



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:54 PM GMT

PDB ID : 4DPG  
Title : Crystal Structure of Human LysRS: P38/AIMP2 Complex I  
Authors : Fang, P.; Wang, J.; Bennett, S.P.; Guo, M.  
Deposited on : 2012-02-13  
Resolution : 2.84 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

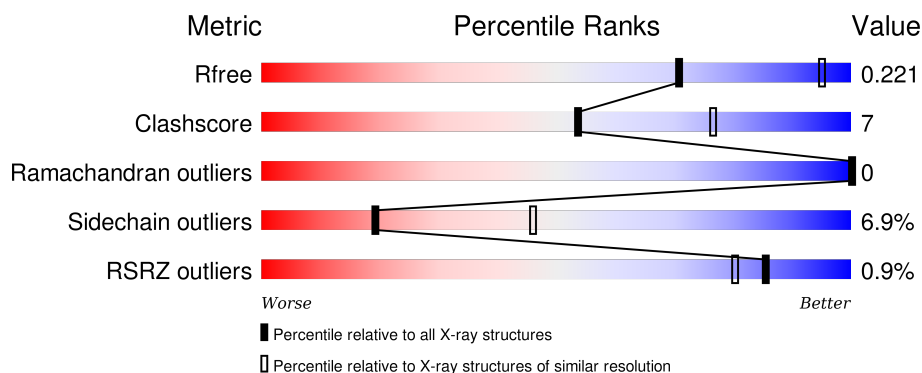
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.84 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.






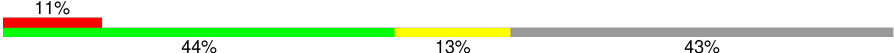
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 91344                       | 3170 (2.88-2.80)                                      |
| Clashscore            | 102246                      | 3658 (2.88-2.80)                                      |
| Ramachandran outliers | 100387                      | 3591 (2.88-2.80)                                      |
| Sidechain outliers    | 100360                      | 3594 (2.88-2.80)                                      |
| RSRZ outliers         | 91569                       | 3184 (2.88-2.80)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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     | 513    | <div> <div>77%</div> <div>18%</div> <div>..</div> </div>               |
| 1   | B     | 513    | <div> <div>83%</div> <div>14%</div> <div>..</div> </div>               |
| 1   | C     | 513    | <div> <div>%</div> <div>75%</div> <div>19%</div> <div>..</div> </div>  |
| 1   | D     | 513    | <div> <div>%</div> <div>80%</div> <div>16%</div> <div>...</div> </div> |
| 1   | E     | 513    | <div> <div>78%</div> <div>17%</div> <div>..</div> </div>               |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | F     | 513    |  |
| 1   | G     | 513    |  |
| 1   | H     | 513    |  |
| 2   | I     | 54     |  |
| 2   | J     | 54     |  |
| 2   | K     | 54     |  |
| 2   | L     | 54     |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 4   | APC  | A     | 602 | -         | -        | -       | X                |
| 4   | APC  | B     | 602 | -         | -        | -       | X                |
| 4   | APC  | C     | 602 | -         | -        | -       | X                |
| 4   | APC  | D     | 602 | -         | -        | -       | X                |
| 4   | APC  | E     | 602 | -         | -        | -       | X                |
| 4   | APC  | F     | 602 | -         | -        | -       | X                |
| 4   | APC  | G     | 602 | -         | -        | -       | X                |
| 4   | APC  | H     | 603 | -         | -        | -       | X                |

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 33740 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 Lysine-tRNA ligase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 501      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3932  | 2519 | 668 | 718 | 27 |         |         |       |
| 1   | B     | 506      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4055  | 2596 | 687 | 744 | 28 |         |         |       |
| 1   | C     | 501      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3989  | 2553 | 677 | 731 | 28 |         |         |       |
| 1   | D     | 505      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4031  | 2588 | 685 | 730 | 28 |         |         |       |
| 1   | E     | 500      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3969  | 2540 | 671 | 730 | 28 |         |         |       |
| 1   | F     | 505      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4023  | 2580 | 685 | 730 | 28 |         |         |       |
| 1   | G     | 501      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3921  | 2507 | 667 | 719 | 28 |         |         |       |
| 1   | H     | 505      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4045  | 2590 | 685 | 742 | 28 |         |         |       |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 69      | MET      | -      | EXPRESSION TAG | UNP Q15046 |
| B     | 69      | MET      | -      | EXPRESSION TAG | UNP Q15046 |
| C     | 69      | MET      | -      | EXPRESSION TAG | UNP Q15046 |
| D     | 69      | MET      | -      | EXPRESSION TAG | UNP Q15046 |
| E     | 69      | MET      | -      | EXPRESSION TAG | UNP Q15046 |
| F     | 69      | MET      | -      | EXPRESSION TAG | UNP Q15046 |
| G     | 69      | MET      | -      | EXPRESSION TAG | UNP Q15046 |
| H     | 69      | MET      | -      | EXPRESSION TAG | UNP Q15046 |

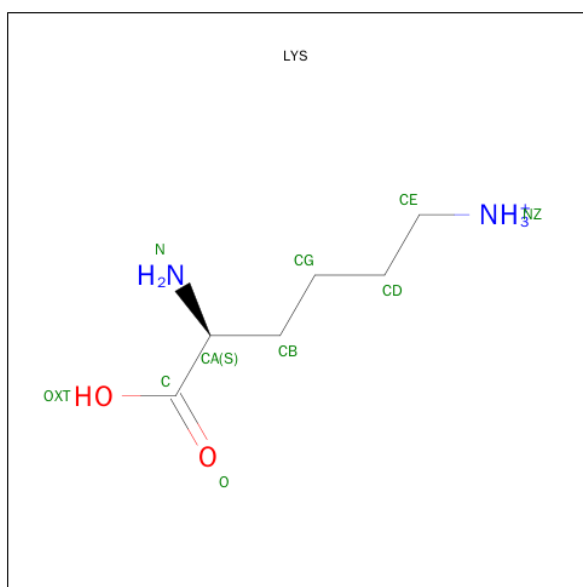
- Molecule 2 is a protein called Aminoacyl tRNA synthase complex-interacting multifunctional protein 2.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 2   | I     | 31       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 224   | 144 | 40 | 37 | 3 |         |         |       |
| 2   | J     | 31       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 226   | 146 | 40 | 37 | 3 |         |         |       |
| 2   | K     | 31       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 224   | 144 | 40 | 37 | 3 |         |         |       |
| 2   | L     | 31       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 230   | 148 | 40 | 39 | 3 |         |         |       |

There are 24 discrepancies between the modelled and reference sequences:

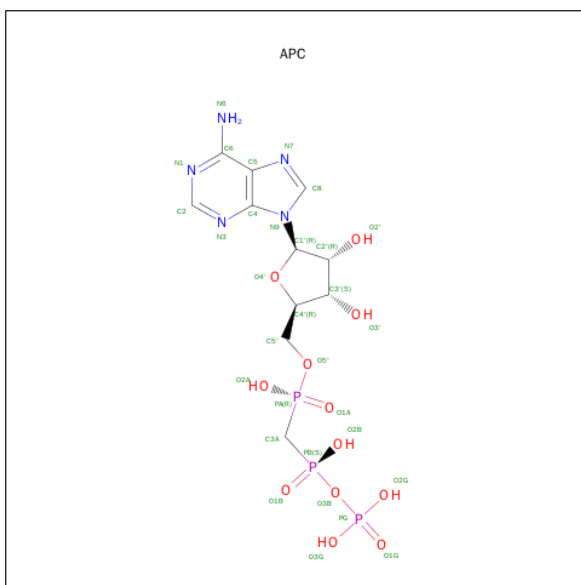
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| I     | 49      | HIS      | -      | EXPRESSION TAG | UNP Q13155 |
| I     | 50      | HIS      | -      | EXPRESSION TAG | UNP Q13155 |
| I     | 51      | HIS      | -      | EXPRESSION TAG | UNP Q13155 |
| I     | 52      | HIS      | -      | EXPRESSION TAG | UNP Q13155 |
| I     | 53      | HIS      | -      | EXPRESSION TAG | UNP Q13155 |
| I     | 54      | HIS      | -      | EXPRESSION TAG | UNP Q13155 |
| J     | 49      | HIS      | -      | EXPRESSION TAG | UNP Q13155 |
| J     | 50      | HIS      | -      | EXPRESSION TAG | UNP Q13155 |
| J     | 51      | HIS      | -      | EXPRESSION TAG | UNP Q13155 |
| J     | 52      | HIS      | -      | EXPRESSION TAG | UNP Q13155 |
| J     | 53      | HIS      | -      | EXPRESSION TAG | UNP Q13155 |
| J     | 54      | HIS      | -      | EXPRESSION TAG | UNP Q13155 |
| K     | 49      | HIS      | -      | EXPRESSION TAG | UNP Q13155 |
| K     | 50      | HIS      | -      | EXPRESSION TAG | UNP Q13155 |
| K     | 51      | HIS      | -      | EXPRESSION TAG | UNP Q13155 |
| K     | 52      | HIS      | -      | EXPRESSION TAG | UNP Q13155 |
| K     | 53      | HIS      | -      | EXPRESSION TAG | UNP Q13155 |
| K     | 54      | HIS      | -      | EXPRESSION TAG | UNP Q13155 |
| L     | 49      | HIS      | -      | EXPRESSION TAG | UNP Q13155 |
| L     | 50      | HIS      | -      | EXPRESSION TAG | UNP Q13155 |
| L     | 51      | HIS      | -      | EXPRESSION TAG | UNP Q13155 |
| L     | 52      | HIS      | -      | EXPRESSION TAG | UNP Q13155 |
| L     | 53      | HIS      | -      | EXPRESSION TAG | UNP Q13155 |
| L     | 54      | HIS      | -      | EXPRESSION TAG | UNP Q13155 |

- Molecule 3 is LYSINE (three-letter code: LYS) (formula:  $C_6H_{15}N_2O_2$ ).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 3   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 10    | 6 | 2 | 2 |         |         |
| 3   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 10    | 6 | 2 | 2 |         |         |
| 3   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 10    | 6 | 2 | 2 |         |         |
| 3   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 10    | 6 | 2 | 2 |         |         |
| 3   | E     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 10    | 6 | 2 | 2 |         |         |
| 3   | F     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 10    | 6 | 2 | 2 |         |         |
| 3   | G     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 10    | 6 | 2 | 2 |         |         |
| 3   | H     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 10    | 6 | 2 | 2 |         |         |

- Molecule 4 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: APC) (formula:  $C_{11}H_{18}N_5O_{12}P_3$ ).



| Mol | Chain | Residues | Atoms       |         |        |         |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|---------|
| 4   | A     | 1        | Total<br>27 | C<br>11 | N<br>5 | O<br>9  | P<br>2 | 0       | 0       |
| 4   | B     | 1        | Total<br>31 | C<br>11 | N<br>5 | O<br>12 | P<br>3 | 0       | 0       |
| 4   | C     | 1        | Total<br>27 | C<br>11 | N<br>5 | O<br>9  | P<br>2 | 0       | 0       |
| 4   | D     | 1        | Total<br>31 | C<br>11 | N<br>5 | O<br>12 | P<br>3 | 0       | 0       |
| 4   | E     | 1        | Total<br>27 | C<br>11 | N<br>5 | O<br>9  | P<br>2 | 0       | 0       |
| 4   | F     | 1        | Total<br>31 | C<br>11 | N<br>5 | O<br>12 | P<br>3 | 0       | 0       |
| 4   | G     | 1        | Total<br>27 | C<br>11 | N<br>5 | O<br>9  | P<br>2 | 0       | 0       |
| 4   | H     | 1        | Total<br>31 | C<br>11 | N<br>5 | O<br>12 | P<br>3 | 0       | 0       |

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

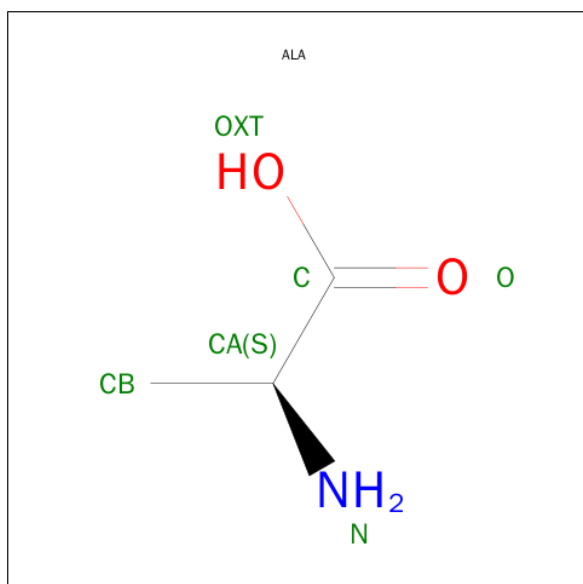
| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 5   | G     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 5   | J     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 5   | D     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 5   | E     | 1        | Total Mg<br>1 1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | H     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 5   | B     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 5   | C     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 5   | A     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 5   | L     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 5   | F     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 6 is ALANINE (three-letter code: ALA) (formula:  $C_3H_7NO_2$ ).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 6   | H     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 5     | 3 | 1 | 1 |         |         |

- Molecule 7 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 7   | A     | 47       | Total | O  | 0       | 0       |
|     |       |          | 47    | 47 |         |         |
| 7   | B     | 85       | Total | O  | 0       | 0       |
|     |       |          | 85    | 85 |         |         |

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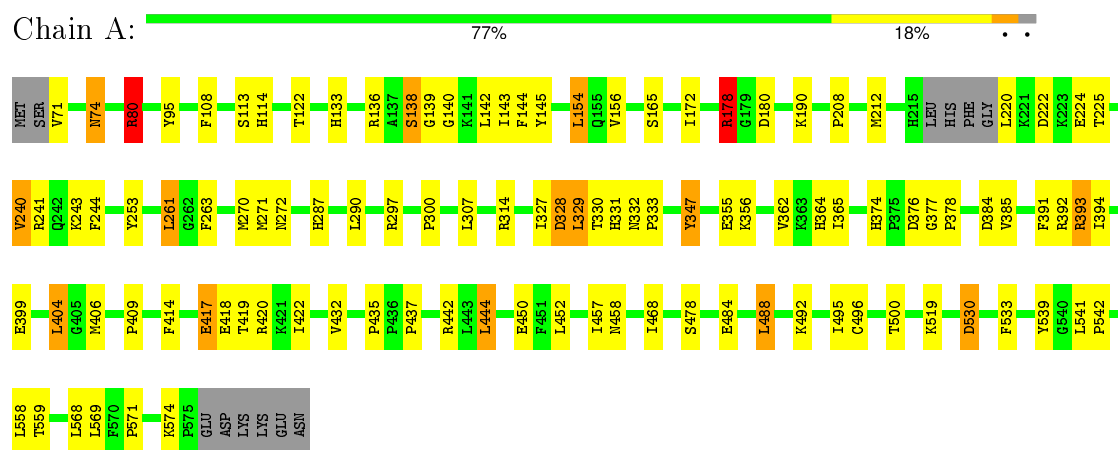
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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 7   | C     | 55       | Total<br>55 | O<br>55 | 0       | 0       |
| 7   | D     | 71       | Total<br>71 | O<br>71 | 0       | 0       |
| 7   | E     | 66       | Total<br>66 | O<br>66 | 0       | 0       |
| 7   | F     | 81       | Total<br>81 | O<br>81 | 0       | 0       |
| 7   | G     | 43       | Total<br>43 | O<br>43 | 0       | 0       |
| 7   | H     | 62       | Total<br>62 | O<br>62 | 0       | 0       |
| 7   | I     | 6        | Total<br>6  | O<br>6  | 0       | 0       |
| 7   | J     | 3        | Total<br>3  | O<br>3  | 0       | 0       |
| 7   | K     | 10       | Total<br>10 | O<br>10 | 0       | 0       |
| 7   | L     | 13       | Total<br>13 | O<br>13 | 0       | 0       |

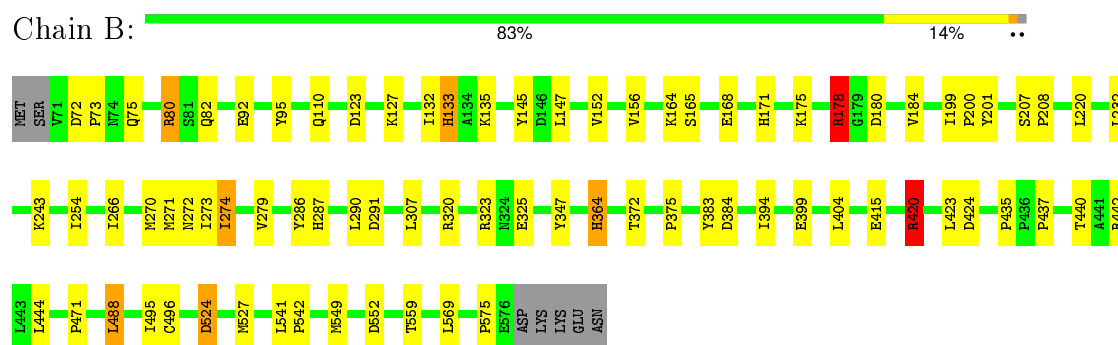
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

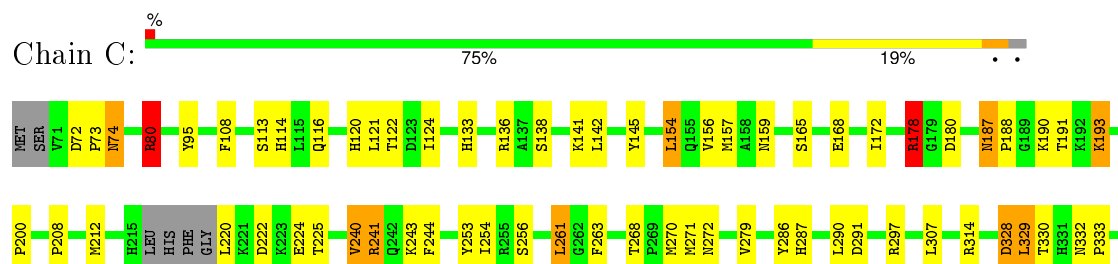
#### • Molecule 1: Lysine-tRNA ligase

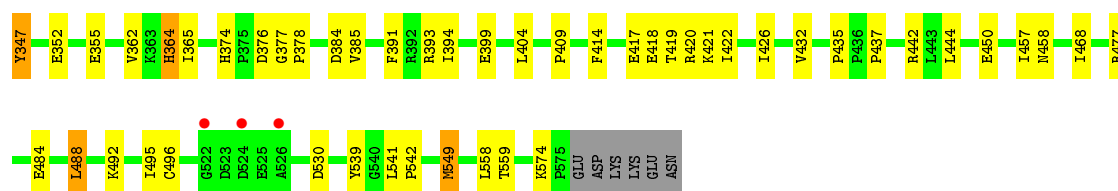


#### • Molecule 1: Lysine-tRNA ligase

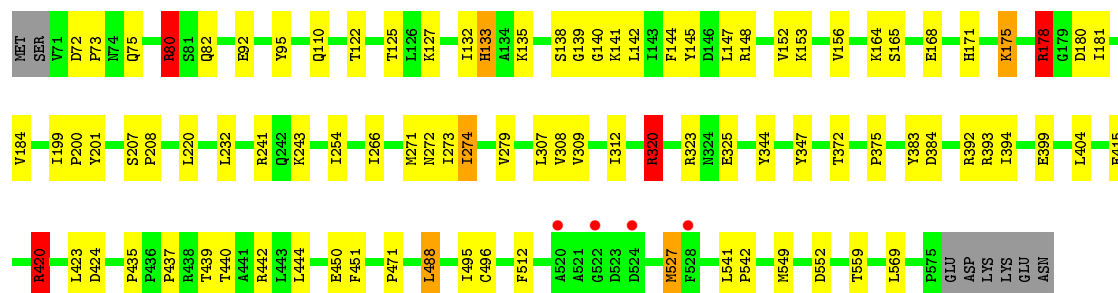
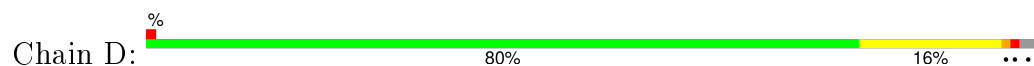


#### • Molecule 1: Lysine-tRNA ligase

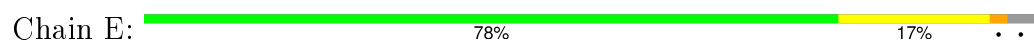




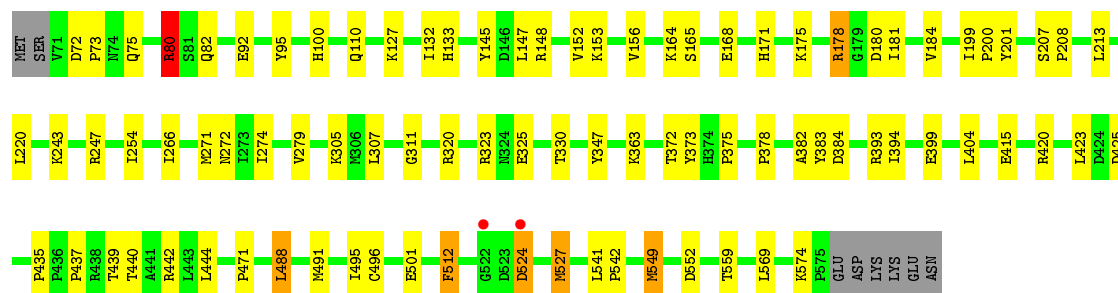
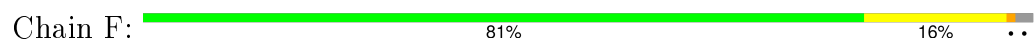
• Molecule 1: Lysine–tRNA ligase



• Molecule 1: Lysine–tRNA ligase

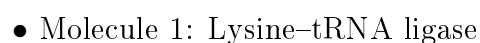


• Molecule 1: Lysine–tRNA ligase



• Molecule 1: Lysine–tRNA ligase

17%



78%



39%

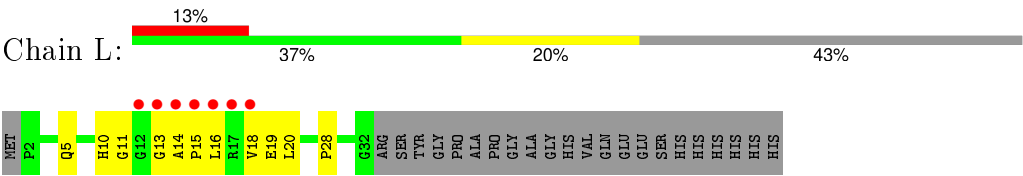


11%



13%

● Molecule 2: Aminoacyl tRNA synthase complex-interacting multifunctional protein 2



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 79.20 Å 122.01 Å 149.20 Å<br>89.16° 85.58° 89.71°           | Depositor        |
| Resolution (Å)  | 46.84 – 2.84<br>47.84 – 2.84                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.5 (46.84-2.84)<br>95.8 (47.84-2.84)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.10  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.59 (at 2.86 Å)  | Xtriage          |
| Refinement program  | PHENIX (phenix.refine: 1.7.2_869)                           | Depositor        |
| R, $R_{free}$   | 0.185 , 0.223<br>0.186 , 0.221                              | Depositor<br>DCC |
| $R_{free}$ test set   | 6481 reflections (5.30%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 38.4  | Xtriage          |
| Anisotropy  | 0.002   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 14.9   | EDS              |
| Estimated twinning fraction   | 0.339 for -h,k,-l   | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Outliers  | 0 of 128809 reflections                                     | Xtriage          |
| $F_o, F_c$ correlation  | 0.94  | EDS              |
| Total number of atoms   | 33740   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 42.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: APC, MG

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     | 0.51         | 0/4025      | 0.82        | 12/5457 (0.2%)  |
| 1   | B     | 0.50         | 0/4152      | 0.75        | 10/5619 (0.2%)  |
| 1   | C     | 0.48         | 0/4082      | 0.72        | 12/5526 (0.2%)  |
| 1   | D     | 0.52         | 0/4128      | 0.91        | 14/5586 (0.3%)  |
| 1   | E     | 0.48         | 0/4062      | 0.81        | 14/5503 (0.3%)  |
| 1   | F     | 0.50         | 0/4120      | 0.73        | 12/5577 (0.2%)  |
| 1   | G     | 0.49         | 0/4012      | 0.72        | 10/5440 (0.2%)  |
| 1   | H     | 0.51         | 0/4142      | 0.73        | 10/5607 (0.2%)  |
| 2   | I     | 0.49         | 0/233       | 0.78        | 0/319           |
| 2   | J     | 0.60         | 0/235       | 0.75        | 0/322           |
| 2   | K     | 0.58         | 0/233       | 0.78        | 0/319           |
| 2   | L     | 0.57         | 0/239       | 0.67        | 0/327           |
| All | All   | 0.50         | 0/33663     | 0.77        | 94/45602 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | B     | 0                   | 1                   |
| 1   | C     | 0                   | 1                   |
| 1   | E     | 0                   | 1                   |
| 1   | G     | 0                   | 1                   |
| All | All   | 0                   | 5                   |

There are no bond length outliers.

All (94) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | D     | 320 | ARG  | NE-CZ-NH2 | 21.80  | 131.20      | 120.30   |
| 1   | A     | 241 | ARG  | NE-CZ-NH2 | 20.63  | 130.61      | 120.30   |
| 1   | D     | 393 | ARG  | NE-CZ-NH2 | 19.46  | 130.03      | 120.30   |
| 1   | D     | 320 | ARG  | NE-CZ-NH1 | -19.00 | 110.80      | 120.30   |
| 1   | E     | 477 | ARG  | NE-CZ-NH1 | 18.84  | 129.72      | 120.30   |
| 1   | A     | 241 | ARG  | NE-CZ-NH1 | -18.77 | 110.92      | 120.30   |
| 1   | E     | 477 | ARG  | NE-CZ-NH2 | -17.75 | 111.42      | 120.30   |
| 1   | D     | 393 | ARG  | NE-CZ-NH1 | -17.20 | 111.70      | 120.30   |
| 1   | D     | 178 | ARG  | NE-CZ-NH2 | 16.11  | 128.35      | 120.30   |
| 1   | B     | 178 | ARG  | NE-CZ-NH2 | 15.24  | 127.92      | 120.30   |
| 1   | D     | 420 | ARG  | NE-CZ-NH1 | 14.71  | 127.65      | 120.30   |
| 1   | E     | 178 | ARG  | NE-CZ-NH2 | 14.69  | 127.64      | 120.30   |
| 1   | H     | 420 | ARG  | NE-CZ-NH2 | 14.36  | 127.48      | 120.30   |
| 1   | G     | 178 | ARG  | NE-CZ-NH2 | 14.33  | 127.46      | 120.30   |
| 1   | G     | 393 | ARG  | NE-CZ-NH2 | 14.23  | 127.41      | 120.30   |
| 1   | B     | 420 | ARG  | NE-CZ-NH1 | 14.10  | 127.35      | 120.30   |
| 1   | F     | 420 | ARG  | NE-CZ-NH2 | 13.61  | 127.11      | 120.30   |
| 1   | A     | 178 | ARG  | NE-CZ-NH1 | 13.55  | 127.07      | 120.30   |
| 1   | C     | 178 | ARG  | NE-CZ-NH1 | 13.48  | 127.04      | 120.30   |
| 1   | E     | 393 | ARG  | NE-CZ-NH2 | 13.16  | 126.88      | 120.30   |
| 1   | D     | 420 | ARG  | NE-CZ-NH2 | -13.05 | 113.77      | 120.30   |
| 1   | C     | 80  | ARG  | NE-CZ-NH2 | 12.65  | 126.63      | 120.30   |
| 1   | F     | 420 | ARG  | NE-CZ-NH1 | -12.52 | 114.04      | 120.30   |
| 1   | A     | 393 | ARG  | NE-CZ-NH1 | 12.31  | 126.45      | 120.30   |
| 1   | C     | 393 | ARG  | NE-CZ-NH1 | 12.20  | 126.40      | 120.30   |
| 1   | A     | 80  | ARG  | NE-CZ-NH2 | 12.15  | 126.37      | 120.30   |
| 1   | H     | 420 | ARG  | NE-CZ-NH1 | -11.96 | 114.32      | 120.30   |
| 1   | B     | 420 | ARG  | NE-CZ-NH2 | -11.78 | 114.41      | 120.30   |
| 1   | B     | 178 | ARG  | NE-CZ-NH1 | -11.75 | 114.43      | 120.30   |
| 1   | F     | 178 | ARG  | NE-CZ-NH1 | 11.73  | 126.17      | 120.30   |
| 1   | H     | 178 | ARG  | NE-CZ-NH1 | 11.62  | 126.11      | 120.30   |
| 1   | E     | 178 | ARG  | NE-CZ-NH1 | -11.56 | 114.52      | 120.30   |
| 1   | D     | 178 | ARG  | NE-CZ-NH1 | -11.41 | 114.59      | 120.30   |
| 1   | G     | 178 | ARG  | NE-CZ-NH1 | -11.14 | 114.73      | 120.30   |
| 1   | G     | 393 | ARG  | NE-CZ-NH1 | -10.97 | 114.81      | 120.30   |
| 1   | A     | 80  | ARG  | NE-CZ-NH1 | -10.79 | 114.90      | 120.30   |
| 1   | H     | 178 | ARG  | NE-CZ-NH2 | -10.79 | 114.91      | 120.30   |
| 1   | F     | 178 | ARG  | NE-CZ-NH2 | -10.64 | 114.98      | 120.30   |
| 1   | F     | 80  | ARG  | NE-CZ-NH2 | 10.58  | 125.59      | 120.30   |
| 1   | A     | 178 | ARG  | NE-CZ-NH2 | -10.49 | 115.06      | 120.30   |
| 1   | H     | 80  | ARG  | NE-CZ-NH2 | 10.44  | 125.52      | 120.30   |
| 1   | C     | 178 | ARG  | NE-CZ-NH2 | -10.36 | 115.12      | 120.30   |
| 1   | E     | 393 | ARG  | NE-CZ-NH1 | -10.24 | 115.18      | 120.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | D     | 320 | ARG  | CD-NE-CZ  | 10.20 | 137.88      | 123.60   |
| 1   | G     | 80  | ARG  | NE-CZ-NH1 | 10.12 | 125.36      | 120.30   |
| 1   | C     | 393 | ARG  | NE-CZ-NH2 | -9.91 | 115.35      | 120.30   |
| 1   | A     | 393 | ARG  | NE-CZ-NH2 | -9.71 | 115.45      | 120.30   |
| 1   | C     | 80  | ARG  | NE-CZ-NH1 | -9.67 | 115.46      | 120.30   |
| 1   | E     | 80  | ARG  | NE-CZ-NH1 | 9.51  | 125.06      | 120.30   |
| 1   | A     | 241 | ARG  | CD-NE-CZ  | 9.22  | 136.50      | 123.60   |
| 1   | B     | 80  | ARG  | NE-CZ-NH1 | 9.05  | 124.82      | 120.30   |
| 1   | D     | 393 | ARG  | CD-NE-CZ  | 8.40  | 135.36      | 123.60   |
| 1   | E     | 477 | ARG  | CD-NE-CZ  | 8.32  | 135.24      | 123.60   |
| 1   | G     | 80  | ARG  | NE-CZ-NH2 | -8.10 | 116.25      | 120.30   |
| 1   | F     | 80  | ARG  | NE-CZ-NH1 | -8.02 | 116.29      | 120.30   |
| 1   | G     | 241 | ARG  | NE-CZ-NH1 | 7.91  | 124.25      | 120.30   |
| 1   | H     | 320 | ARG  | NE-CZ-NH1 | 7.76  | 124.18      | 120.30   |
| 1   | H     | 80  | ARG  | NE-CZ-NH1 | -7.63 | 116.48      | 120.30   |
| 1   | D     | 80  | ARG  | NE-CZ-NH1 | 7.59  | 124.10      | 120.30   |
| 1   | B     | 320 | ARG  | NE-CZ-NH1 | 7.57  | 124.09      | 120.30   |
| 1   | C     | 241 | ARG  | NE-CZ-NH1 | 7.20  | 123.90      | 120.30   |
| 1   | H     | 420 | ARG  | CD-NE-CZ  | 7.14  | 133.59      | 123.60   |
| 1   | E     | 80  | ARG  | NE-CZ-NH2 | -7.11 | 116.75      | 120.30   |
| 1   | E     | 241 | ARG  | NE-CZ-NH1 | 7.06  | 123.83      | 120.30   |
| 1   | H     | 320 | ARG  | NE-CZ-NH2 | -6.82 | 116.89      | 120.30   |
| 1   | F     | 420 | ARG  | CD-NE-CZ  | 6.77  | 133.07      | 123.60   |
| 1   | F     | 178 | ARG  | CD-NE-CZ  | 6.65  | 132.91      | 123.60   |
| 1   | H     | 178 | ARG  | CD-NE-CZ  | 6.63  | 132.88      | 123.60   |
| 1   | D     | 178 | ARG  | CD-NE-CZ  | 6.46  | 132.65      | 123.60   |
| 1   | G     | 178 | ARG  | CD-NE-CZ  | 6.44  | 132.61      | 123.60   |
| 1   | D     | 420 | ARG  | CD-NE-CZ  | 6.43  | 132.60      | 123.60   |
| 1   | B     | 178 | ARG  | CD-NE-CZ  | 6.42  | 132.59      | 123.60   |
| 1   | B     | 420 | ARG  | CD-NE-CZ  | 6.41  | 132.57      | 123.60   |
| 1   | E     | 178 | ARG  | CD-NE-CZ  | 6.37  | 132.51      | 123.60   |
| 1   | F     | 320 | ARG  | NE-CZ-NH1 | 6.32  | 123.46      | 120.30   |
| 1   | G     | 241 | ARG  | NE-CZ-NH2 | -6.09 | 117.26      | 120.30   |
| 1   | A     | 178 | ARG  | CD-NE-CZ  | 5.98  | 131.97      | 123.60   |
| 1   | B     | 320 | ARG  | NE-CZ-NH2 | -5.93 | 117.33      | 120.30   |
| 1   | E     | 241 | ARG  | NE-CZ-NH2 | -5.93 | 117.34      | 120.30   |
| 1   | C     | 178 | ARG  | CD-NE-CZ  | 5.87  | 131.82      | 123.60   |
| 1   | E     | 393 | ARG  | CD-NE-CZ  | 5.87  | 131.82      | 123.60   |
| 1   | B     | 80  | ARG  | NE-CZ-NH2 | -5.71 | 117.45      | 120.30   |
| 1   | C     | 241 | ARG  | NE-CZ-NH2 | -5.67 | 117.46      | 120.30   |
| 1   | G     | 393 | ARG  | CD-NE-CZ  | 5.62  | 131.47      | 123.60   |
| 1   | A     | 393 | ARG  | CD-NE-CZ  | 5.62  | 131.46      | 123.60   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | C     | 393 | ARG  | CD-NE-CZ  | 5.43  | 131.20      | 123.60   |
| 1   | F     | 320 | ARG  | NE-CZ-NH2 | -5.40 | 117.60      | 120.30   |
| 1   | E     | 477 | ARG  | CB-CG-CD  | -5.38 | 97.62       | 111.60   |
| 1   | C     | 80  | ARG  | CD-NE-CZ  | 5.35  | 131.09      | 123.60   |
| 1   | A     | 80  | ARG  | CD-NE-CZ  | 5.28  | 131.00      | 123.60   |
| 1   | F     | 393 | ARG  | NE-CZ-NH1 | 5.17  | 122.88      | 120.30   |
| 1   | D     | 80  | ARG  | NE-CZ-NH2 | -5.15 | 117.72      | 120.30   |
| 1   | C     | 477 | ARG  | NE-CZ-NH2 | 5.04  | 122.82      | 120.30   |
| 1   | F     | 80  | ARG  | CD-NE-CZ  | 5.03  | 130.64      | 123.60   |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 574 | LYS  | Peptide |
| 1   | B     | 575 | PRO  | Peptide |
| 1   | C     | 574 | LYS  | Peptide |
| 1   | E     | 574 | LYS  | Peptide |
| 1   | G     | 574 | LYS  | Peptide |

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3932  | 0        | 3804     | 59      | 0            |
| 1   | B     | 4055  | 0        | 3984     | 41      | 0            |
| 1   | C     | 3989  | 0        | 3910     | 72      | 0            |
| 1   | D     | 4031  | 0        | 3977     | 51      | 0            |
| 1   | E     | 3969  | 0        | 3873     | 61      | 0            |
| 1   | F     | 4023  | 0        | 3964     | 42      | 0            |
| 1   | G     | 3921  | 0        | 3801     | 47      | 0            |
| 1   | H     | 4045  | 0        | 3981     | 61      | 0            |
| 2   | I     | 224   | 0        | 200      | 6       | 0            |
| 2   | J     | 226   | 0        | 207      | 3       | 0            |
| 2   | K     | 224   | 0        | 200      | 12      | 0            |
| 2   | L     | 230   | 0        | 211      | 15      | 0            |
| 3   | A     | 10    | 0        | 12       | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | B     | 10    | 0        | 12       | 0       | 0            |
| 3   | C     | 10    | 0        | 12       | 0       | 0            |
| 3   | D     | 10    | 0        | 12       | 0       | 0            |
| 3   | E     | 10    | 0        | 12       | 0       | 0            |
| 3   | F     | 10    | 0        | 12       | 0       | 0            |
| 3   | G     | 10    | 0        | 12       | 0       | 0            |
| 3   | H     | 10    | 0        | 12       | 0       | 0            |
| 4   | A     | 27    | 0        | 14       | 1       | 0            |
| 4   | B     | 31    | 0        | 14       | 0       | 0            |
| 4   | C     | 27    | 0        | 14       | 1       | 0            |
| 4   | D     | 31    | 0        | 14       | 0       | 0            |
| 4   | E     | 27    | 0        | 14       | 2       | 0            |
| 4   | F     | 31    | 0        | 14       | 0       | 0            |
| 4   | G     | 27    | 0        | 14       | 0       | 0            |
| 4   | H     | 31    | 0        | 14       | 0       | 0            |
| 5   | A     | 1     | 0        | 0        | 0       | 0            |
| 5   | B     | 1     | 0        | 0        | 0       | 0            |
| 5   | C     | 1     | 0        | 0        | 0       | 0            |
| 5   | D     | 1     | 0        | 0        | 0       | 0            |
| 5   | E     | 1     | 0        | 0        | 0       | 0            |
| 5   | F     | 2     | 0        | 0        | 0       | 0            |
| 5   | G     | 1     | 0        | 0        | 0       | 0            |
| 5   | H     | 2     | 0        | 0        | 0       | 0            |
| 5   | J     | 1     | 0        | 0        | 0       | 0            |
| 5   | L     | 1     | 0        | 0        | 0       | 0            |
| 6   | H     | 5     | 0        | 4        | 1       | 0            |
| 7   | A     | 47    | 0        | 0        | 2       | 0            |
| 7   | B     | 85    | 0        | 0        | 3       | 0            |
| 7   | C     | 55    | 0        | 0        | 4       | 0            |
| 7   | D     | 71    | 0        | 0        | 3       | 0            |
| 7   | E     | 66    | 0        | 0        | 1       | 0            |
| 7   | F     | 81    | 0        | 0        | 2       | 0            |
| 7   | G     | 43    | 0        | 0        | 1       | 0            |
| 7   | H     | 62    | 0        | 0        | 3       | 0            |
| 7   | I     | 6     | 0        | 0        | 0       | 0            |
| 7   | J     | 3     | 0        | 0        | 0       | 0            |
| 7   | K     | 10    | 0        | 0        | 0       | 0            |
| 7   | L     | 13    | 0        | 0        | 1       | 0            |
| All | All   | 33740 | 0        | 32324    | 428     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (428) 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:C:270:MET:HE3  | 7:C:739:HOH:O    | 1.63                     | 0.97              |
| 1:C:124:ILE:O    | 1:C:187:ASN:HB3  | 1.68                     | 0.92              |
| 7:B:776:HOH:O    | 2:I:14:ALA:HB2   | 1.72                     | 0.88              |
| 1:C:256:SER:OG   | 2:K:14:ALA:HB1   | 1.73                     | 0.88              |
| 1:G:427:CYS:SG   | 1:G:438:ARG:NH1  | 2.51                     | 0.84              |
| 1:B:394:ILE:HB   | 1:B:399:GLU:HG3  | 1.64                     | 0.80              |
| 1:E:120:HIS:CD2  | 1:E:122:THR:HG23 | 2.17                     | 0.78              |
| 1:H:394:ILE:HB   | 1:H:399:GLU:HG3  | 1.65                     | 0.77              |
| 1:C:270:MET:CE   | 7:C:739:HOH:O    | 2.23                     | 0.77              |
| 1:F:394:ILE:HB   | 1:F:399:GLU:HG3  | 1.66                     | 0.77              |
| 1:E:287:HIS:CD2  | 1:E:290:LEU:HG   | 2.21                     | 0.76              |
| 1:D:394:ILE:HB   | 1:D:399:GLU:HG3  | 1.66                     | 0.75              |
| 1:C:287:HIS:HD2  | 1:C:290:LEU:HG   | 1.49                     | 0.75              |
| 1:A:327:ILE:HD12 | 1:B:290:LEU:HD11 | 1.68                     | 0.75              |
| 1:C:287:HIS:CD2  | 1:C:290:LEU:HG   | 2.22                     | 0.75              |
| 1:E:287:HIS:HD2  | 1:E:290:LEU:HG   | 1.51                     | 0.73              |
| 1:G:409:PRO:HG2  | 1:G:419:THR:HG23 | 1.69                     | 0.73              |
| 1:G:287:HIS:CD2  | 1:G:290:LEU:HG   | 2.24                     | 0.73              |
| 2:J:15:PRO:O     | 2:J:16:LEU:CB    | 2.35                     | 0.73              |
| 1:A:409:PRO:HG2  | 1:A:419:THR:HG23 | 1.70                     | 0.72              |
| 2:I:15:PRO:O     | 2:I:16:LEU:CB    | 2.37                     | 0.71              |
| 1:C:409:PRO:HG2  | 1:C:419:THR:HG23 | 1.71                     | 0.71              |
| 1:G:287:HIS:HD2  | 1:G:290:LEU:HG   | 1.56                     | 0.71              |
| 1:B:435:PRO:O    | 1:B:442:ARG:NH2  | 2.24                     | 0.70              |
| 1:E:328:ASP:C    | 1:E:328:ASP:OD1  | 2.30                     | 0.69              |
| 1:C:133:HIS:O    | 1:C:178:ARG:HD2  | 1.92                     | 0.69              |
| 1:C:193:LYS:H    | 1:C:193:LYS:HE3  | 1.58                     | 0.69              |
| 1:D:435:PRO:O    | 1:D:442:ARG:NH2  | 2.27                     | 0.68              |
| 1:H:488:LEU:HB2  | 1:H:496:CYS:HB2  | 1.75                     | 0.68              |
| 1:C:256:SER:HB3  | 2:K:15:PRO:O     | 1.94                     | 0.68              |
| 1:E:253:TYR:HD1  | 2:L:15:PRO:HB3   | 1.58                     | 0.68              |
| 1:E:409:PRO:HG2  | 1:E:419:THR:HG23 | 1.75                     | 0.67              |
| 1:B:133:HIS:O    | 1:B:178:ARG:HD2  | 1.94                     | 0.67              |
| 1:A:133:HIS:O    | 1:A:178:ARG:HD2  | 1.94                     | 0.66              |
| 1:G:113:SER:O    | 1:G:190:LYS:NZ   | 2.27                     | 0.66              |
| 1:D:241:ARG:NH2  | 7:D:727:HOH:O    | 2.29                     | 0.66              |
| 1:E:328:ASP:OD1  | 1:E:330:THR:N    | 2.29                     | 0.65              |
| 1:E:253:TYR:CD1  | 2:L:15:PRO:HB3   | 2.32                     | 0.65              |
| 1:B:488:LEU:HB2  | 1:B:496:CYS:HB2  | 1.77                     | 0.65              |
| 1:G:328:ASP:OD1  | 1:G:329:LEU:N    | 2.30                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:15:PRO:O     | 2:K:16:LEU:CB    | 2.42                     | 0.65              |
| 1:H:575:PRO:C    | 6:H:601:ALA:N    | 2.50                     | 0.65              |
| 2:L:11:GLY:HA2   | 7:L:211:HOH:O    | 1.96                     | 0.65              |
| 1:F:435:PRO:O    | 1:F:442:ARG:NH2  | 2.30                     | 0.65              |
| 1:E:328:ASP:OD1  | 1:E:329:LEU:N    | 2.30                     | 0.64              |
| 1:C:328:ASP:OD1  | 1:C:329:LEU:N    | 2.29                     | 0.64              |
| 1:B:364:HIS:HD1  | 1:B:364:HIS:C    | 2.01                     | 0.64              |
| 1:E:120:HIS:HD2  | 1:E:122:THR:HG23 | 1.62                     | 0.64              |
| 1:H:133:HIS:HB3  | 7:H:739:HOH:O    | 1.96                     | 0.64              |
| 1:F:488:LEU:HB2  | 1:F:496:CYS:HB2  | 1.77                     | 0.64              |
| 1:E:113:SER:O    | 1:E:190:LYS:NZ   | 2.31                     | 0.64              |
| 1:A:328:ASP:OD1  | 1:A:329:LEU:N    | 2.30                     | 0.64              |
| 1:H:328:ASP:OD1  | 1:H:331:HIS:ND1  | 2.30                     | 0.64              |
| 1:C:116:GLN:HE22 | 1:F:382:ALA:H    | 1.43                     | 0.64              |
| 1:C:253:TYR:HD1  | 2:K:15:PRO:HB3   | 1.63                     | 0.63              |
| 1:G:541:LEU:HD12 | 1:G:542:PRO:HD2  | 1.80                     | 0.63              |
| 1:C:74:ASN:OD1   | 1:C:74:ASN:N     | 2.31                     | 0.63              |
| 1:E:256:SER:OG   | 2:L:15:PRO:HD2   | 1.98                     | 0.63              |
| 1:H:435:PRO:O    | 1:H:442:ARG:NH2  | 2.32                     | 0.63              |
| 1:D:541:LEU:HD12 | 1:D:542:PRO:HD2  | 1.79                     | 0.63              |
| 1:A:253:TYR:HD1  | 1:A:364:HIS:HD2  | 1.47                     | 0.63              |
| 1:A:541:LEU:HD12 | 1:A:542:PRO:HD2  | 1.81                     | 0.62              |
| 1:B:541:LEU:HD12 | 1:B:542:PRO:HD2  | 1.81                     | 0.62              |
| 1:A:74:ASN:N     | 1:A:74:ASN:OD1   | 2.31                     | 0.62              |
| 1:E:541:LEU:HD12 | 1:E:542:PRO:HD2  | 1.80                     | 0.62              |
| 1:G:74:ASN:N     | 1:G:74:ASN:OD1   | 2.30                     | 0.62              |
| 1:B:164:LYS:HB3  | 1:B:201:TYR:CZ   | 2.35                     | 0.62              |
| 1:B:273:ILE:HG13 | 1:B:274:ILE:HG12 | 1.80                     | 0.62              |
| 1:A:113:SER:O    | 1:A:190:LYS:NZ   | 2.33                     | 0.62              |
| 1:C:488:LEU:HB2  | 1:C:496:CYS:HB2  | 1.81                     | 0.62              |
| 1:A:114:HIS:NE2  | 1:H:378:PRO:O    | 2.31                     | 0.62              |
| 1:A:328:ASP:OD1  | 1:A:330:THR:N    | 2.30                     | 0.62              |
| 1:A:328:ASP:OD2  | 1:A:331:HIS:ND1  | 2.30                     | 0.62              |
| 1:H:328:ASP:OD1  | 1:H:331:HIS:CG   | 2.53                     | 0.62              |
| 1:H:273:ILE:HG13 | 1:H:274:ILE:HG12 | 1.82                     | 0.62              |
| 1:D:133:HIS:O    | 1:D:178:ARG:HD2  | 1.98                     | 0.61              |
| 1:C:253:TYR:CD1  | 2:K:15:PRO:HB3   | 2.35                     | 0.61              |
| 1:E:74:ASN:N     | 1:E:74:ASN:OD1   | 2.33                     | 0.61              |
| 1:D:273:ILE:HG13 | 1:D:274:ILE:HG12 | 1.81                     | 0.60              |
| 1:H:524:ASP:OD2  | 1:H:524:ASP:N    | 2.28                     | 0.60              |
| 1:C:80:ARG:NH1   | 1:C:180:ASP:OD2  | 2.33                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:113:SER:O    | 1:C:190:LYS:NZ   | 2.34                     | 0.60              |
| 1:F:95:TYR:CE2   | 1:F:208:PRO:HD2  | 2.37                     | 0.59              |
| 1:G:488:LEU:HB2  | 1:G:496:CYS:HB2  | 1.83                     | 0.59              |
| 1:F:80:ARG:NH1   | 1:F:180:ASP:OD1  | 2.36                     | 0.59              |
| 1:F:541:LEU:HD12 | 1:F:542:PRO:HD2  | 1.83                     | 0.59              |
| 1:A:270:MET:HE1  | 7:B:770:HOH:O    | 2.02                     | 0.59              |
| 1:A:80:ARG:NH1   | 1:A:180:ASP:OD2  | 2.34                     | 0.59              |
| 1:H:95:TYR:CE2   | 1:H:208:PRO:HD2  | 2.37                     | 0.59              |
| 1:A:488:LEU:HB2  | 1:A:496:CYS:HB2  | 1.84                     | 0.59              |
| 1:C:328:ASP:OD1  | 1:C:330:THR:N    | 2.30                     | 0.59              |
| 1:H:541:LEU:HD12 | 1:H:542:PRO:HD2  | 1.84                     | 0.59              |
| 1:C:253:TYR:HD1  | 1:C:364:HIS:HD2  | 1.51                     | 0.59              |
| 1:D:95:TYR:CE2   | 1:D:208:PRO:HD2  | 2.38                     | 0.58              |
| 1:A:488:LEU:HD13 | 1:A:495:ILE:HD11 | 1.86                     | 0.58              |
| 1:E:327:ILE:O    | 1:E:327:ILE:HG22 | 2.02                     | 0.58              |
| 1:E:488:LEU:HB2  | 1:E:496:CYS:HB2  | 1.86                     | 0.58              |
| 1:E:488:LEU:HD13 | 1:E:495:ILE:HD11 | 1.86                     | 0.58              |
| 1:G:145:TYR:HB2  | 1:G:156:VAL:HB   | 1.86                     | 0.58              |
| 1:B:286:TYR:OH   | 1:B:291:ASP:OD1  | 2.21                     | 0.57              |
| 1:E:270:MET:HA   | 1:E:297:ARG:HD3  | 1.86                     | 0.57              |
| 1:D:488:LEU:HB2  | 1:D:496:CYS:HB2  | 1.85                     | 0.57              |
| 7:E:762:HOH:O    | 2:L:19:GLU:HG3   | 2.05                     | 0.57              |
| 1:H:164:LYS:HB3  | 1:H:201:TYR:CZ   | 2.38                     | 0.57              |
| 1:G:270:MET:HA   | 1:G:297:ARG:HD3  | 1.87                     | 0.57              |
| 1:D:139:GLY:HA3  | 1:D:140:GLY:C    | 2.24                     | 0.57              |
| 1:C:541:LEU:HD12 | 1:C:542:PRO:HD2  | 1.86                     | 0.57              |
| 1:C:145:TYR:HB2  | 1:C:156:VAL:HB   | 1.87                     | 0.57              |
| 1:F:323:ARG:NH1  | 1:F:325:GLU:OE2  | 2.37                     | 0.57              |
| 1:C:142:LEU:HD13 | 1:C:159:ASN:HB3  | 1.87                     | 0.57              |
| 1:B:95:TYR:CE2   | 1:B:208:PRO:HD2  | 2.40                     | 0.56              |
| 1:H:323:ARG:NH1  | 1:H:325:GLU:OE2  | 2.36                     | 0.56              |
| 1:B:323:ARG:NH1  | 1:B:325:GLU:OE2  | 2.37                     | 0.56              |
| 1:E:256:SER:OG   | 2:L:14:ALA:HB1   | 2.06                     | 0.56              |
| 1:E:145:TYR:HB2  | 1:E:156:VAL:HB   | 1.87                     | 0.56              |
| 1:A:145:TYR:HB2  | 1:A:156:VAL:HB   | 1.88                     | 0.56              |
| 1:G:142:LEU:HD13 | 1:G:159:ASN:HB3  | 1.87                     | 0.56              |
| 1:A:253:TYR:CD1  | 1:A:364:HIS:HD2  | 2.23                     | 0.56              |
| 1:F:164:LYS:HB3  | 1:F:201:TYR:CZ   | 2.41                     | 0.56              |
| 1:D:323:ARG:NH1  | 1:D:325:GLU:OE2  | 2.38                     | 0.56              |
| 1:A:138:SER:HB2  | 1:A:142:LEU:HD23 | 1.88                     | 0.55              |
| 1:E:142:LEU:HD13 | 1:E:159:ASN:HB3  | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:254:ILE:HD11 | 1:H:549:MET:CE   | 2.36                     | 0.55              |
| 1:H:286:TYR:OH   | 1:H:291:ASP:OD1  | 2.20                     | 0.55              |
| 1:E:256:SER:HB3  | 2:L:15:PRO:O     | 2.07                     | 0.54              |
| 1:F:145:TYR:HB2  | 1:F:156:VAL:HB   | 1.89                     | 0.54              |
| 1:H:80:ARG:NH1   | 1:H:180:ASP:OD1  | 2.40                     | 0.54              |
| 1:G:287:HIS:HD2  | 1:G:290:LEU:CG   | 2.21                     | 0.54              |
| 1:C:120:HIS:NE2  | 1:C:187:ASN:OD1  | 2.40                     | 0.54              |
| 1:H:488:LEU:HD13 | 1:H:495:ILE:HD11 | 1.89                     | 0.54              |
| 1:H:423:LEU:HD12 | 1:H:440:THR:HG23 | 1.90                     | 0.53              |
| 1:B:364:HIS:ND1  | 1:B:364:HIS:C    | 2.62                     | 0.53              |
| 1:E:307:LEU:HD11 | 1:F:569:LEU:HD13 | 1.91                     | 0.53              |
| 1:C:488:LEU:HD13 | 1:C:495:ILE:HD11 | 1.90                     | 0.53              |
| 1:C:364:HIS:CD2  | 2:K:15:PRO:HB3   | 2.44                     | 0.53              |
| 1:C:240:VAL:HG12 | 1:C:244:PHE:HE2  | 1.74                     | 0.53              |
| 1:D:164:LYS:HB3  | 1:D:201:TYR:CZ   | 2.43                     | 0.53              |
| 1:E:240:VAL:HG12 | 1:E:244:PHE:HE2  | 1.73                     | 0.53              |
| 1:H:145:TYR:HB2  | 1:H:156:VAL:HB   | 1.90                     | 0.53              |
| 1:C:253:TYR:CD1  | 1:C:364:HIS:HD2  | 2.27                     | 0.53              |
| 1:F:132:ILE:HD12 | 1:F:180:ASP:HB2  | 1.91                     | 0.53              |
| 1:C:116:GLN:NE2  | 1:F:382:ALA:H    | 2.07                     | 0.52              |
| 1:C:270:MET:HA   | 1:C:297:ARG:HD3  | 1.90                     | 0.52              |
| 1:D:139:GLY:CA   | 1:D:140:GLY:C    | 2.75                     | 0.52              |
| 1:A:222:ASP:OD1  | 1:A:225:THR:OG1  | 2.27                     | 0.52              |
| 1:G:417:GLU:OE2  | 1:G:420:ARG:NE   | 2.42                     | 0.52              |
| 1:B:270:MET:HE3  | 7:B:770:HOH:O    | 2.09                     | 0.52              |
| 1:A:270:MET:HA   | 1:A:297:ARG:HD3  | 1.91                     | 0.51              |
| 1:H:142:LEU:HD12 | 1:H:143:ILE:N    | 2.25                     | 0.51              |
| 1:D:92:GLU:OE1   | 1:D:171:HIS:NE2  | 2.42                     | 0.51              |
| 1:E:435:PRO:O    | 1:E:442:ARG:NH2  | 2.43                     | 0.51              |
| 1:H:305:LYS:NZ   | 1:H:501:GLU:OE1  | 2.37                     | 0.51              |
| 1:G:222:ASP:OD1  | 1:G:225:THR:OG1  | 2.28                     | 0.51              |
| 1:B:92:GLU:OE1   | 1:B:171:HIS:NE2  | 2.43                     | 0.51              |
| 1:A:394:ILE:HD12 | 1:A:452:LEU:HD22 | 1.93                     | 0.51              |
| 1:A:143:ILE:HG22 | 1:A:144:PHE:N    | 2.25                     | 0.51              |
| 1:A:243:LYS:HG2  | 1:A:559:THR:HB   | 1.92                     | 0.51              |
| 1:B:145:TYR:HB2  | 1:B:156:VAL:HB   | 1.91                     | 0.51              |
| 1:B:254:ILE:HD11 | 1:B:549:MET:CE   | 2.41                     | 0.51              |
| 1:A:287:HIS:CE1  | 1:A:290:LEU:HG   | 2.45                     | 0.51              |
| 1:A:240:VAL:HG12 | 1:A:244:PHE:HE2  | 1.76                     | 0.51              |
| 1:D:423:LEU:HD12 | 1:D:440:THR:HG23 | 1.92                     | 0.51              |
| 1:A:307:LEU:HD11 | 1:B:569:LEU:HD13 | 1.93                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:132:ILE:HD12 | 1:B:180:ASP:HB2  | 1.92                     | 0.50              |
| 1:C:243:LYS:HG2  | 1:C:559:THR:HB   | 1.93                     | 0.50              |
| 1:E:253:TYR:CD1  | 2:L:15:PRO:CB    | 2.94                     | 0.50              |
| 1:G:488:LEU:HD13 | 1:G:495:ILE:HD11 | 1.92                     | 0.50              |
| 1:G:307:LEU:HD11 | 1:H:569:LEU:HD13 | 1.94                     | 0.50              |
| 1:G:422:ILE:O    | 1:G:426:ILE:HG13 | 2.11                     | 0.50              |
| 1:D:145:TYR:HB2  | 1:D:156:VAL:HB   | 1.94                     | 0.50              |
| 1:B:123:ASP:HB3  | 1:F:425:ASP:HB3  | 1.93                     | 0.50              |
| 1:A:327:ILE:CD1  | 1:B:290:LEU:HD11 | 2.39                     | 0.50              |
| 1:A:287:HIS:ND1  | 1:A:290:LEU:HG   | 2.27                     | 0.50              |
| 1:E:347:TYR:CE1  | 1:E:484:GLU:HB3  | 2.46                     | 0.50              |
| 1:F:254:ILE:HD11 | 1:F:549:MET:CE   | 2.41                     | 0.50              |
| 1:B:423:LEU:HD12 | 1:B:440:THR:HG23 | 1.94                     | 0.50              |
| 1:E:95:TYR:CE2   | 1:E:208:PRO:HD2  | 2.46                     | 0.50              |
| 1:H:92:GLU:OE1   | 1:H:171:HIS:NE2  | 2.45                     | 0.50              |
| 1:G:240:VAL:HG12 | 1:G:244:PHE:HE2  | 1.76                     | 0.50              |
| 1:E:222:ASP:OD1  | 1:E:225:THR:OG1  | 2.27                     | 0.50              |
| 1:A:417:GLU:OE2  | 1:A:420:ARG:NE   | 2.43                     | 0.50              |
| 1:G:347:TYR:CE1  | 1:G:484:GLU:HB3  | 2.47                     | 0.50              |
| 1:C:95:TYR:CE2   | 1:C:208:PRO:HD2  | 2.47                     | 0.50              |
| 1:E:330:THR:O    | 1:E:330:THR:OG1  | 2.30                     | 0.49              |
| 1:H:132:ILE:HD12 | 1:H:180:ASP:HB2  | 1.93                     | 0.49              |
| 1:E:385:VAL:HG13 | 1:E:458:ASN:HA   | 1.94                     | 0.49              |
| 1:F:92:GLU:OE1   | 1:F:171:HIS:NE2  | 2.45                     | 0.49              |
| 1:F:488:LEU:HD13 | 1:F:495:ILE:HD11 | 1.93                     | 0.49              |
| 1:A:457:ILE:HD11 | 1:A:492:LYS:HE3  | 1.95                     | 0.49              |
| 1:E:253:TYR:HA   | 2:L:15:PRO:HB2   | 1.95                     | 0.49              |
| 1:G:95:TYR:CE2   | 1:G:208:PRO:HD2  | 2.47                     | 0.49              |
| 1:H:98:LYS:HA    | 7:H:706:HOH:O    | 2.13                     | 0.49              |
| 1:C:417:GLU:OE2  | 1:C:420:ARG:NE   | 2.43                     | 0.49              |
| 1:C:261:LEU:HD13 | 2:K:20:LEU:HD22  | 1.95                     | 0.49              |
| 1:D:175:LYS:HE3  | 7:D:723:HOH:O    | 2.12                     | 0.49              |
| 1:B:524:ASP:OD2  | 1:B:524:ASP:N    | 2.26                     | 0.49              |
| 1:D:254:ILE:HD11 | 1:D:549:MET:CE   | 2.43                     | 0.49              |
| 1:D:471:PRO:HG2  | 1:D:527:MET:HE3  | 1.94                     | 0.49              |
| 1:C:362:VAL:HG22 | 1:C:558:LEU:HD21 | 1.93                     | 0.49              |
| 1:H:330:THR:O    | 1:H:331:HIS:HD2  | 1.96                     | 0.48              |
| 1:C:268:THR:O    | 1:D:320:ARG:NH1  | 2.36                     | 0.48              |
| 1:B:437:PRO:O    | 1:B:442:ARG:HD3  | 2.12                     | 0.48              |
| 1:A:435:PRO:O    | 1:A:442:ARG:NH2  | 2.46                     | 0.48              |
| 1:G:243:LYS:HG2  | 1:G:559:THR:HB   | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:364:HIS:HD2  | 2:K:15:PRO:HB3   | 1.78                     | 0.48              |
| 1:D:437:PRO:O    | 1:D:442:ARG:HD3  | 2.14                     | 0.48              |
| 1:C:418:GLU:O    | 1:C:422:ILE:HG13 | 2.14                     | 0.48              |
| 1:C:222:ASP:OD1  | 1:C:225:THR:OG1  | 2.30                     | 0.48              |
| 1:G:394:ILE:HD12 | 1:G:452:LEU:HD22 | 1.96                     | 0.48              |
| 1:C:114:HIS:NE2  | 1:F:378:PRO:O    | 2.44                     | 0.48              |
| 1:C:253:TYR:CD1  | 2:K:15:PRO:CB    | 2.96                     | 0.48              |
| 1:A:138:SER:CB   | 1:A:142:LEU:HD23 | 2.44                     | 0.48              |
| 7:A:726:HOH:O    | 2:I:31:HIS:HE1   | 1.97                     | 0.48              |
| 1:H:140:GLY:O    | 1:H:141:LYS:CB   | 2.60                     | 0.48              |
| 1:G:385:VAL:HG13 | 1:G:458:ASN:HA   | 1.96                     | 0.48              |
| 1:C:435:PRO:O    | 1:C:442:ARG:NH2  | 2.46                     | 0.48              |
| 1:E:418:GLU:O    | 1:E:422:ILE:HG13 | 2.14                     | 0.48              |
| 1:E:120:HIS:CD2  | 1:E:122:THR:CG2  | 2.95                     | 0.47              |
| 1:D:148:ARG:HD3  | 1:D:153:LYS:HB3  | 1.96                     | 0.47              |
| 1:A:385:VAL:HG13 | 1:A:458:ASN:HA   | 1.95                     | 0.47              |
| 1:G:355:GLU:OE2  | 1:G:393:ARG:NH2  | 2.47                     | 0.47              |
| 1:A:488:LEU:CB   | 1:A:496:CYS:HB2  | 2.43                     | 0.47              |
| 1:G:241:ARG:NH2  | 1:H:311:GLY:O    | 2.48                     | 0.47              |
| 1:A:347:TYR:CE1  | 1:A:484:GLU:HB3  | 2.49                     | 0.47              |
| 1:H:328:ASP:OD1  | 1:H:331:HIS:HB2  | 2.15                     | 0.47              |
| 1:E:394:ILE:HB   | 1:E:399:GLU:HG3  | 1.96                     | 0.47              |
| 1:F:423:LEU:HD12 | 1:F:440:THR:HG23 | 1.96                     | 0.47              |
| 1:D:140:GLY:O    | 1:D:141:LYS:HB2  | 2.15                     | 0.47              |
| 1:F:471:PRO:HG2  | 1:F:527:MET:HE3  | 1.96                     | 0.47              |
| 1:E:331:HIS:HD2  | 4:E:602:APC:C6   | 2.27                     | 0.47              |
| 1:G:263:PHE:CD2  | 1:G:314:ARG:HB3  | 2.50                     | 0.47              |
| 1:F:305:LYS:NZ   | 1:F:501:GLU:OE1  | 2.37                     | 0.47              |
| 1:A:418:GLU:O    | 1:A:422:ILE:HG13 | 2.15                     | 0.47              |
| 1:A:332:ASN:CG   | 1:A:333:PRO:HD2  | 2.35                     | 0.47              |
| 1:D:444:LEU:HD12 | 1:D:444:LEU:HA   | 1.67                     | 0.47              |
| 1:E:374:HIS:HB3  | 1:E:377:GLY:O    | 2.15                     | 0.47              |
| 1:H:72:ASP:HA    | 1:H:73:PRO:HD3   | 1.83                     | 0.47              |
| 1:A:263:PHE:CD2  | 1:A:314:ARG:HB3  | 2.50                     | 0.47              |
| 1:E:355:GLU:OE2  | 1:E:393:ARG:NH2  | 2.49                     | 0.46              |
| 1:F:524:ASP:N    | 1:F:524:ASP:OD2  | 2.29                     | 0.46              |
| 1:E:362:VAL:HG22 | 1:E:558:LEU:HD21 | 1.96                     | 0.46              |
| 1:A:374:HIS:HB3  | 1:A:377:GLY:O    | 2.16                     | 0.46              |
| 1:A:95:TYR:CE2   | 1:A:208:PRO:HD2  | 2.50                     | 0.46              |
| 1:H:437:PRO:O    | 1:H:442:ARG:HD3  | 2.15                     | 0.46              |
| 1:G:374:HIS:HB3  | 1:G:377:GLY:O    | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:127:LYS:HA   | 1:B:184:VAL:O    | 2.16                     | 0.46              |
| 1:B:488:LEU:HD13 | 1:B:495:ILE:HD11 | 1.97                     | 0.46              |
| 1:D:420:ARG:NH2  | 1:D:424:ASP:OD1  | 2.49                     | 0.46              |
| 1:A:139:GLY:HA2  | 1:A:140:GLY:HA2  | 1.61                     | 0.46              |
| 1:A:362:VAL:HG22 | 1:A:558:LEU:HD21 | 1.97                     | 0.46              |
| 1:D:142:LEU:HG   | 1:D:144:PHE:CE1  | 2.51                     | 0.46              |
| 7:G:711:HOH:O    | 2:J:31:HIS:HE1   | 1.99                     | 0.46              |
| 1:B:243:LYS:HG2  | 1:B:559:THR:HB   | 1.98                     | 0.46              |
| 1:F:437:PRO:O    | 1:F:442:ARG:HD3  | 2.16                     | 0.46              |
| 1:D:488:LEU:HD13 | 1:D:495:ILE:HD11 | 1.96                     | 0.46              |
| 1:D:135:LYS:HG3  | 1:D:145:TYR:CE2  | 2.50                     | 0.46              |
| 1:D:132:ILE:HD12 | 1:D:180:ASP:HB2  | 1.98                     | 0.46              |
| 1:A:432:VAL:HG22 | 1:A:450:GLU:HG3  | 1.98                     | 0.45              |
| 1:G:364:HIS:C    | 1:G:364:HIS:HD1  | 2.20                     | 0.45              |
| 1:C:385:VAL:HG13 | 1:C:458:ASN:HA   | 1.98                     | 0.45              |
| 1:C:286:TYR:OH   | 1:C:291:ASP:HA   | 2.16                     | 0.45              |
| 1:C:307:LEU:HD11 | 1:D:569:LEU:HD13 | 1.97                     | 0.45              |
| 1:H:139:GLY:HA2  | 7:H:754:HOH:O    | 2.16                     | 0.45              |
| 1:C:121:LEU:O    | 1:C:187:ASN:HB2  | 2.15                     | 0.45              |
| 1:C:347:TYR:CE1  | 1:C:484:GLU:HB3  | 2.51                     | 0.45              |
| 1:A:399:GLU:HB3  | 1:A:452:LEU:HD21 | 1.97                     | 0.45              |
| 1:C:422:ILE:O    | 1:C:426:ILE:HG13 | 2.15                     | 0.45              |
| 1:A:261:LEU:HD13 | 2:I:20:LEU:HD22  | 1.97                     | 0.45              |
| 1:G:539:TYR:CE1  | 1:H:232:LEU:HD21 | 2.52                     | 0.45              |
| 1:E:542:PRO:HB3  | 1:F:181:ILE:HG21 | 1.99                     | 0.45              |
| 1:D:423:LEU:HD13 | 1:D:444:LEU:HD13 | 1.99                     | 0.45              |
| 1:G:418:GLU:O    | 1:G:422:ILE:HG13 | 2.16                     | 0.45              |
| 1:B:471:PRO:HG2  | 1:B:527:MET:HE3  | 1.99                     | 0.45              |
| 1:C:374:HIS:HB3  | 1:C:377:GLY:O    | 2.17                     | 0.45              |
| 1:A:394:ILE:HB   | 1:A:399:GLU:HG3  | 1.97                     | 0.45              |
| 1:A:539:TYR:CE1  | 1:B:232:LEU:HD21 | 2.50                     | 0.45              |
| 1:F:127:LYS:HA   | 1:F:184:VAL:O    | 2.17                     | 0.45              |
| 1:E:263:PHE:CD2  | 1:E:314:ARG:HB3  | 2.52                     | 0.45              |
| 1:E:394:ILE:HD12 | 1:E:452:LEU:HD22 | 1.98                     | 0.45              |
| 2:L:13:GLY:HA2   | 2:L:14:ALA:HA    | 1.59                     | 0.45              |
| 1:F:423:LEU:HD13 | 1:F:444:LEU:HD13 | 1.99                     | 0.45              |
| 1:D:199:ILE:HA   | 1:D:200:PRO:HD3  | 1.79                     | 0.45              |
| 7:C:730:HOH:O    | 1:D:344:TYR:HA   | 2.17                     | 0.45              |
| 1:G:400:LEU:HD12 | 1:G:400:LEU:HA   | 1.80                     | 0.45              |
| 1:B:375:PRO:HG3  | 1:B:383:TYR:CE2  | 2.51                     | 0.45              |
| 1:D:375:PRO:HG3  | 1:D:383:TYR:CE2  | 2.52                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:10:HIS:HB2   | 2:K:11:GLY:H     | 1.31                     | 0.44              |
| 1:E:243:LYS:HG2  | 1:E:559:THR:HB   | 1.98                     | 0.44              |
| 1:H:127:LYS:HA   | 1:H:184:VAL:O    | 2.17                     | 0.44              |
| 1:B:135:LYS:HG3  | 1:B:145:TYR:CE2  | 2.52                     | 0.44              |
| 1:F:375:PRO:HG3  | 1:F:383:TYR:CE2  | 2.53                     | 0.44              |
| 1:E:457:ILE:HD11 | 1:E:492:LYS:HE3  | 1.99                     | 0.44              |
| 1:H:444:LEU:HA   | 1:H:444:LEU:HD12 | 1.66                     | 0.44              |
| 1:D:392:ARG:NH2  | 7:D:771:HOH:O    | 2.49                     | 0.44              |
| 1:C:157:MET:O    | 1:C:200:PRO:HD2  | 2.18                     | 0.44              |
| 1:G:414:PHE:HE2  | 1:G:444:LEU:HD11 | 1.82                     | 0.44              |
| 1:C:191:THR:HB   | 1:C:193:LYS:NZ   | 2.32                     | 0.44              |
| 1:C:377:GLY:HA2  | 1:C:378:PRO:HD3  | 1.84                     | 0.44              |
| 1:F:165:SER:HB2  | 1:F:168:GLU:H    | 1.82                     | 0.44              |
| 1:B:165:SER:HB2  | 1:B:168:GLU:H    | 1.83                     | 0.44              |
| 1:G:362:VAL:HG22 | 1:G:558:LEU:HD21 | 1.99                     | 0.44              |
| 1:B:199:ILE:HA   | 1:B:200:PRO:HD3  | 1.74                     | 0.44              |
| 1:F:372:THR:HG22 | 1:F:384:ASP:OD2  | 2.18                     | 0.44              |
| 1:C:108:PHE:CE2  | 1:C:154:LEU:HD11 | 2.53                     | 0.44              |
| 1:H:330:THR:O    | 1:H:331:HIS:CD2  | 2.71                     | 0.44              |
| 1:A:355:GLU:OE2  | 1:A:393:ARG:NH2  | 2.51                     | 0.44              |
| 1:E:261:LEU:HA   | 1:E:261:LEU:HD12 | 1.85                     | 0.44              |
| 1:C:187:ASN:CB   | 1:C:188:PRO:HD2  | 2.48                     | 0.44              |
| 1:H:164:LYS:HE2  | 1:H:168:GLU:OE1  | 2.17                     | 0.44              |
| 1:H:372:THR:HG22 | 1:H:384:ASP:OD2  | 2.18                     | 0.44              |
| 1:H:519:LYS:HE2  | 1:H:528:PHE:CE2  | 2.52                     | 0.43              |
| 1:E:399:GLU:HB3  | 1:E:452:LEU:HD21 | 1.98                     | 0.43              |
| 1:E:261:LEU:HD13 | 2:L:20:LEU:HD22  | 1.99                     | 0.43              |
| 1:E:241:ARG:NH2  | 1:F:311:GLY:O    | 2.51                     | 0.43              |
| 1:C:457:ILE:HD11 | 1:C:492:LYS:HE3  | 1.99                     | 0.43              |
| 1:E:437:PRO:O    | 1:E:442:ARG:HD3  | 2.17                     | 0.43              |
| 1:G:394:ILE:HB   | 1:G:399:GLU:HG3  | 2.00                     | 0.43              |
| 1:A:530:ASP:HB3  | 1:A:533:PHE:HB3  | 2.00                     | 0.43              |
| 1:E:414:PHE:HE2  | 1:E:444:LEU:HD11 | 1.84                     | 0.43              |
| 1:E:267:GLU:OE2  | 1:F:247:ARG:NH2  | 2.45                     | 0.43              |
| 1:H:519:LYS:HE2  | 1:H:528:PHE:CZ   | 2.53                     | 0.43              |
| 1:C:263:PHE:CD2  | 1:C:314:ARG:HB3  | 2.53                     | 0.43              |
| 1:B:444:LEU:HA   | 1:B:444:LEU:HD12 | 1.66                     | 0.43              |
| 1:D:254:ILE:HD11 | 1:D:549:MET:HE1  | 2.00                     | 0.43              |
| 1:D:165:SER:HB2  | 1:D:168:GLU:H    | 1.83                     | 0.43              |
| 1:E:286:TYR:OH   | 1:E:291:ASP:HA   | 2.18                     | 0.43              |
| 1:H:375:PRO:HG3  | 1:H:383:TYR:CE2  | 2.53                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:254:ILE:HD11 | 1:B:549:MET:HE1  | 2.01                     | 0.43              |
| 1:D:372:THR:HG22 | 1:D:384:ASP:OD2  | 2.19                     | 0.43              |
| 1:G:349:ASP:OD2  | 1:H:98:LYS:NZ    | 2.48                     | 0.43              |
| 1:G:399:GLU:HB3  | 1:G:452:LEU:HD21 | 2.00                     | 0.43              |
| 1:C:488:LEU:CB   | 1:C:496:CYS:HB2  | 2.48                     | 0.43              |
| 1:G:98:LYS:NZ    | 1:H:349:ASP:OD2  | 2.51                     | 0.43              |
| 1:F:72:ASP:HA    | 1:F:73:PRO:HD3   | 1.80                     | 0.43              |
| 1:A:568:LEU:O    | 1:A:571:PRO:HD3  | 2.19                     | 0.43              |
| 1:C:542:PRO:HB3  | 1:D:181:ILE:HG21 | 2.01                     | 0.42              |
| 1:C:241:ARG:NH1  | 7:C:715:HOH:O    | 2.51                     | 0.42              |
| 1:E:400:LEU:HD12 | 1:E:400:LEU:HA   | 1.82                     | 0.42              |
| 1:B:488:LEU:HD23 | 1:B:488:LEU:HA   | 1.87                     | 0.42              |
| 1:C:332:ASN:CG   | 1:C:333:PRO:HD2  | 2.39                     | 0.42              |
| 1:D:125:THR:HG21 | 1:H:405:GLY:O    | 2.19                     | 0.42              |
| 1:C:254:ILE:HD11 | 1:C:549:MET:CE   | 2.50                     | 0.42              |
| 1:D:243:LYS:HG2  | 1:D:559:THR:HB   | 2.01                     | 0.42              |
| 7:F:760:HOH:O    | 2:L:28:PRO:HD3   | 2.18                     | 0.42              |
| 1:D:72:ASP:HA    | 1:D:73:PRO:HD3   | 1.80                     | 0.42              |
| 1:H:178:ARG:NH1  | 1:H:213:LEU:O    | 2.52                     | 0.42              |
| 1:H:213:LEU:HA   | 1:H:214:PRO:HD3  | 1.89                     | 0.42              |
| 1:D:450:GLU:HG2  | 1:D:451:PHE:CE1  | 2.54                     | 0.42              |
| 2:I:11:GLY:HA3   | 2:I:12:GLY:C     | 2.40                     | 0.42              |
| 1:F:266:ILE:HD13 | 1:F:307:LEU:CD1  | 2.50                     | 0.42              |
| 1:C:394:ILE:HB   | 1:C:399:GLU:HG3  | 2.01                     | 0.42              |
| 1:C:193:LYS:N    | 1:C:193:LYS:HE3  | 2.31                     | 0.42              |
| 2:I:10:HIS:HB2   | 2:I:11:GLY:H     | 1.38                     | 0.42              |
| 1:B:372:THR:HG22 | 1:B:384:ASP:OD2  | 2.19                     | 0.42              |
| 1:C:329:LEU:HD22 | 1:C:329:LEU:HA   | 1.86                     | 0.42              |
| 1:H:135:LYS:HG3  | 1:H:145:TYR:CE2  | 2.54                     | 0.42              |
| 1:F:243:LYS:HG2  | 1:F:559:THR:HB   | 2.01                     | 0.42              |
| 2:J:31:HIS:HA    | 2:J:32:GLY:HA2   | 1.69                     | 0.42              |
| 1:H:347:TYR:CE1  | 1:H:484:GLU:HB3  | 2.55                     | 0.42              |
| 1:C:355:GLU:HA   | 1:C:391:PHE:CE2  | 2.55                     | 0.42              |
| 1:B:420:ARG:NH2  | 1:B:424:ASP:OD1  | 2.53                     | 0.42              |
| 1:H:471:PRO:HG2  | 1:H:527:MET:HE3  | 2.01                     | 0.42              |
| 1:D:232:LEU:HA   | 1:D:232:LEU:HD23 | 1.90                     | 0.42              |
| 4:A:602:APC:O2A  | 4:A:602:APC:O3B  | 2.38                     | 0.42              |
| 1:D:439:THR:OG1  | 1:D:442:ARG:HG3  | 2.20                     | 0.42              |
| 1:F:373:TYR:CD1  | 1:F:491:MET:HG3  | 2.54                     | 0.42              |
| 1:D:122:THR:O    | 1:H:406:MET:SD   | 2.77                     | 0.42              |
| 1:G:488:LEU:CB   | 1:G:496:CYS:HB2  | 2.47                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:437:PRO:O    | 1:C:442:ARG:HD3  | 2.20                     | 0.41              |
| 1:E:220:LEU:HD13 | 1:E:226:ARG:HG2  | 2.01                     | 0.41              |
| 1:A:569:LEU:HD13 | 1:B:307:LEU:HD11 | 2.02                     | 0.41              |
| 1:D:127:LYS:HA   | 1:D:184:VAL:O    | 2.20                     | 0.41              |
| 1:B:72:ASP:HA    | 1:B:73:PRO:HD3   | 1.81                     | 0.41              |
| 1:C:253:TYR:HA   | 2:K:15:PRO:HB2   | 2.02                     | 0.41              |
| 1:E:488:LEU:CB   | 1:E:496:CYS:HB2  | 2.50                     | 0.41              |
| 1:F:148:ARG:HD3  | 1:F:153:LYS:HB3  | 2.02                     | 0.41              |
| 1:G:72:ASP:HA    | 1:G:73:PRO:HD3   | 1.88                     | 0.41              |
| 1:H:408:LEU:HA   | 1:H:408:LEU:HD23 | 1.95                     | 0.41              |
| 1:A:484:GLU:HB2  | 1:A:500:THR:HB   | 2.03                     | 0.41              |
| 1:A:108:PHE:CE2  | 1:A:154:LEU:HD11 | 2.56                     | 0.41              |
| 1:H:243:LYS:HG2  | 1:H:559:THR:HB   | 2.02                     | 0.41              |
| 1:E:300:PRO:HD3  | 1:E:321:GLN:NE2  | 2.35                     | 0.41              |
| 1:C:72:ASP:HA    | 1:C:73:PRO:HD3   | 1.88                     | 0.41              |
| 1:H:423:LEU:HD13 | 1:H:444:LEU:HD13 | 2.03                     | 0.41              |
| 1:E:266:ILE:HD13 | 1:E:307:LEU:HD12 | 2.03                     | 0.41              |
| 1:G:355:GLU:HA   | 1:G:391:PHE:CE2  | 2.55                     | 0.41              |
| 4:E:602:APC:O2A  | 4:E:602:APC:O3B  | 2.39                     | 0.41              |
| 1:D:308:VAL:HA   | 1:D:312:ILE:O    | 2.21                     | 0.41              |
| 1:F:100:HIS:HB2  | 7:F:738:HOH:O    | 2.21                     | 0.41              |
| 1:H:373:TYR:CD1  | 1:H:491:MET:HG3  | 2.56                     | 0.41              |
| 1:E:257:PHE:HA   | 2:L:16:LEU:CB    | 2.51                     | 0.41              |
| 2:L:15:PRO:O     | 2:L:16:LEU:CB    | 2.69                     | 0.41              |
| 1:D:309:VAL:HG22 | 1:D:541:LEU:HA   | 2.03                     | 0.41              |
| 1:C:539:TYR:CE1  | 1:D:232:LEU:HD21 | 2.55                     | 0.41              |
| 1:G:127:LYS:HA   | 1:G:184:VAL:O    | 2.21                     | 0.41              |
| 1:H:199:ILE:HA   | 1:H:200:PRO:HD3  | 1.74                     | 0.41              |
| 1:G:286:TYR:OH   | 1:G:291:ASP:HA   | 2.21                     | 0.41              |
| 4:C:602:APC:O2A  | 4:C:602:APC:O3B  | 2.38                     | 0.41              |
| 1:A:414:PHE:HE2  | 1:A:444:LEU:HD11 | 1.85                     | 0.41              |
| 1:A:300:PRO:HG3  | 7:A:711:HOH:O    | 2.19                     | 0.41              |
| 1:D:266:ILE:HD13 | 1:D:307:LEU:CD1  | 2.51                     | 0.41              |
| 1:F:199:ILE:HA   | 1:F:200:PRO:HD3  | 1.81                     | 0.41              |
| 1:A:404:LEU:HB3  | 1:A:406:MET:HG2  | 2.02                     | 0.41              |
| 1:E:530:ASP:HB3  | 1:E:533:PHE:HB3  | 2.02                     | 0.41              |
| 1:C:414:PHE:HE2  | 1:C:444:LEU:HD11 | 1.86                     | 0.40              |
| 1:G:569:LEU:HD13 | 1:H:307:LEU:HD11 | 2.03                     | 0.40              |
| 1:G:332:ASN:CG   | 1:G:333:PRO:HD2  | 2.42                     | 0.40              |
| 1:F:439:THR:OG1  | 1:F:442:ARG:HG3  | 2.21                     | 0.40              |
| 1:H:164:LYS:HB2  | 1:H:164:LYS:HE3  | 1.90                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:444:LEU:HD12 | 1:F:444:LEU:HA   | 1.69                     | 0.40              |
| 1:E:332:ASN:CG   | 1:E:333:PRO:HD2  | 2.41                     | 0.40              |
| 1:C:193:LYS:H    | 1:C:193:LYS:CE   | 2.30                     | 0.40              |
| 1:A:377:GLY:HA2  | 1:A:378:PRO:HD3  | 1.83                     | 0.40              |
| 1:D:80:ARG:NH1   | 1:D:180:ASP:OD1  | 2.55                     | 0.40              |
| 2:L:20:LEU:HD23  | 2:L:20:LEU:HA    | 1.97                     | 0.40              |
| 1:F:178:ARG:NH1  | 1:F:213:LEU:O    | 2.55                     | 0.40              |
| 1:G:509:ARG:NH2  | 1:G:538:GLU:OE2  | 2.52                     | 0.40              |
| 1:H:266:ILE:HD11 | 1:H:304:HIS:CE1  | 2.57                     | 0.40              |
| 1:G:479:LYS:HD3  | 1:G:482:LEU:HD12 | 2.04                     | 0.40              |
| 1:E:232:LEU:HD23 | 1:E:232:LEU:HA   | 1.92                     | 0.40              |
| 1:A:355:GLU:HA   | 1:A:391:PHE:CE2  | 2.56                     | 0.40              |
| 1:B:266:ILE:HD13 | 1:B:307:LEU:CD1  | 2.51                     | 0.40              |
| 1:H:172:ILE:HD12 | 1:H:172:ILE:HA   | 1.90                     | 0.40              |
| 2:K:13:GLY:HA2   | 2:K:14:ALA:HA    | 1.67                     | 0.40              |
| 1:H:133:HIS:CD2  | 1:H:148:ARG:HG3  | 2.57                     | 0.40              |
| 1:A:437:PRO:O    | 1:A:442:ARG:HD3  | 2.22                     | 0.40              |
| 1:C:432:VAL:HG22 | 1:C:450:GLU:HG3  | 2.02                     | 0.40              |
| 1:F:512:PHE:HA   | 1:F:512:PHE:HD2  | 1.78                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 497/513 (97%) | 477 (96%) | 20 (4%) | 0        | 100         | 100 |
| 1   | B     | 504/513 (98%) | 495 (98%) | 9 (2%)  | 0        | 100         | 100 |
| 1   | C     | 497/513 (97%) | 479 (96%) | 18 (4%) | 0        | 100         | 100 |
| 1   | D     | 503/513 (98%) | 493 (98%) | 10 (2%) | 0        | 100         | 100 |
| 1   | E     | 496/513 (97%) | 478 (96%) | 18 (4%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | F     | 503/513 (98%)   | 495 (98%)  | 8 (2%)   | 0        | 100         | 100 |
| 1   | G     | 497/513 (97%)   | 477 (96%)  | 20 (4%)  | 0        | 100         | 100 |
| 1   | H     | 503/513 (98%)   | 493 (98%)  | 10 (2%)  | 0        | 100         | 100 |
| 2   | I     | 29/54 (54%)     | 25 (86%)   | 4 (14%)  | 0        | 100         | 100 |
| 2   | J     | 29/54 (54%)     | 24 (83%)   | 5 (17%)  | 0        | 100         | 100 |
| 2   | K     | 29/54 (54%)     | 23 (79%)   | 6 (21%)  | 0        | 100         | 100 |
| 2   | L     | 29/54 (54%)     | 26 (90%)   | 3 (10%)  | 0        | 100         | 100 |
| All | All   | 4116/4320 (95%) | 3985 (97%) | 131 (3%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 409/455 (90%)   | 376 (92%)  | 33 (8%)  | 15          | 37 |
| 1   | B     | 435/455 (96%)   | 411 (94%)  | 24 (6%)  | 27          | 58 |
| 1   | C     | 425/455 (93%)   | 390 (92%)  | 35 (8%)  | 14          | 37 |
| 1   | D     | 430/455 (94%)   | 405 (94%)  | 25 (6%)  | 25          | 55 |
| 1   | E     | 422/455 (93%)   | 391 (93%)  | 31 (7%)  | 17          | 43 |
| 1   | F     | 430/455 (94%)   | 404 (94%)  | 26 (6%)  | 24          | 54 |
| 1   | G     | 410/455 (90%)   | 378 (92%)  | 32 (8%)  | 16          | 39 |
| 1   | H     | 436/455 (96%)   | 410 (94%)  | 26 (6%)  | 24          | 54 |
| 2   | I     | 21/44 (48%)     | 18 (86%)   | 3 (14%)  | 4           | 11 |
| 2   | J     | 22/44 (50%)     | 19 (86%)   | 3 (14%)  | 5           | 13 |
| 2   | K     | 21/44 (48%)     | 20 (95%)   | 1 (5%)   | 31          | 64 |
| 2   | L     | 23/44 (52%)     | 20 (87%)   | 3 (13%)  | 5           | 14 |
| All | All   | 3484/3816 (91%) | 3242 (93%) | 242 (7%) | 19          | 46 |

All (242) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 71  | VAL  |
| 1   | A     | 74  | ASN  |
| 1   | A     | 80  | ARG  |
| 1   | A     | 122 | THR  |
| 1   | A     | 136 | ARG  |
| 1   | A     | 138 | SER  |
| 1   | A     | 154 | LEU  |
| 1   | A     | 165 | SER  |
| 1   | A     | 172 | ILE  |
| 1   | A     | 178 | ARG  |
| 1   | A     | 212 | MET  |
| 1   | A     | 220 | LEU  |
| 1   | A     | 224 | GLU  |
| 1   | A     | 240 | VAL  |
| 1   | A     | 261 | LEU  |
| 1   | A     | 271 | MET  |
| 1   | A     | 272 | ASN  |
| 1   | A     | 328 | ASP  |
| 1   | A     | 329 | LEU  |
| 1   | A     | 347 | TYR  |
| 1   | A     | 356 | LYS  |
| 1   | A     | 365 | ILE  |
| 1   | A     | 376 | ASP  |
| 1   | A     | 384 | ASP  |
| 1   | A     | 392 | ARG  |
| 1   | A     | 404 | LEU  |
| 1   | A     | 417 | GLU  |
| 1   | A     | 444 | LEU  |
| 1   | A     | 468 | ILE  |
| 1   | A     | 478 | SER  |
| 1   | A     | 488 | LEU  |
| 1   | A     | 519 | LYS  |
| 1   | A     | 530 | ASP  |
| 1   | B     | 75  | GLN  |
| 1   | B     | 80  | ARG  |
| 1   | B     | 82  | GLN  |
| 1   | B     | 110 | GLN  |
| 1   | B     | 133 | HIS  |
| 1   | B     | 147 | LEU  |
| 1   | B     | 152 | VAL  |
| 1   | B     | 175 | LYS  |
| 1   | B     | 178 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 207 | SER  |
| 1   | B     | 220 | LEU  |
| 1   | B     | 271 | MET  |
| 1   | B     | 272 | ASN  |
| 1   | B     | 274 | ILE  |
| 1   | B     | 279 | VAL  |
| 1   | B     | 287 | HIS  |
| 1   | B     | 347 | TYR  |
| 1   | B     | 364 | HIS  |
| 1   | B     | 404 | LEU  |
| 1   | B     | 415 | GLU  |
| 1   | B     | 420 | ARG  |
| 1   | B     | 488 | LEU  |
| 1   | B     | 524 | ASP  |
| 1   | B     | 552 | ASP  |
| 1   | C     | 74  | ASN  |
| 1   | C     | 80  | ARG  |
| 1   | C     | 122 | THR  |
| 1   | C     | 136 | ARG  |
| 1   | C     | 138 | SER  |
| 1   | C     | 141 | LYS  |
| 1   | C     | 154 | LEU  |
| 1   | C     | 165 | SER  |
| 1   | C     | 168 | GLU  |
| 1   | C     | 172 | ILE  |
| 1   | C     | 178 | ARG  |
| 1   | C     | 187 | ASN  |
| 1   | C     | 193 | LYS  |
| 1   | C     | 212 | MET  |
| 1   | C     | 220 | LEU  |
| 1   | C     | 224 | GLU  |
| 1   | C     | 240 | VAL  |
| 1   | C     | 261 | LEU  |
| 1   | C     | 271 | MET  |
| 1   | C     | 272 | ASN  |
| 1   | C     | 279 | VAL  |
| 1   | C     | 328 | ASP  |
| 1   | C     | 329 | LEU  |
| 1   | C     | 347 | TYR  |
| 1   | C     | 352 | GLU  |
| 1   | C     | 364 | HIS  |
| 1   | C     | 365 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 376 | ASP  |
| 1   | C     | 384 | ASP  |
| 1   | C     | 404 | LEU  |
| 1   | C     | 421 | LYS  |
| 1   | C     | 468 | ILE  |
| 1   | C     | 488 | LEU  |
| 1   | C     | 530 | ASP  |
| 1   | C     | 549 | MET  |
| 1   | D     | 75  | GLN  |
| 1   | D     | 80  | ARG  |
| 1   | D     | 82  | GLN  |
| 1   | D     | 110 | GLN  |
| 1   | D     | 133 | HIS  |
| 1   | D     | 138 | SER  |
| 1   | D     | 147 | LEU  |
| 1   | D     | 152 | VAL  |
| 1   | D     | 175 | LYS  |
| 1   | D     | 178 | ARG  |
| 1   | D     | 207 | SER  |
| 1   | D     | 220 | LEU  |
| 1   | D     | 271 | MET  |
| 1   | D     | 272 | ASN  |
| 1   | D     | 274 | ILE  |
| 1   | D     | 279 | VAL  |
| 1   | D     | 320 | ARG  |
| 1   | D     | 347 | TYR  |
| 1   | D     | 404 | LEU  |
| 1   | D     | 415 | GLU  |
| 1   | D     | 420 | ARG  |
| 1   | D     | 488 | LEU  |
| 1   | D     | 512 | PHE  |
| 1   | D     | 527 | MET  |
| 1   | D     | 552 | ASP  |
| 1   | E     | 74  | ASN  |
| 1   | E     | 75  | GLN  |
| 1   | E     | 80  | ARG  |
| 1   | E     | 82  | GLN  |
| 1   | E     | 111 | LYS  |
| 1   | E     | 122 | THR  |
| 1   | E     | 136 | ARG  |
| 1   | E     | 138 | SER  |
| 1   | E     | 154 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 165 | SER  |
| 1   | E     | 172 | ILE  |
| 1   | E     | 187 | ASN  |
| 1   | E     | 212 | MET  |
| 1   | E     | 220 | LEU  |
| 1   | E     | 224 | GLU  |
| 1   | E     | 240 | VAL  |
| 1   | E     | 261 | LEU  |
| 1   | E     | 271 | MET  |
| 1   | E     | 272 | ASN  |
| 1   | E     | 327 | ILE  |
| 1   | E     | 328 | ASP  |
| 1   | E     | 347 | TYR  |
| 1   | E     | 352 | GLU  |
| 1   | E     | 365 | ILE  |
| 1   | E     | 376 | ASP  |
| 1   | E     | 379 | GLU  |
| 1   | E     | 393 | ARG  |
| 1   | E     | 404 | LEU  |
| 1   | E     | 468 | ILE  |
| 1   | E     | 488 | LEU  |
| 1   | E     | 530 | ASP  |
| 1   | F     | 75  | GLN  |
| 1   | F     | 80  | ARG  |
| 1   | F     | 82  | GLN  |
| 1   | F     | 110 | GLN  |
| 1   | F     | 133 | HIS  |
| 1   | F     | 147 | LEU  |
| 1   | F     | 152 | VAL  |
| 1   | F     | 175 | LYS  |
| 1   | F     | 207 | SER  |
| 1   | F     | 220 | LEU  |
| 1   | F     | 271 | MET  |
| 1   | F     | 272 | ASN  |
| 1   | F     | 274 | ILE  |
| 1   | F     | 279 | VAL  |
| 1   | F     | 330 | THR  |
| 1   | F     | 347 | TYR  |
| 1   | F     | 363 | LYS  |
| 1   | F     | 404 | LEU  |
| 1   | F     | 415 | GLU  |
| 1   | F     | 488 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 512 | PHE  |
| 1   | F     | 524 | ASP  |
| 1   | F     | 527 | MET  |
| 1   | F     | 549 | MET  |
| 1   | F     | 552 | ASP  |
| 1   | F     | 574 | LYS  |
| 1   | G     | 74  | ASN  |
| 1   | G     | 80  | ARG  |
| 1   | G     | 122 | THR  |
| 1   | G     | 136 | ARG  |
| 1   | G     | 138 | SER  |
| 1   | G     | 154 | LEU  |
| 1   | G     | 165 | SER  |
| 1   | G     | 172 | ILE  |
| 1   | G     | 212 | MET  |
| 1   | G     | 220 | LEU  |
| 1   | G     | 224 | GLU  |
| 1   | G     | 240 | VAL  |
| 1   | G     | 261 | LEU  |
| 1   | G     | 271 | MET  |
| 1   | G     | 272 | ASN  |
| 1   | G     | 321 | GLN  |
| 1   | G     | 347 | TYR  |
| 1   | G     | 352 | GLU  |
| 1   | G     | 365 | ILE  |
| 1   | G     | 376 | ASP  |
| 1   | G     | 384 | ASP  |
| 1   | G     | 392 | ARG  |
| 1   | G     | 393 | ARG  |
| 1   | G     | 404 | LEU  |
| 1   | G     | 407 | LYS  |
| 1   | G     | 417 | GLU  |
| 1   | G     | 427 | CYS  |
| 1   | G     | 444 | LEU  |
| 1   | G     | 468 | ILE  |
| 1   | G     | 488 | LEU  |
| 1   | G     | 530 | ASP  |
| 1   | G     | 549 | MET  |
| 1   | H     | 71  | VAL  |
| 1   | H     | 75  | GLN  |
| 1   | H     | 80  | ARG  |
| 1   | H     | 82  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 110 | GLN  |
| 1   | H     | 133 | HIS  |
| 1   | H     | 142 | LEU  |
| 1   | H     | 147 | LEU  |
| 1   | H     | 152 | VAL  |
| 1   | H     | 175 | LYS  |
| 1   | H     | 207 | SER  |
| 1   | H     | 220 | LEU  |
| 1   | H     | 221 | LYS  |
| 1   | H     | 271 | MET  |
| 1   | H     | 272 | ASN  |
| 1   | H     | 274 | ILE  |
| 1   | H     | 279 | VAL  |
| 1   | H     | 327 | ILE  |
| 1   | H     | 328 | ASP  |
| 1   | H     | 330 | THR  |
| 1   | H     | 347 | TYR  |
| 1   | H     | 363 | LYS  |
| 1   | H     | 404 | LEU  |
| 1   | H     | 488 | LEU  |
| 1   | H     | 524 | ASP  |
| 1   | H     | 552 | ASP  |
| 2   | I     | 5   | GLN  |
| 2   | I     | 20  | LEU  |
| 2   | I     | 30  | VAL  |
| 2   | J     | 5   | GLN  |
| 2   | J     | 20  | LEU  |
| 2   | J     | 30  | VAL  |
| 2   | K     | 5   | GLN  |
| 2   | L     | 5   | GLN  |
| 2   | L     | 10  | HIS  |
| 2   | L     | 18  | VAL  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 364 | HIS  |
| 1   | C     | 116 | GLN  |
| 1   | C     | 287 | HIS  |
| 1   | C     | 364 | HIS  |
| 1   | E     | 120 | HIS  |
| 1   | E     | 187 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 287 | HIS  |
| 1   | G     | 187 | ASN  |
| 1   | G     | 287 | HIS  |
| 1   | H     | 331 | HIS  |
| 2   | I     | 31  | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 12 are monoatomic - leaving 17 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | LYS  | A     | 601 | -    | 6,9,9        | 0.28 | 0           | 4,10,10     | 0.46 | 0           |
| 4   | APC  | A     | 602 | -    | 22,29,33     | 1.52 | 5 (22%)     | 27,45,52    | 2.27 | 3 (11%)     |
| 3   | LYS  | B     | 601 | -    | 6,9,9        | 0.32 | 0           | 4,10,10     | 0.42 | 0           |
| 4   | APC  | B     | 602 | 5    | 25,33,33     | 1.62 | 6 (24%)     | 30,52,52    | 2.12 | 5 (16%)     |
| 3   | LYS  | C     | 601 | -    | 6,9,9        | 0.37 | 0           | 4,10,10     | 0.48 | 0           |
| 4   | APC  | C     | 602 | -    | 22,29,33     | 1.54 | 5 (22%)     | 27,45,52    | 2.32 | 3 (11%)     |
| 3   | LYS  | D     | 601 | -    | 6,9,9        | 0.49 | 0           | 4,10,10     | 0.41 | 0           |
| 4   | APC  | D     | 602 | 5    | 25,33,33     | 1.64 | 6 (24%)     | 30,52,52    | 2.11 | 4 (13%)     |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | LYS  | E     | 601 | -    | 6,9,9        | 0.38 | 0        | 4,10,10     | 0.43 | 0        |
| 4   | APC  | E     | 602 | -    | 22,29,33     | 1.53 | 5 (22%)  | 27,45,52    | 2.32 | 3 (11%)  |
| 3   | LYS  | F     | 601 | -    | 6,9,9        | 0.41 | 0        | 4,10,10     | 0.42 | 0        |
| 4   | APC  | F     | 602 | 5    | 25,33,33     | 1.63 | 5 (20%)  | 30,52,52    | 2.23 | 4 (13%)  |
| 3   | LYS  | G     | 601 | -    | 6,9,9        | 0.34 | 0        | 4,10,10     | 0.51 | 0        |
| 4   | APC  | G     | 602 | -    | 22,29,33     | 1.57 | 5 (22%)  | 27,45,52    | 2.27 | 3 (11%)  |
| 6   | ALA  | H     | 601 | -    | 3,4,5        | 0.84 | 0        | 0,4,6       | 0.00 | -        |
| 3   | LYS  | H     | 602 | -    | 6,9,9        | 0.44 | 0        | 4,10,10     | 0.37 | 0        |
| 4   | APC  | H     | 603 | 5    | 25,33,33     | 1.59 | 6 (24%)  | 30,52,52    | 2.24 | 4 (13%)  |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 3   | LYS  | A     | 601 | -    | -       | 0/5/9/9    | 0/0/0/0 |
| 4   | APC  | A     | 602 | -    | -       | 0/12/32/38 | 0/3/3/3 |
| 3   | LYS  | B     | 601 | -    | -       | 0/5/9/9    | 0/0/0/0 |
| 4   | APC  | B     | 602 | 5    | -       | 0/15/38/38 | 0/3/3/3 |
| 3   | LYS  | C     | 601 | -    | -       | 0/5/9/9    | 0/0/0/0 |
| 4   | APC  | C     | 602 | -    | -       | 0/12/32/38 | 0/3/3/3 |
| 3   | LYS  | D     | 601 | -    | -       | 0/5/9/9    | 0/0/0/0 |
| 4   | APC  | D     | 602 | 5    | -       | 0/15/38/38 | 0/3/3/3 |
| 3   | LYS  | E     | 601 | -    | -       | 0/5/9/9    | 0/0/0/0 |
| 4   | APC  | E     | 602 | -    | -       | 0/12/32/38 | 0/3/3/3 |
| 3   | LYS  | F     | 601 | -    | -       | 0/5/9/9    | 0/0/0/0 |
| 4   | APC  | F     | 602 | 5    | -       | 0/15/38/38 | 0/3/3/3 |
| 3   | LYS  | G     | 601 | -    | -       | 0/5/9/9    | 0/0/0/0 |
| 4   | APC  | G     | 602 | -    | -       | 0/12/32/38 | 0/3/3/3 |
| 6   | ALA  | H     | 601 | -    | -       | 0/0/2/4    | 0/0/0/0 |
| 3   | LYS  | H     | 602 | -    | -       | 0/5/9/9    | 0/0/0/0 |
| 4   | APC  | H     | 603 | 5    | -       | 0/15/38/38 | 0/3/3/3 |

All (43) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 4   | H     | 603 | APC  | PB-O2B | 2.04 | 1.61        | 1.56     |
| 4   | D     | 602 | APC  | PA-O2A | 2.04 | 1.61        | 1.56     |
| 4   | B     | 602 | APC  | PA-O2A | 2.05 | 1.61        | 1.56     |
| 4   | H     | 603 | APC  | PA-O2A | 2.08 | 1.61        | 1.56     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4   | B     | 602 | APC  | PB-O2B  | 2.13 | 1.61        | 1.56     |
| 4   | F     | 602 | APC  | PB-O2B  | 2.14 | 1.61        | 1.56     |
| 4   | A     | 602 | APC  | O4'-C1' | 2.16 | 1.43        | 1.41     |
| 4   | E     | 602 | APC  | O4'-C1' | 2.16 | 1.43        | 1.41     |
| 4   | C     | 602 | APC  | O4'-C1' | 2.23 | 1.44        | 1.41     |
| 4   | D     | 602 | APC  | PB-O2B  | 2.23 | 1.61        | 1.56     |
| 4   | G     | 602 | APC  | O4'-C1' | 2.27 | 1.44        | 1.41     |
| 4   | E     | 602 | APC  | PA-O2A  | 2.31 | 1.61        | 1.56     |
| 4   | A     | 602 | APC  | PA-O2A  | 2.32 | 1.62        | 1.56     |
| 4   | G     | 602 | APC  | PA-O2A  | 2.32 | 1.62        | 1.56     |
| 4   | C     | 602 | APC  | PA-O2A  | 2.34 | 1.62        | 1.56     |
| 4   | B     | 602 | APC  | O4'-C1' | 2.39 | 1.44        | 1.41     |
| 4   | D     | 602 | APC  | O4'-C1' | 2.43 | 1.44        | 1.41     |
| 4   | F     | 602 | APC  | O4'-C1' | 2.53 | 1.44        | 1.41     |
| 4   | H     | 603 | APC  | O4'-C1' | 2.56 | 1.44        | 1.41     |
| 4   | E     | 602 | APC  | PB-O2B  | 2.64 | 1.61        | 1.54     |
| 4   | C     | 602 | APC  | PB-O2B  | 2.71 | 1.61        | 1.54     |
| 4   | A     | 602 | APC  | PB-O2B  | 2.71 | 1.61        | 1.54     |
| 4   | C     | 602 | APC  | PB-O3B  | 2.76 | 1.61        | 1.54     |
| 4   | E     | 602 | APC  | PB-O3B  | 2.89 | 1.61        | 1.54     |
| 4   | G     | 602 | APC  | PB-O2B  | 2.98 | 1.62        | 1.54     |
| 4   | A     | 602 | APC  | PB-O3B  | 3.06 | 1.62        | 1.54     |
| 4   | G     | 602 | APC  | PB-O3B  | 3.09 | 1.62        | 1.54     |
| 4   | H     | 603 | APC  | PG-O1G  | 3.10 | 1.61        | 1.51     |
| 4   | F     | 602 | APC  | PG-O1G  | 3.15 | 1.61        | 1.51     |
| 4   | B     | 602 | APC  | PG-O1G  | 3.16 | 1.61        | 1.51     |
| 4   | H     | 603 | APC  | PB-O3B  | 3.19 | 1.62        | 1.58     |
| 4   | D     | 602 | APC  | PB-O3B  | 3.21 | 1.62        | 1.58     |
| 4   | D     | 602 | APC  | PG-O1G  | 3.22 | 1.61        | 1.51     |
| 4   | F     | 602 | APC  | PB-O3B  | 3.31 | 1.62        | 1.58     |
| 4   | B     | 602 | APC  | PB-O3B  | 3.37 | 1.62        | 1.58     |
| 4   | H     | 603 | APC  | PA-O5'  | 3.64 | 1.61        | 1.57     |
| 4   | B     | 602 | APC  | PA-O5'  | 3.93 | 1.61        | 1.57     |
| 4   | F     | 602 | APC  | PA-O5'  | 3.94 | 1.61        | 1.57     |
| 4   | D     | 602 | APC  | PA-O5'  | 4.06 | 1.61        | 1.57     |
| 4   | A     | 602 | APC  | PA-O5'  | 4.08 | 1.62        | 1.57     |
| 4   | G     | 602 | APC  | PA-O5'  | 4.10 | 1.62        | 1.57     |
| 4   | E     | 602 | APC  | PA-O5'  | 4.14 | 1.62        | 1.57     |
| 4   | C     | 602 | APC  | PA-O5'  | 4.29 | 1.62        | 1.57     |

All (29) bond angle outliers are listed below:



| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 4   | C     | 602 | APC  | N3-C2-N1    | -10.39 | 120.94      | 128.89   |
| 4   | E     | 602 | APC  | N3-C2-N1    | -10.36 | 120.96      | 128.89   |
| 4   | A     | 602 | APC  | N3-C2-N1    | -10.17 | 121.11      | 128.89   |
| 4   | G     | 602 | APC  | N3-C2-N1    | -10.16 | 121.12      | 128.89   |
| 4   | H     | 603 | APC  | N3-C2-N1    | -10.08 | 121.17      | 128.89   |
| 4   | F     | 602 | APC  | N3-C2-N1    | -10.00 | 121.24      | 128.89   |
| 4   | B     | 602 | APC  | N3-C2-N1    | -9.40  | 121.69      | 128.89   |
| 4   | D     | 602 | APC  | N3-C2-N1    | -9.20  | 121.85      | 128.89   |
| 4   | H     | 603 | APC  | PG-O3B-PB   | -3.19  | 121.97      | 132.67   |
| 4   | D     | 602 | APC  | C2'-C1'-N9  | -3.18  | 109.44      | 114.29   |
| 4   | D     | 602 | APC  | PG-O3B-PB   | -3.15  | 122.11      | 132.67   |
| 4   | F     | 602 | APC  | PG-O3B-PB   | -3.12  | 122.20      | 132.67   |
| 4   | B     | 602 | APC  | PG-O3B-PB   | -3.10  | 122.27      | 132.67   |
| 4   | H     | 603 | APC  | C2'-C1'-N9  | -3.07  | 109.59      | 114.29   |
| 4   | F     | 602 | APC  | C2'-C1'-N9  | -3.06  | 109.61      | 114.29   |
| 4   | B     | 602 | APC  | C2'-C1'-N9  | -2.83  | 109.97      | 114.29   |
| 4   | D     | 602 | APC  | C4-C5-N7    | -2.60  | 107.08      | 109.48   |
| 4   | B     | 602 | APC  | C4-C5-N7    | -2.50  | 107.17      | 109.48   |
| 4   | C     | 602 | APC  | C4-C5-N7    | -2.33  | 107.33      | 109.48   |
| 4   | G     | 602 | APC  | O5'-PA-O1A  | -2.23  | 108.05      | 113.98   |
| 4   | F     | 602 | APC  | C4-C5-N7    | -2.21  | 107.45      | 109.48   |
| 4   | E     | 602 | APC  | C4-C5-N7    | -2.20  | 107.46      | 109.48   |
| 4   | E     | 602 | APC  | O5'-PA-O1A  | -2.19  | 108.16      | 113.98   |
| 4   | H     | 603 | APC  | C4-C5-N7    | -2.18  | 107.47      | 109.48   |
| 4   | A     | 602 | APC  | C4-C5-N7    | -2.12  | 107.53      | 109.48   |
| 4   | A     | 602 | APC  | O5'-PA-O1A  | -2.10  | 108.39      | 113.98   |
| 4   | C     | 602 | APC  | O5'-PA-O1A  | -2.08  | 108.45      | 113.98   |
| 4   | G     | 602 | APC  | C4'-O4'-C1' | 2.02   | 111.94      | 109.72   |
| 4   | B     | 602 | APC  | C2'-C3'-C4' | 2.03   | 106.79      | 102.61   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | A     | 602 | APC  | 1       | 0            |
| 4   | C     | 602 | APC  | 1       | 0            |
| 4   | E     | 602 | APC  | 2       | 0            |
| 6   | H     | 601 | ALA  | 1       | 0            |

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 501/513 (97%)   | -0.34  | 0 100 100     | 17, 49, 84, 100       | 0     |
| 1   | B     | 506/513 (98%)   | -0.56  | 0 100 100     | 17, 33, 66, 82        | 0     |
| 1   | C     | 501/513 (97%)   | -0.47  | 3 (0%) 90 87  | 16, 40, 74, 97        | 0     |
| 1   | D     | 505/513 (98%)   | -0.49  | 4 (0%) 87 82  | 16, 34, 70, 112       | 0     |
| 1   | E     | 500/513 (97%)   | -0.50  | 2 (0%) 93 90  | 16, 39, 75, 114       | 0     |
| 1   | F     | 505/513 (98%)   | -0.53  | 2 (0%) 93 90  | 16, 33, 72, 117       | 0     |
| 1   | G     | 501/513 (97%)   | -0.35  | 2 (0%) 93 90  | 19, 49, 83, 108       | 0     |
| 1   | H     | 505/513 (98%)   | -0.46  | 0 100 100     | 18, 33, 65, 91        | 0     |
| 2   | I     | 31/54 (57%)     | 0.56   | 6 (19%) 1 1   | 23, 50, 114, 118      | 0     |
| 2   | J     | 31/54 (57%)     | 0.75   | 6 (19%) 1 1   | 21, 53, 115, 125      | 0     |
| 2   | K     | 31/54 (57%)     | 0.85   | 7 (22%) 1 1   | 21, 53, 113, 118      | 0     |
| 2   | L     | 31/54 (57%)     | 0.95   | 7 (22%) 1 1   | 20, 49, 114, 116      | 0     |
| All | All   | 4148/4320 (96%) | -0.43  | 39 (0%) 85 80 | 16, 37, 79, 125       | 0     |

All (39) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | L     | 12  | GLY  | 8.4  |
| 2   | J     | 14  | ALA  | 8.3  |
| 2   | L     | 13  | GLY  | 8.1  |
| 1   | D     | 524 | ASP  | 6.7  |
| 2   | J     | 12  | GLY  | 6.3  |
| 2   | I     | 14  | ALA  | 6.2  |
| 2   | K     | 18  | VAL  | 6.0  |
| 2   | K     | 14  | ALA  | 6.0  |
| 2   | J     | 18  | VAL  | 5.7  |
| 2   | L     | 18  | VAL  | 5.5  |
| 2   | K     | 13  | GLY  | 5.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | L     | 14  | ALA  | 5.3  |
| 1   | F     | 524 | ASP  | 5.2  |
| 2   | I     | 12  | GLY  | 4.8  |
| 2   | K     | 15  | PRO  | 4.6  |
| 1   | D     | 522 | GLY  | 4.5  |
| 2   | J     | 15  | PRO  | 4.4  |
| 2   | I     | 13  | GLY  | 4.0  |
| 2   | L     | 15  | PRO  | 3.9  |
| 2   | K     | 12  | GLY  | 3.5  |
| 1   | E     | 524 | ASP  | 3.2  |
| 2   | J     | 13  | GLY  | 3.2  |
| 2   | J     | 17  | ARG  | 3.2  |
| 2   | K     | 20  | LEU  | 3.1  |
| 1   | C     | 524 | ASP  | 3.0  |
| 1   | F     | 522 | GLY  | 2.9  |
| 2   | L     | 17  | ARG  | 2.9  |
| 2   | K     | 19  | GLU  | 2.8  |
| 2   | I     | 18  | VAL  | 2.6  |
| 1   | C     | 526 | ALA  | 2.5  |
| 2   | I     | 15  | PRO  | 2.5  |
| 2   | I     | 17  | ARG  | 2.4  |
| 2   | L     | 16  | LEU  | 2.4  |
| 1   | G     | 405 | GLY  | 2.4  |
| 1   | C     | 522 | GLY  | 2.2  |
| 1   | D     | 528 | PHE  | 2.2  |
| 1   | E     | 528 | PHE  | 2.1  |
| 1   | D     | 520 | ALA  | 2.1  |
| 1   | G     | 426 | ILE  | 2.0  |

## 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 4   | APC  | A     | 602 | 27/31 | 0.80 | 0.42 | 7.24  | 73,101,138,154             | 0     |
| 4   | APC  | G     | 602 | 27/31 | 0.75 | 0.41 | 6.05  | 83,111,142,148             | 0     |
| 4   | APC  | B     | 602 | 31/31 | 0.81 | 0.28 | 4.81  | 57,101,132,156             | 0     |
| 4   | APC  | H     | 603 | 31/31 | 0.80 | 0.29 | 4.34  | 56,105,139,158             | 0     |
| 4   | APC  | E     | 602 | 27/31 | 0.80 | 0.28 | 3.91  | 74,99,127,160              | 0     |
| 4   | APC  | F     | 602 | 31/31 | 0.79 | 0.28 | 2.79  | 61,107,145,155             | 0     |
| 4   | APC  | C     | 602 | 27/31 | 0.78 | 0.34 | 2.77  | 72,101,131,155             | 0     |
| 4   | APC  | D     | 602 | 31/31 | 0.81 | 0.27 | 2.16  | 60,108,149,152             | 0     |
| 3   | LYS  | C     | 601 | 10/10 | 0.96 | 0.20 | 1.14  | 15,19,42,44                | 0     |
| 3   | LYS  | A     | 601 | 10/10 | 0.97 | 0.19 | 0.96  | 16,24,46,61                | 0     |
| 3   | LYS  | G     | 601 | 10/10 | 0.95 | 0.17 | 0.53  | 17,33,43,52                | 0     |
| 3   | LYS  | H     | 602 | 10/10 | 0.97 | 0.16 | 0.52  | 18,22,30,32                | 0     |
| 3   | LYS  | B     | 601 | 10/10 | 0.97 | 0.15 | 0.50  | 15,24,32,35                | 0     |
| 3   | LYS  | D     | 601 | 10/10 | 0.96 | 0.15 | 0.19  | 15,31,36,38                | 0     |
| 3   | LYS  | F     | 601 | 10/10 | 0.96 | 0.15 | -0.31 | 17,30,36,39                | 0     |
| 3   | LYS  | E     | 601 | 10/10 | 0.97 | 0.14 | -0.81 | 15,22,45,49                | 0     |
| 5   | MG   | D     | 603 | 1/1   | 0.76 | 0.12 | -     | 68,68,68,68                | 0     |
| 5   | MG   | F     | 604 | 1/1   | 0.96 | 0.21 | -     | 12,12,12,12                | 0     |
| 5   | MG   | H     | 604 | 1/1   | 0.77 | 0.09 | -     | 66,66,66,66                | 0     |
| 5   | MG   | C     | 603 | 1/1   | 0.94 | 0.15 | -     | 59,59,59,59                | 0     |
| 5   | MG   | H     | 605 | 1/1   | 0.93 | 0.26 | -     | 13,13,13,13                | 0     |
| 5   | MG   | E     | 603 | 1/1   | 0.95 | 0.09 | -     | 53,53,53,53                | 0     |
| 5   | MG   | L     | 101 | 1/1   | 0.96 | 0.30 | -     | 20,20,20,20                | 0     |
| 5   | MG   | B     | 603 | 1/1   | 0.77 | 0.17 | -     | 63,63,63,63                | 0     |
| 6   | ALA  | H     | 601 | 5/6   | 0.73 | 0.20 | -     | 69,76,79,80                | 0     |
| 5   | MG   | J     | 101 | 1/1   | 0.84 | 0.27 | -     | 21,21,21,21                | 0     |
| 5   | MG   | F     | 603 | 1/1   | 0.72 | 0.09 | -     | 59,59,59,59                | 0     |
| 5   | MG   | A     | 603 | 1/1   | 0.89 | 0.09 | -     | 53,53,53,53                | 0     |
| 5   | MG   | G     | 603 | 1/1   | 0.93 | 0.12 | -     | 55,55,55,55                | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.