1   | B     | 270 | ILE  |
| 1   | B     | 272 | LEU  |
| 1   | B     | 284 | VAL  |
| 1   | B     | 287 | VAL  |
| 1   | B     | 293 | LYS  |
| 1   | B     | 304 | LEU  |
| 1   | B     | 313 | SER  |
| 1   | B     | 323 | VAL  |
| 1   | B     | 325 | LEU  |
| 1   | B     | 331 | LEU  |
| 1   | B     | 333 | ILE  |
| 1   | B     | 359 | GLU  |
| 1   | B     | 360 | ASN  |
| 1   | B     | 367 | VAL  |
| 1   | B     | 368 | LEU  |
| 1   | B     | 370 | LEU  |
| 1   | B     | 371 | THR  |
| 1   | B     | 373 | GLU  |
| 1   | B     | 375 | LEU  |
| 1   | C     | 3   | LEU  |
| 1   | C     | 5   | LYS  |
| 1   | C     | 6   | VAL  |
| 1   | C     | 8   | LEU  |
| 1   | C     | 11  | THR  |
| 1   | C     | 12  | LEU  |
| 1   | C     | 22  | LYS  |
| 1   | C     | 24  | THR  |
| 1   | C     | 33  | ILE  |
| 1   | C     | 47  | LEU  |
| 1   | C     | 64  | LEU  |
| 1   | C     | 82  | ILE  |
| 1   | C     | 83  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 88  | TYR  |
| 1   | C     | 90  | VAL  |
| 1   | C     | 103 | ASP  |
| 1   | C     | 104 | ILE  |
| 1   | C     | 107 | LYS  |
| 1   | C     | 120 | THR  |
| 1   | C     | 123 | ILE  |
| 1   | C     | 145 | VAL  |
| 1   | C     | 163 | ILE  |
| 1   | C     | 168 | ILE  |
| 1   | C     | 170 | LYS  |
| 1   | C     | 220 | ILE  |
| 1   | C     | 255 | GLN  |
| 1   | C     | 270 | ILE  |
| 1   | C     | 272 | LEU  |
| 1   | C     | 284 | VAL  |
| 1   | C     | 287 | VAL  |
| 1   | C     | 293 | LYS  |
| 1   | C     | 304 | LEU  |
| 1   | C     | 313 | SER  |
| 1   | C     | 323 | VAL  |
| 1   | C     | 325 | LEU  |
| 1   | C     | 331 | LEU  |
| 1   | C     | 333 | ILE  |
| 1   | C     | 359 | GLU  |
| 1   | C     | 360 | ASN  |
| 1   | C     | 367 | VAL  |
| 1   | C     | 368 | LEU  |
| 1   | C     | 370 | LEU  |
| 1   | C     | 371 | THR  |
| 1   | C     | 373 | GLU  |
| 1   | C     | 375 | LEU  |
| 1   | D     | 3   | LEU  |
| 1   | D     | 5   | LYS  |
| 1   | D     | 6   | VAL  |
| 1   | D     | 8   | LEU  |
| 1   | D     | 11  | THR  |
| 1   | D     | 12  | LEU  |
| 1   | D     | 22  | LYS  |
| 1   | D     | 33  | ILE  |
| 1   | D     | 47  | LEU  |
| 1   | D     | 64  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 82  | ILE  |
| 1   | D     | 83  | LEU  |
| 1   | D     | 88  | TYR  |
| 1   | D     | 90  | VAL  |
| 1   | D     | 103 | ASP  |
| 1   | D     | 104 | ILE  |
| 1   | D     | 107 | LYS  |
| 1   | D     | 120 | THR  |
| 1   | D     | 123 | ILE  |
| 1   | D     | 145 | VAL  |
| 1   | D     | 163 | ILE  |
| 1   | D     | 168 | ILE  |
| 1   | D     | 170 | LYS  |
| 1   | D     | 220 | ILE  |
| 1   | D     | 255 | GLN  |
| 1   | D     | 270 | ILE  |
| 1   | D     | 272 | LEU  |
| 1   | D     | 284 | VAL  |
| 1   | D     | 287 | VAL  |
| 1   | D     | 293 | LYS  |
| 1   | D     | 304 | LEU  |
| 1   | D     | 313 | SER  |
| 1   | D     | 323 | VAL  |
| 1   | D     | 325 | LEU  |
| 1   | D     | 331 | LEU  |
| 1   | D     | 333 | ILE  |
| 1   | D     | 359 | GLU  |
| 1   | D     | 360 | ASN  |
| 1   | D     | 367 | VAL  |
| 1   | D     | 368 | LEU  |
| 1   | D     | 370 | LEU  |
| 1   | D     | 371 | THR  |
| 1   | D     | 373 | GLU  |
| 1   | D     | 375 | LEU  |
| 1   | E     | 3   | LEU  |
| 1   | E     | 5   | LYS  |
| 1   | E     | 6   | VAL  |
| 1   | E     | 8   | LEU  |
| 1   | E     | 11  | THR  |
| 1   | E     | 12  | LEU  |
| 1   | E     | 22  | LYS  |
| 1   | E     | 24  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 33  | ILE  |
| 1   | E     | 47  | LEU  |
| 1   | E     | 64  | LEU  |
| 1   | E     | 82  | ILE  |
| 1   | E     | 83  | LEU  |
| 1   | E     | 88  | TYR  |
| 1   | E     | 90  | VAL  |
| 1   | E     | 103 | ASP  |
| 1   | E     | 104 | ILE  |
| 1   | E     | 107 | LYS  |
| 1   | E     | 120 | THR  |
| 1   | E     | 123 | ILE  |
| 1   | E     | 145 | VAL  |
| 1   | E     | 163 | ILE  |
| 1   | E     | 168 | ILE  |
| 1   | E     | 170 | LYS  |
| 1   | E     | 220 | ILE  |
| 1   | E     | 255 | GLN  |
| 1   | E     | 270 | ILE  |
| 1   | E     | 272 | LEU  |
| 1   | E     | 284 | VAL  |
| 1   | E     | 287 | VAL  |
| 1   | E     | 293 | LYS  |
| 1   | E     | 304 | LEU  |
| 1   | E     | 313 | SER  |
| 1   | E     | 323 | VAL  |
| 1   | E     | 325 | LEU  |
| 1   | E     | 331 | LEU  |
| 1   | E     | 333 | ILE  |
| 1   | E     | 359 | GLU  |
| 1   | E     | 360 | ASN  |
| 1   | E     | 367 | VAL  |
| 1   | E     | 368 | LEU  |
| 1   | E     | 370 | LEU  |
| 1   | E     | 371 | THR  |
| 1   | E     | 373 | GLU  |
| 1   | E     | 375 | LEU  |
| 1   | F     | 3   | LEU  |
| 1   | F     | 5   | LYS  |
| 1   | F     | 6   | VAL  |
| 1   | F     | 8   | LEU  |
| 1   | F     | 11  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 12  | LEU  |
| 1   | F     | 22  | LYS  |
| 1   | F     | 24  | THR  |
| 1   | F     | 33  | ILE  |
| 1   | F     | 47  | LEU  |
| 1   | F     | 64  | LEU  |
| 1   | F     | 82  | ILE  |
| 1   | F     | 83  | LEU  |
| 1   | F     | 88  | TYR  |
| 1   | F     | 90  | VAL  |
| 1   | F     | 103 | ASP  |
| 1   | F     | 104 | ILE  |
| 1   | F     | 107 | LYS  |
| 1   | F     | 120 | THR  |
| 1   | F     | 123 | ILE  |
| 1   | F     | 145 | VAL  |
| 1   | F     | 163 | ILE  |
| 1   | F     | 168 | ILE  |
| 1   | F     | 170 | LYS  |
| 1   | F     | 220 | ILE  |
| 1   | F     | 255 | GLN  |
| 1   | F     | 270 | ILE  |
| 1   | F     | 272 | LEU  |
| 1   | F     | 284 | VAL  |
| 1   | F     | 287 | VAL  |
| 1   | F     | 293 | LYS  |
| 1   | F     | 304 | LEU  |
| 1   | F     | 313 | SER  |
| 1   | F     | 323 | VAL  |
| 1   | F     | 325 | LEU  |
| 1   | F     | 331 | LEU  |
| 1   | F     | 333 | ILE  |
| 1   | F     | 359 | GLU  |
| 1   | F     | 360 | ASN  |
| 1   | F     | 367 | VAL  |
| 1   | F     | 368 | LEU  |
| 1   | F     | 370 | LEU  |
| 1   | F     | 371 | THR  |
| 1   | F     | 373 | GLU  |
| 1   | F     | 375 | LEU  |
| 1   | G     | 3   | LEU  |
| 1   | G     | 5   | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 6   | VAL  |
| 1   | G     | 8   | LEU  |
| 1   | G     | 11  | THR  |
| 1   | G     | 12  | LEU  |
| 1   | G     | 22  | LYS  |
| 1   | G     | 24  | THR  |
| 1   | G     | 33  | ILE  |
| 1   | G     | 47  | LEU  |
| 1   | G     | 64  | LEU  |
| 1   | G     | 82  | ILE  |
| 1   | G     | 83  | LEU  |
| 1   | G     | 88  | TYR  |
| 1   | G     | 90  | VAL  |
| 1   | G     | 103 | ASP  |
| 1   | G     | 104 | ILE  |
| 1   | G     | 107 | LYS  |
| 1   | G     | 120 | THR  |
| 1   | G     | 123 | ILE  |
| 1   | G     | 145 | VAL  |
| 1   | G     | 163 | ILE  |
| 1   | G     | 168 | ILE  |
| 1   | G     | 170 | LYS  |
| 1   | G     | 220 | ILE  |
| 1   | G     | 255 | GLN  |
| 1   | G     | 270 | ILE  |
| 1   | G     | 272 | LEU  |
| 1   | G     | 284 | VAL  |
| 1   | G     | 287 | VAL  |
| 1   | G     | 293 | LYS  |
| 1   | G     | 304 | LEU  |
| 1   | G     | 313 | SER  |
| 1   | G     | 323 | VAL  |
| 1   | G     | 325 | LEU  |
| 1   | G     | 331 | LEU  |
| 1   | G     | 333 | ILE  |
| 1   | G     | 359 | GLU  |
| 1   | G     | 360 | ASN  |
| 1   | G     | 367 | VAL  |
| 1   | G     | 368 | LEU  |
| 1   | G     | 370 | LEU  |
| 1   | G     | 371 | THR  |
| 1   | G     | 373 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 375 | LEU  |
| 1   | H     | 3   | LEU  |
| 1   | H     | 5   | LYS  |
| 1   | H     | 6   | VAL  |
| 1   | H     | 8   | LEU  |
| 1   | H     | 11  | THR  |
| 1   | H     | 12  | LEU  |
| 1   | H     | 22  | LYS  |
| 1   | H     | 33  | ILE  |
| 1   | H     | 47  | LEU  |
| 1   | H     | 64  | LEU  |
| 1   | H     | 82  | ILE  |
| 1   | H     | 83  | LEU  |
| 1   | H     | 88  | TYR  |
| 1   | H     | 90  | VAL  |
| 1   | H     | 103 | ASP  |
| 1   | H     | 104 | ILE  |
| 1   | H     | 107 | LYS  |
| 1   | H     | 120 | THR  |
| 1   | H     | 123 | ILE  |
| 1   | H     | 145 | VAL  |
| 1   | H     | 163 | ILE  |
| 1   | H     | 168 | ILE  |
| 1   | H     | 170 | LYS  |
| 1   | H     | 220 | ILE  |
| 1   | H     | 255 | GLN  |
| 1   | H     | 270 | ILE  |
| 1   | H     | 272 | LEU  |
| 1   | H     | 284 | VAL  |
| 1   | H     | 287 | VAL  |
| 1   | H     | 293 | LYS  |
| 1   | H     | 304 | LEU  |
| 1   | H     | 313 | SER  |
| 1   | H     | 323 | VAL  |
| 1   | H     | 325 | LEU  |
| 1   | H     | 331 | LEU  |
| 1   | H     | 333 | ILE  |
| 1   | H     | 359 | GLU  |
| 1   | H     | 360 | ASN  |
| 1   | H     | 367 | VAL  |
| 1   | H     | 368 | LEU  |
| 1   | H     | 370 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 371 | THR  |
| 1   | H     | 373 | GLU  |
| 1   | H     | 375 | LEU  |
| 1   | I     | 3   | LEU  |
| 1   | I     | 5   | LYS  |
| 1   | I     | 6   | VAL  |
| 1   | I     | 8   | LEU  |
| 1   | I     | 11  | THR  |
| 1   | I     | 12  | LEU  |
| 1   | I     | 22  | LYS  |
| 1   | I     | 24  | THR  |
| 1   | I     | 33  | ILE  |
| 1   | I     | 47  | LEU  |
| 1   | I     | 64  | LEU  |
| 1   | I     | 82  | ILE  |
| 1   | I     | 83  | LEU  |
| 1   | I     | 88  | TYR  |
| 1   | I     | 90  | VAL  |
| 1   | I     | 103 | ASP  |
| 1   | I     | 104 | ILE  |
| 1   | I     | 107 | LYS  |
| 1   | I     | 120 | THR  |
| 1   | I     | 123 | ILE  |
| 1   | I     | 145 | VAL  |
| 1   | I     | 163 | ILE  |
| 1   | I     | 168 | ILE  |
| 1   | I     | 170 | LYS  |
| 1   | I     | 220 | ILE  |
| 1   | I     | 255 | GLN  |
| 1   | I     | 270 | ILE  |
| 1   | I     | 272 | LEU  |
| 1   | I     | 284 | VAL  |
| 1   | I     | 287 | VAL  |
| 1   | I     | 293 | LYS  |
| 1   | I     | 304 | LEU  |
| 1   | I     | 313 | SER  |
| 1   | I     | 323 | VAL  |
| 1   | I     | 325 | LEU  |
| 1   | I     | 331 | LEU  |
| 1   | I     | 333 | ILE  |
| 1   | I     | 359 | GLU  |
| 1   | I     | 360 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 367 | VAL  |
| 1   | I     | 368 | LEU  |
| 1   | I     | 370 | LEU  |
| 1   | I     | 371 | THR  |
| 1   | I     | 373 | GLU  |
| 1   | I     | 375 | LEU  |
| 1   | J     | 3   | LEU  |
| 1   | J     | 5   | LYS  |
| 1   | J     | 6   | VAL  |
| 1   | J     | 8   | LEU  |
| 1   | J     | 11  | THR  |
| 1   | J     | 12  | LEU  |
| 1   | J     | 22  | LYS  |
| 1   | J     | 24  | THR  |
| 1   | J     | 33  | ILE  |
| 1   | J     | 47  | LEU  |
| 1   | J     | 64  | LEU  |
| 1   | J     | 82  | ILE  |
| 1   | J     | 83  | LEU  |
| 1   | J     | 88  | TYR  |
| 1   | J     | 90  | VAL  |
| 1   | J     | 103 | ASP  |
| 1   | J     | 104 | ILE  |
| 1   | J     | 107 | LYS  |
| 1   | J     | 120 | THR  |
| 1   | J     | 123 | ILE  |
| 1   | J     | 145 | VAL  |
| 1   | J     | 163 | ILE  |
| 1   | J     | 168 | ILE  |
| 1   | J     | 170 | LYS  |
| 1   | J     | 220 | ILE  |
| 1   | J     | 255 | GLN  |
| 1   | J     | 270 | ILE  |
| 1   | J     | 272 | LEU  |
| 1   | J     | 284 | VAL  |
| 1   | J     | 287 | VAL  |
| 1   | J     | 293 | LYS  |
| 1   | J     | 304 | LEU  |
| 1   | J     | 313 | SER  |
| 1   | J     | 323 | VAL  |
| 1   | J     | 325 | LEU  |
| 1   | J     | 331 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 333 | ILE  |
| 1   | J     | 359 | GLU  |
| 1   | J     | 360 | ASN  |
| 1   | J     | 367 | VAL  |
| 1   | J     | 368 | LEU  |
| 1   | J     | 370 | LEU  |
| 1   | J     | 371 | THR  |
| 1   | J     | 373 | GLU  |
| 1   | J     | 374 | GLU  |
| 1   | J     | 375 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 26  | GLN  |
| 1   | A     | 41  | GLN  |
| 1   | A     | 43  | HIS  |
| 1   | A     | 151 | HIS  |
| 1   | A     | 187 | ASN  |
| 1   | A     | 283 | GLN  |
| 1   | A     | 292 | GLN  |
| 1   | B     | 26  | GLN  |
| 1   | B     | 43  | HIS  |
| 1   | B     | 151 | HIS  |
| 1   | B     | 187 | ASN  |
| 1   | B     | 283 | GLN  |
| 1   | B     | 292 | GLN  |
| 1   | C     | 26  | GLN  |
| 1   | C     | 41  | GLN  |
| 1   | C     | 43  | HIS  |
| 1   | C     | 151 | HIS  |
| 1   | C     | 187 | ASN  |
| 1   | C     | 278 | GLN  |
| 1   | C     | 283 | GLN  |
| 1   | C     | 292 | GLN  |
| 1   | C     | 305 | ASN  |
| 1   | C     | 364 | ASN  |
| 1   | D     | 26  | GLN  |
| 1   | D     | 41  | GLN  |
| 1   | D     | 43  | HIS  |
| 1   | D     | 151 | HIS  |
| 1   | D     | 187 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 283 | GLN  |
| 1   | D     | 364 | ASN  |
| 1   | E     | 151 | HIS  |
| 1   | E     | 187 | ASN  |
| 1   | E     | 225 | HIS  |
| 1   | E     | 278 | GLN  |
| 1   | E     | 305 | ASN  |
| 1   | E     | 364 | ASN  |
| 1   | F     | 26  | GLN  |
| 1   | F     | 43  | HIS  |
| 1   | F     | 151 | HIS  |
| 1   | F     | 187 | ASN  |
| 1   | F     | 283 | GLN  |
| 1   | G     | 89  | HIS  |
| 1   | G     | 151 | HIS  |
| 1   | G     | 187 | ASN  |
| 1   | G     | 292 | GLN  |
| 1   | G     | 305 | ASN  |
| 1   | H     | 41  | GLN  |
| 1   | H     | 43  | HIS  |
| 1   | H     | 89  | HIS  |
| 1   | H     | 151 | HIS  |
| 1   | H     | 187 | ASN  |
| 1   | H     | 225 | HIS  |
| 1   | H     | 283 | GLN  |
| 1   | H     | 305 | ASN  |
| 1   | H     | 364 | ASN  |
| 1   | I     | 26  | GLN  |
| 1   | I     | 41  | GLN  |
| 1   | I     | 43  | HIS  |
| 1   | I     | 151 | HIS  |
| 1   | I     | 187 | ASN  |
| 1   | I     | 278 | GLN  |
| 1   | I     | 283 | GLN  |
| 1   | I     | 305 | ASN  |
| 1   | J     | 26  | GLN  |
| 1   | J     | 151 | HIS  |
| 1   | J     | 187 | ASN  |
| 1   | J     | 283 | GLN  |
| 1   | J     | 292 | GLN  |
| 1   | J     | 305 | ASN  |
| 1   | J     | 364 | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 2   | K     | 69/70 (98%) | 19 (27%)          | 4 (5%)          |

All (19) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | K     | 8   | C    |
| 2   | K     | 11  | C    |
| 2   | K     | 12  | C    |
| 2   | K     | 15  | C    |
| 2   | K     | 17  | C    |
| 2   | K     | 22  | C    |
| 2   | K     | 23  | C    |
| 2   | K     | 29  | C    |
| 2   | K     | 36  | C    |
| 2   | K     | 40  | C    |
| 2   | K     | 43  | C    |
| 2   | K     | 45  | C    |
| 2   | K     | 46  | C    |
| 2   | K     | 47  | C    |
| 2   | K     | 50  | C    |
| 2   | K     | 56  | C    |
| 2   | K     | 57  | C    |
| 2   | K     | 64  | C    |
| 2   | K     | 70  | C    |

All (4) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | K     | 11  | C    |
| 2   | K     | 18  | C    |
| 2   | K     | 25  | C    |
| 2   | K     | 46  | C    |

## 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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     | 375/375 (100%)   | -0.58  | 0 <b>100</b> <b>100</b> | 63, 100, 171, 212     | 0     |
| 1   | B     | 375/375 (100%)   | -0.57  | 1 (0%) 90 75            | 68, 106, 183, 272     | 0     |
| 1   | C     | 375/375 (100%)   | -0.59  | 0 <b>100</b> <b>100</b> | 63, 98, 182, 269      | 0     |
| 1   | D     | 375/375 (100%)   | -0.54  | 1 (0%) 90 75            | 64, 94, 165, 260      | 0     |
| 1   | E     | 375/375 (100%)   | -0.50  | 0 <b>100</b> <b>100</b> | 46, 91, 182, 251      | 0     |
| 1   | F     | 375/375 (100%)   | -0.56  | 0 <b>100</b> <b>100</b> | 50, 86, 173, 231      | 0     |
| 1   | G     | 375/375 (100%)   | -0.62  | 1 (0%) 90 75            | 50, 90, 171, 273      | 0     |
| 1   | H     | 375/375 (100%)   | -0.58  | 1 (0%) 90 75            | 55, 89, 171, 291      | 0     |
| 1   | I     | 375/375 (100%)   | -0.56  | 1 (0%) 90 75            | 56, 90, 181, 334      | 0     |
| 1   | J     | 375/375 (100%)   | -0.47  | 0 <b>100</b> <b>100</b> | 57, 95, 182, 337      | 0     |
| 2   | K     | 70/70 (100%)     | -1.09  | 0 <b>100</b> <b>100</b> | 71, 85, 96, 107       | 0     |
| All | All   | 3820/3820 (100%) | -0.57  | 5 (0%) 92 85            | 46, 93, 178, 337      | 0     |

All (5) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 375 | LEU  | 3.6  |
| 1   | B     | 375 | LEU  | 3.0  |
| 1   | I     | 375 | LEU  | 2.8  |
| 1   | H     | 368 | LEU  | 2.4  |
| 1   | D     | 375 | LEU  | 2.1  |

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.