



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:35 AM UTC

PDB ID : 4MEX / pdb\_00004mex  
Title : Crystal structure of Escherichia coli RNA polymerase in complex with salinamide A  
Authors : Feng, Y.; Zhang, Y.; Arnold, E.; Ebright, R.H.  
Deposited on : 2013-08-27  
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

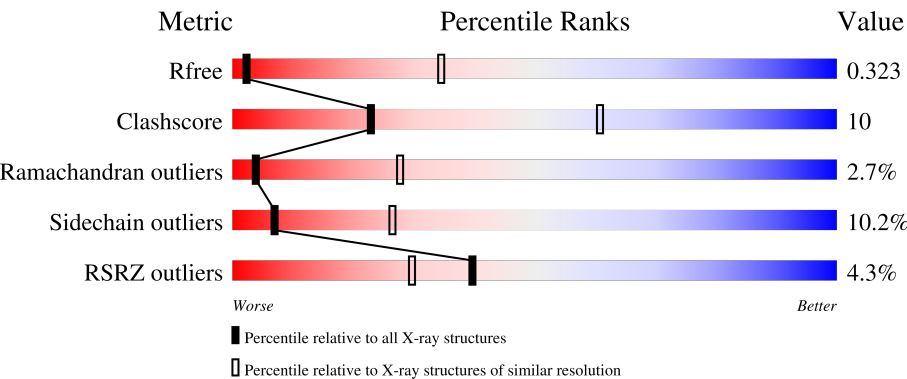
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.90 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1270 (4.10-3.70)                                      |
| Clashscore            | 190562                      | 1034 (4.08-3.72)                                      |
| Ramachandran outliers | 187476                      | 1251 (4.10-3.70)                                      |
| Sidechain outliers    | 187428                      | 1243 (4.10-3.70)                                      |
| RSRZ outliers         | 180081                      | 1269 (4.10-3.70)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                                       |
|-----|-------|--------|--------------------------------------------------------------------------------------------------------|
| 1   | A     | 335    | <div><div>5%</div><div><div></div><div>64%</div><div>20%</div><div>• •</div><div>11%</div></div></div> |
| 1   | B     | 335    | <div><div>7%</div><div><div></div><div>55%</div><div>26%</div><div>5%</div><div>14%</div></div></div>  |
| 1   | G     | 335    | <div><div>3%</div><div><div></div><div>43%</div><div>19%</div><div>•</div><div>36%</div></div></div>   |
| 1   | H     | 335    | <div><div>3%</div><div><div></div><div>45%</div><div>16%</div><div>•</div><div>36%</div></div></div>   |
| 2   | C     | 1342   | <div><div>4%</div><div><div></div><div>80%</div><div>18%</div><div>•</div></div></div>                 |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | I     | 1342   |                  |
| 3   | D     | 1407   |                  |
| 3   | J     | 1407   |                  |
| 4   | E     | 91     |                  |
| 4   | K     | 91     |                  |
| 5   | F     | 613    |                  |
| 5   | L     | 613    |                  |
| 6   | M     | 9      |                  |
| 6   | N     | 9      |                  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 6   | D4P  | M     | 4   | -         | -        | X       | -                |
| 6   | MEA  | M     | 5   | -         | -        | X       | -                |
| 6   | 2TL  | M     | 6   | -         | -        | X       | -                |
| 6   | D4P  | N     | 4   | -         | -        | X       | -                |
| 6   | MEA  | N     | 5   | -         | -        | X       | -                |
| 6   | 2TL  | N     | 6   | -         | -        | X       | -                |

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 50018 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 DNA-directed RNA polymerase subunit alpha.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 298      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2236  | 1405 | 391 | 432 | 8 |         |         |       |
| 1   | B     | 287      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2160  | 1359 | 374 | 419 | 8 |         |         |       |
| 1   | G     | 216      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1618  | 1013 | 282 | 317 | 6 |         |         |       |
| 1   | H     | 215      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1605  | 1005 | 278 | 316 | 6 |         |         |       |

There are 24 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -4      | HIS      | -      | expression tag | UNP P0A7Z4 |
| A     | -3      | HIS      | -      | expression tag | UNP P0A7Z4 |
| A     | -2      | HIS      | -      | expression tag | UNP P0A7Z4 |
| A     | -1      | HIS      | -      | expression tag | UNP P0A7Z4 |
| A     | 0       | HIS      | -      | expression tag | UNP P0A7Z4 |
| A     | 1       | HIS      | -      | expression tag | UNP P0A7Z4 |
| B     | -4      | HIS      | -      | expression tag | UNP P0A7Z4 |
| B     | -3      | HIS      | -      | expression tag | UNP P0A7Z4 |
| B     | -2      | HIS      | -      | expression tag | UNP P0A7Z4 |
| B     | -1      | HIS      | -      | expression tag | UNP P0A7Z4 |
| B     | 0       | HIS      | -      | expression tag | UNP P0A7Z4 |
| B     | 1       | HIS      | -      | expression tag | UNP P0A7Z4 |
| G     | -4      | HIS      | -      | expression tag | UNP P0A7Z4 |
| G     | -3      | HIS      | -      | expression tag | UNP P0A7Z4 |
| G     | -2      | HIS      | -      | expression tag | UNP P0A7Z4 |
| G     | -1      | HIS      | -      | expression tag | UNP P0A7Z4 |
| G     | 0       | HIS      | -      | expression tag | UNP P0A7Z4 |
| G     | 1       | HIS      | -      | expression tag | UNP P0A7Z4 |
| H     | -4      | HIS      | -      | expression tag | UNP P0A7Z4 |
| H     | -3      | HIS      | -      | expression tag | UNP P0A7Z4 |
| H     | -2      | HIS      | -      | expression tag | UNP P0A7Z4 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| H     | -1      | HIS      | -      | expression tag | UNP P0A7Z4 |
| H     | 0       | HIS      | -      | expression tag | UNP P0A7Z4 |
| H     | 1       | HIS      | -      | expression tag | UNP P0A7Z4 |

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2   | C     | 1340     | Total | C    | N    | O    | S  | 3       | 0       | 0     |
|     |       |          | 9522  | 5999 | 1675 | 1829 | 19 |         |         |       |
| 2   | I     | 1340     | Total | C    | N    | O    | S  | 3       | 0       | 0     |
|     |       |          | 9544  | 6013 | 1676 | 1835 | 20 |         |         |       |

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 3   | D     | 1150     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 7572  | 4771 | 1358 | 1415 | 28 |         |         |       |
| 3   | J     | 1143     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 7535  | 4748 | 1351 | 1408 | 28 |         |         |       |

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 4   | E     | 89       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 482   | 299 | 93 | 90 |         |         |       |
| 4   | K     | 75       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 408   | 253 | 79 | 76 |         |         |       |

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 5   | F     | 464      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3592  | 2253 | 643 | 682 | 14 |         |         |       |
| 5   | L     | 464      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3592  | 2253 | 643 | 682 | 14 |         |         |       |

- Molecule 6 is a protein called Salinamide A.

| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 6   | M     | 9        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 73    | 51 | 7 | 15 |         |         |       |

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| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 6   | N     | 9        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 73    | 51 | 7 | 15 |         |         |       |

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 7   | D     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | J     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

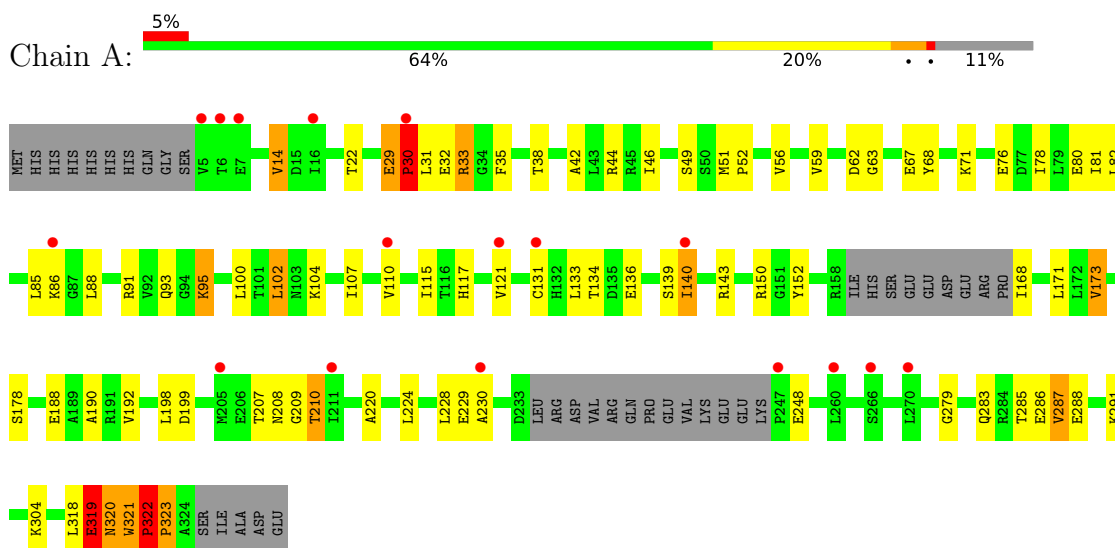
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 8   | D     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 8   | J     | 2        | Total | Zn | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

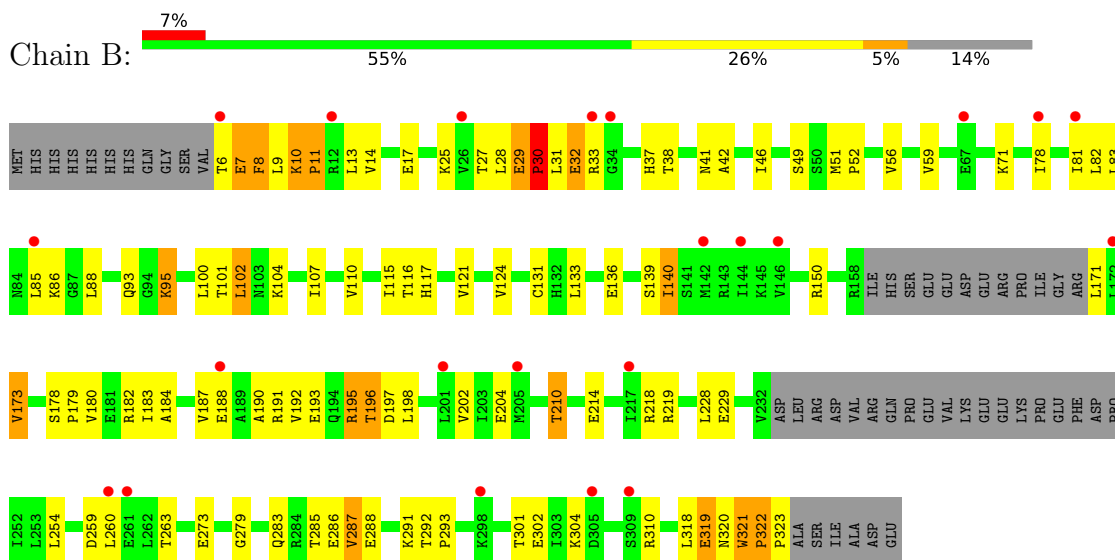
### 3 Residue-property plots [i](#)

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

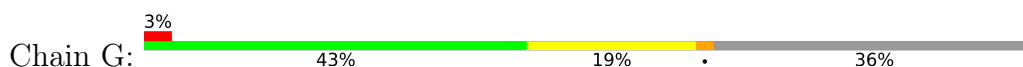
- Molecule 1: DNA-directed RNA polymerase subunit alpha

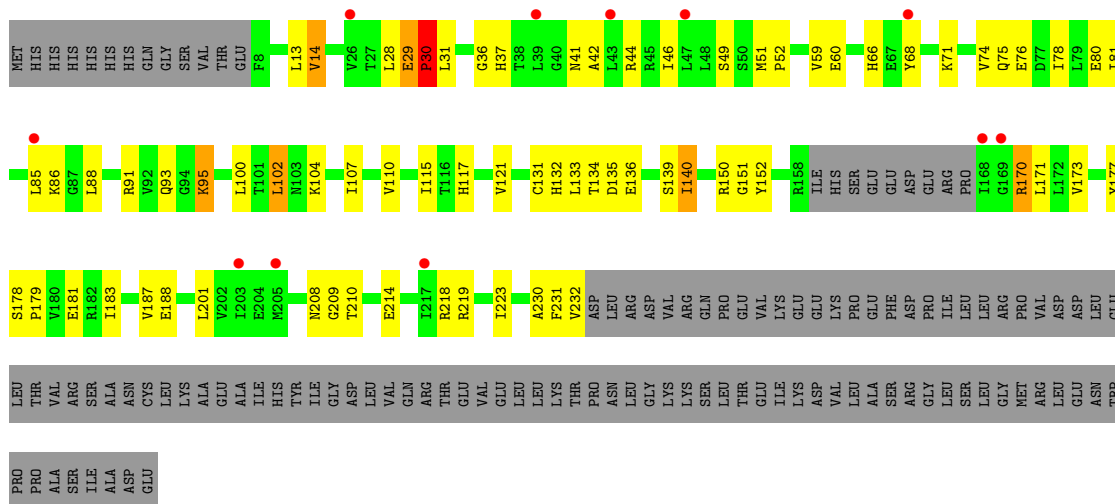


- Molecule 1: DNA-directed RNA polymerase subunit alpha

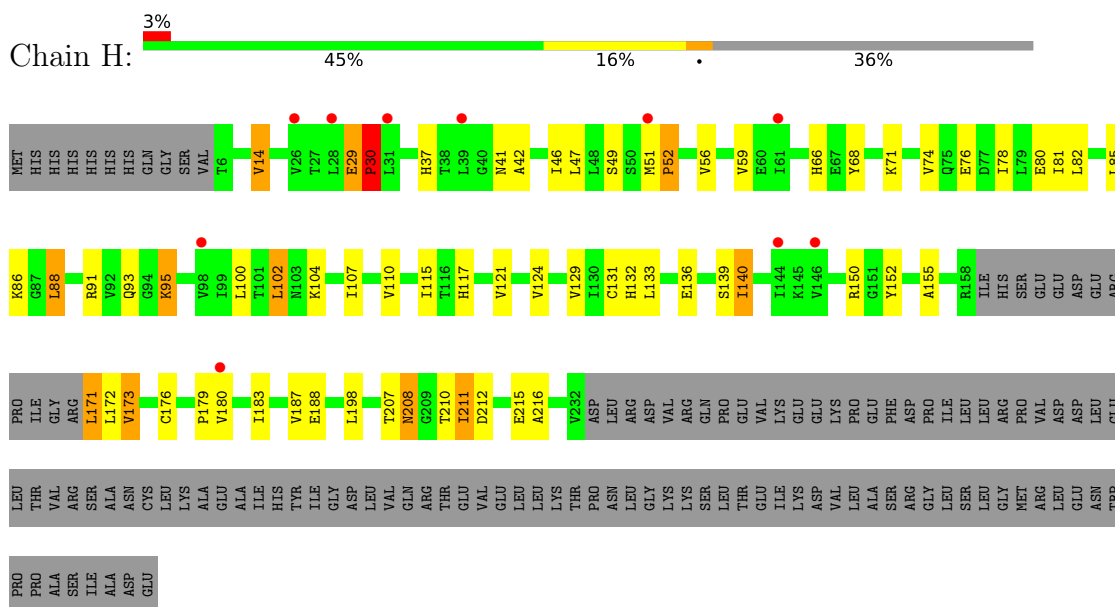


- Molecule 1: DNA-directed RNA polymerase subunit alpha

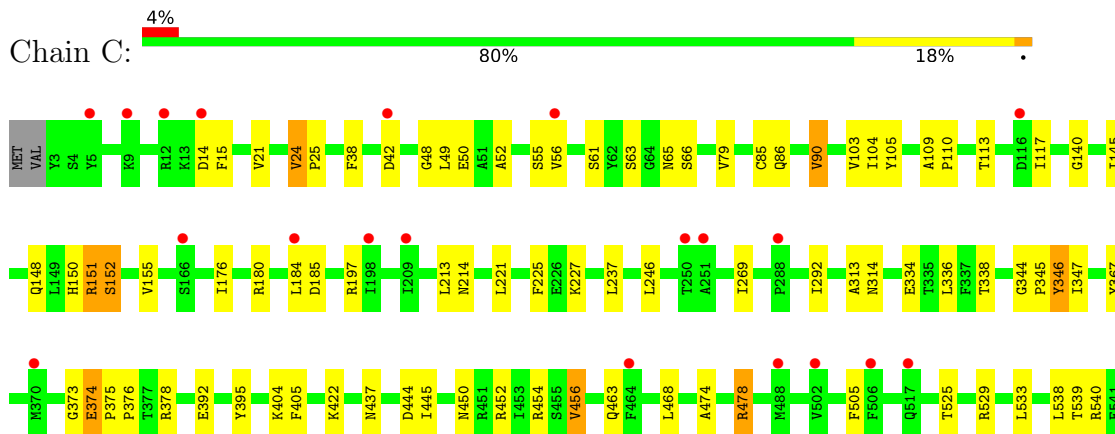




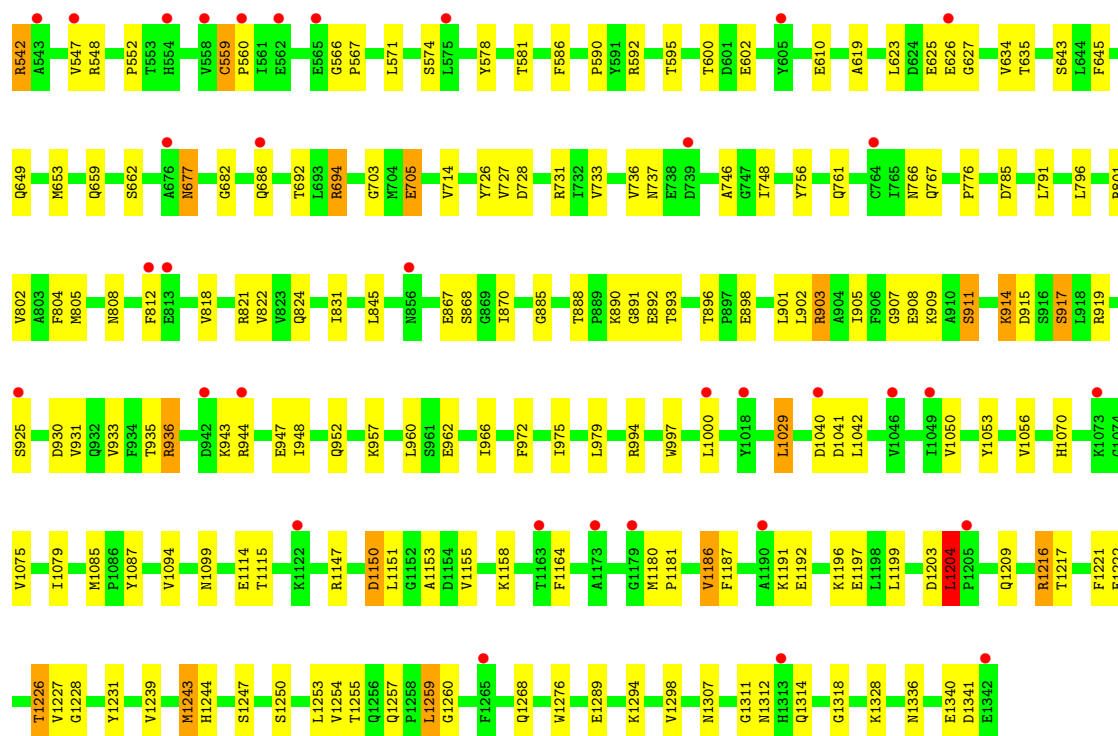
- Molecule 1: DNA-directed RNA polymerase subunit alpha



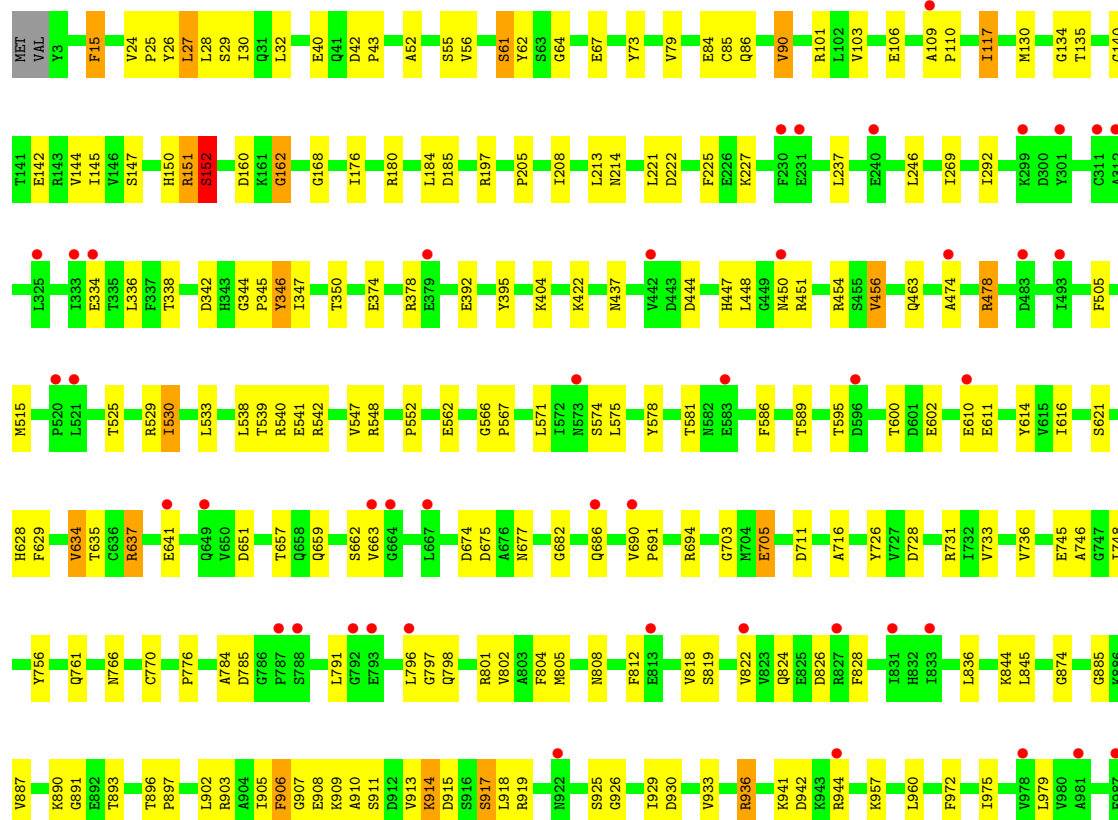
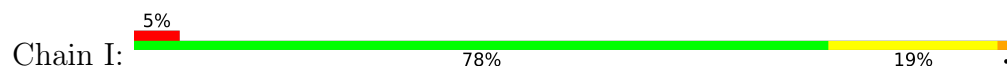
- Molecule 2: DNA-directed RNA polymerase subunit beta

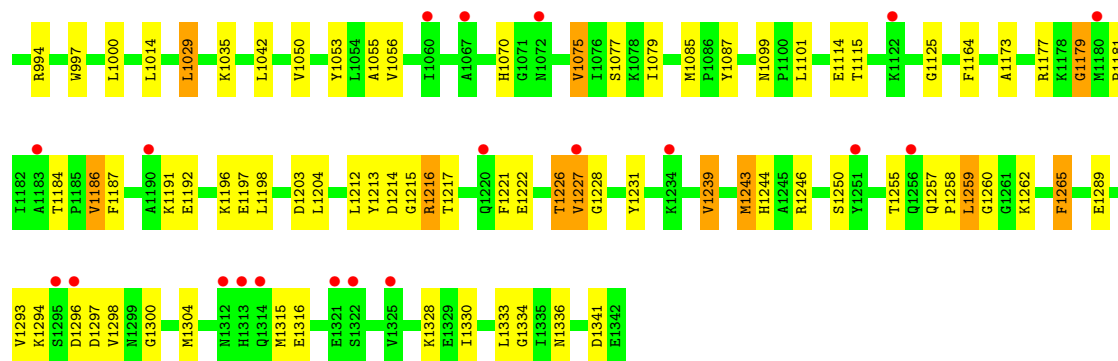




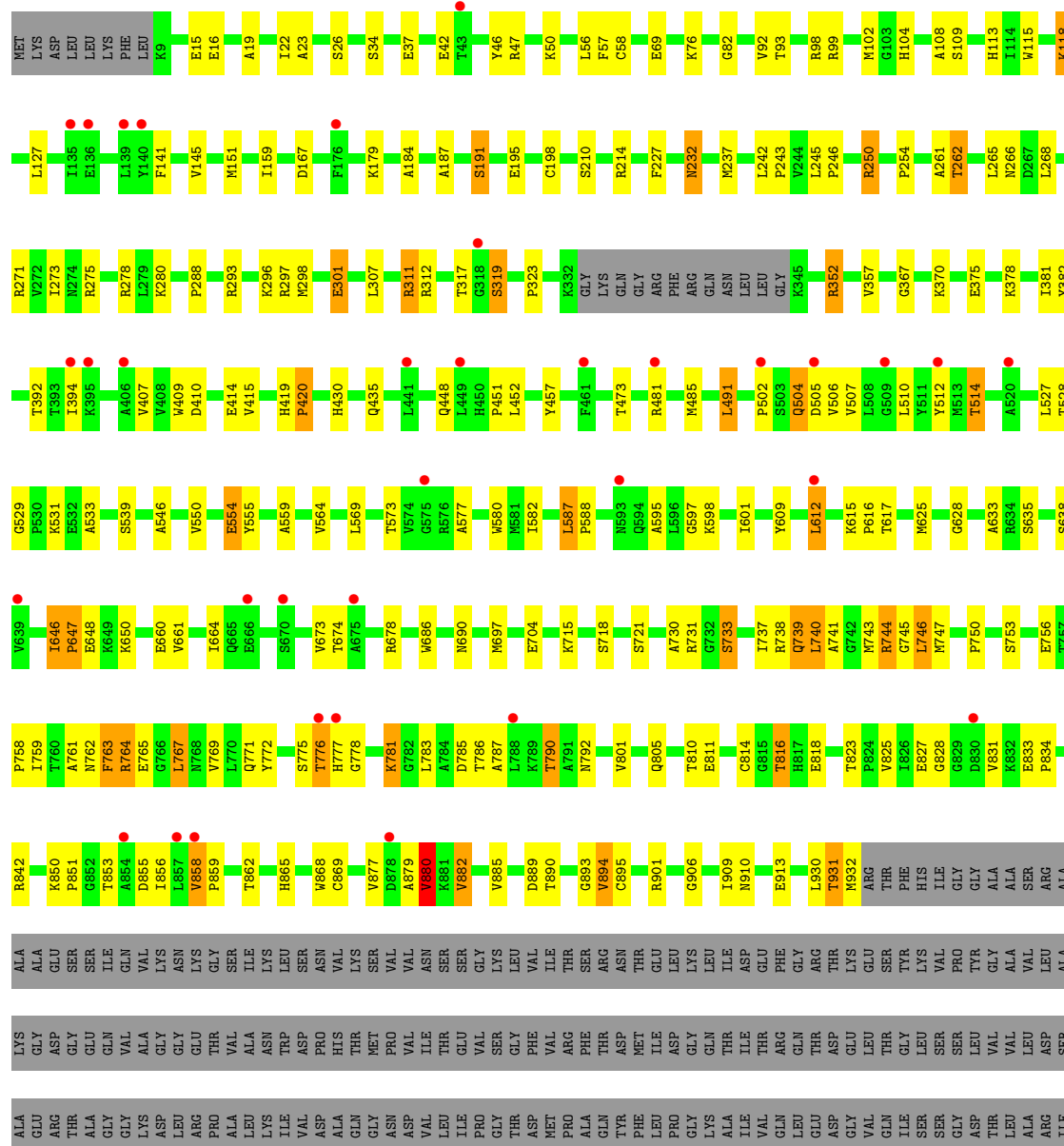


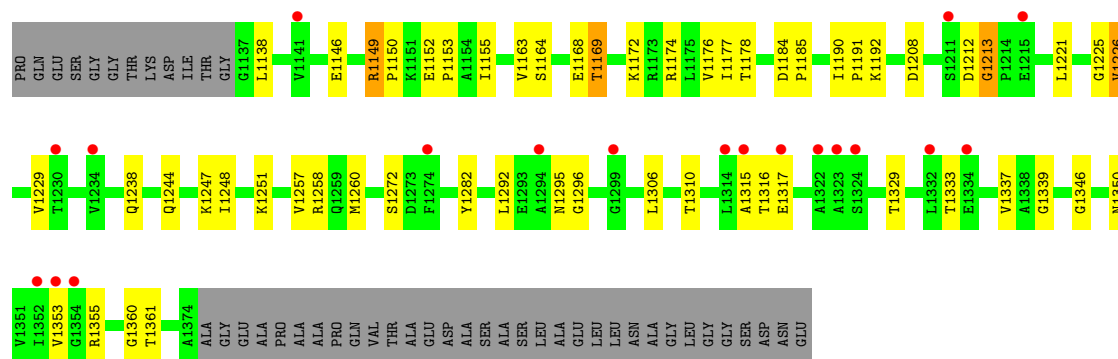
• Molecule 2: DNA-directed RNA polymerase subunit beta



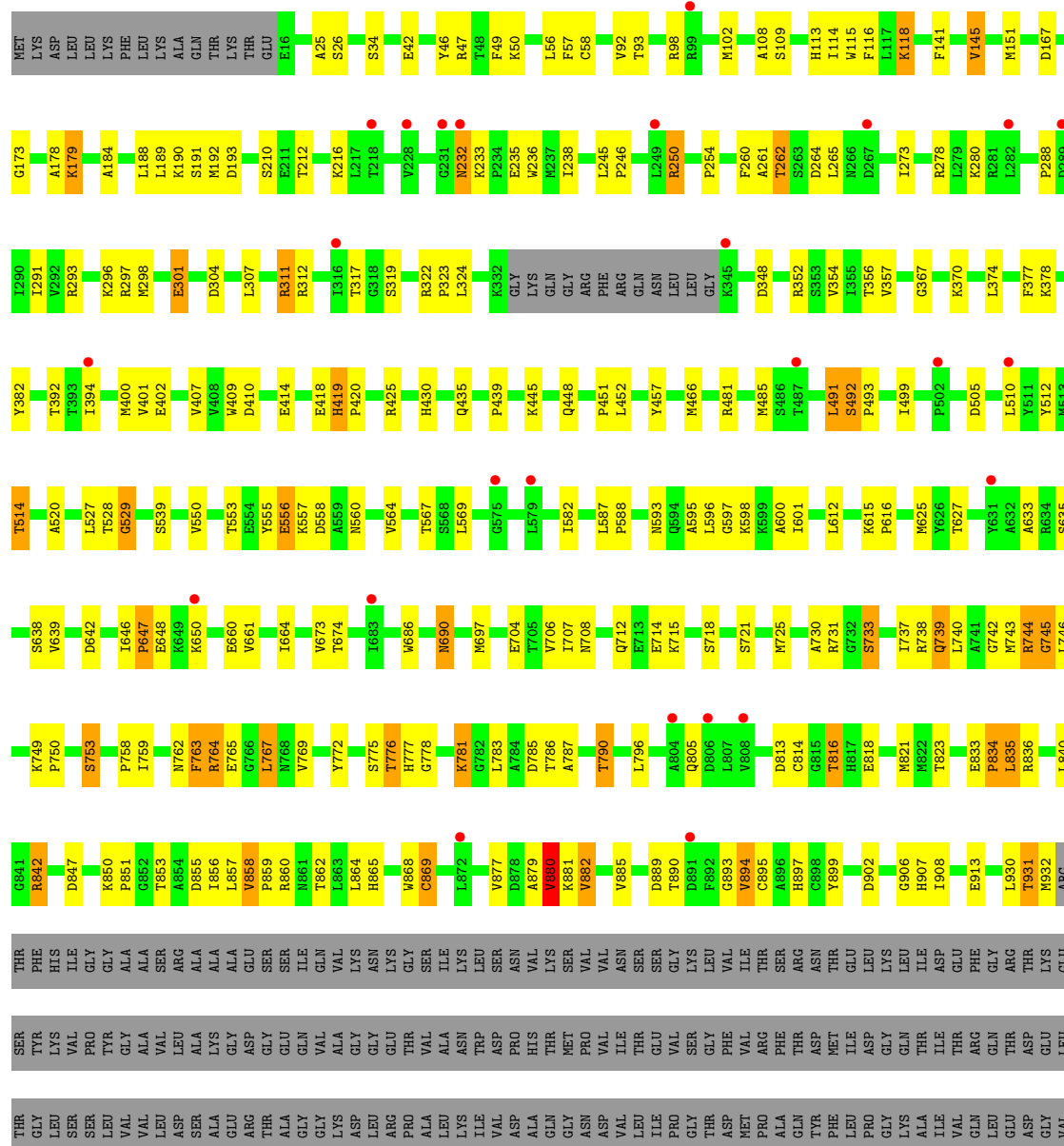


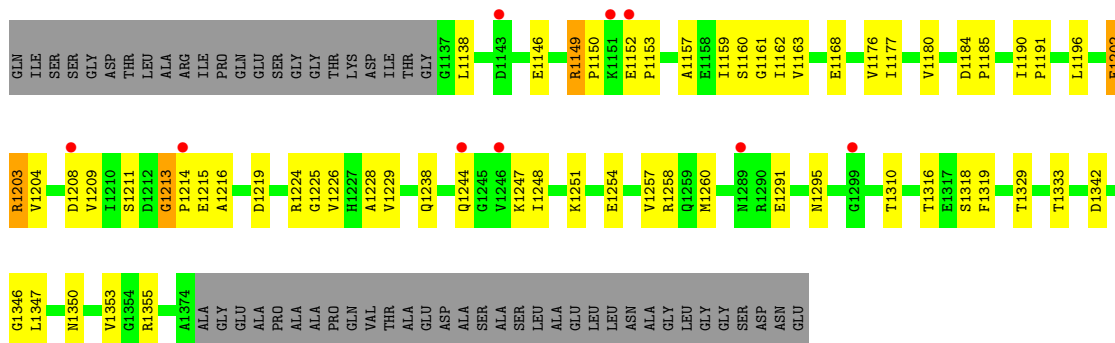
- Molecule 3: DNA-directed RNA polymerase subunit beta'



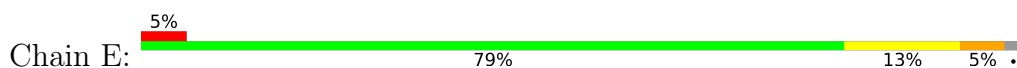


• Molecule 3: DNA-directed RNA polymerase subunit beta'





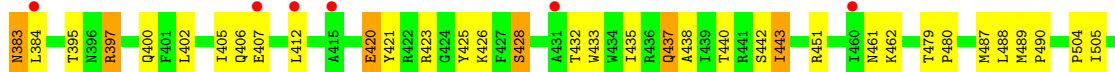
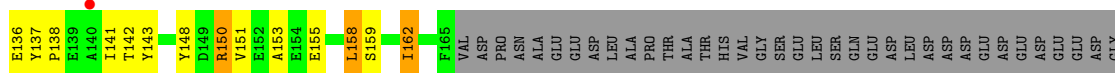
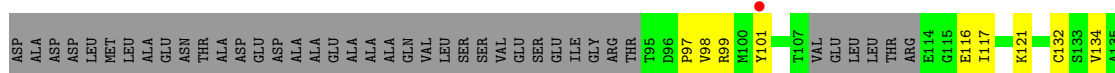
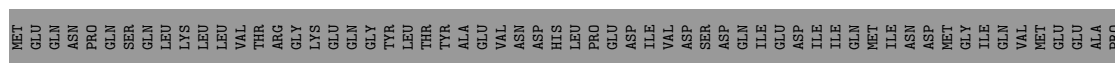
- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 4: DNA-directed RNA polymerase subunit omega

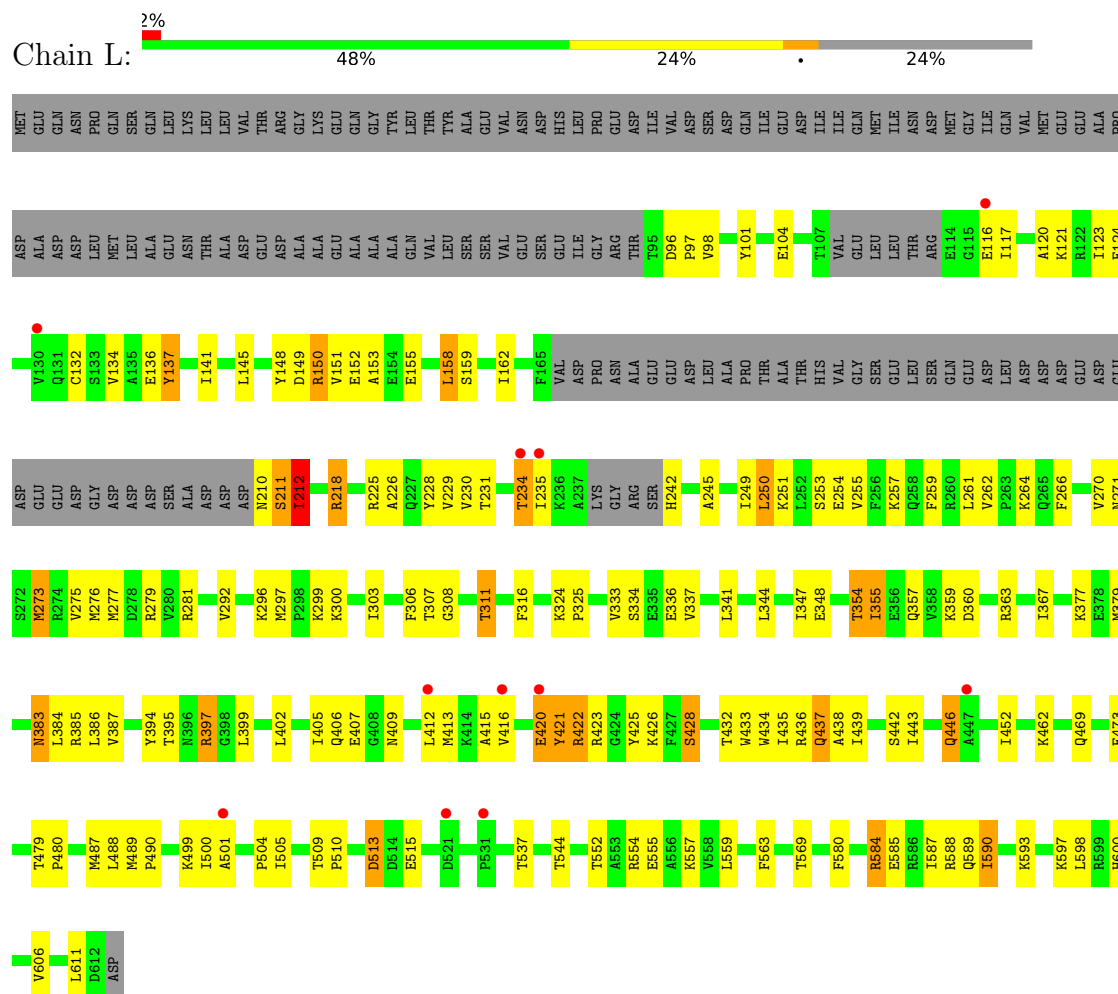


- Molecule 5: RNA polymerase sigma factor RpoD

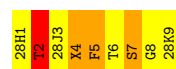




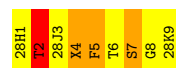
- Molecule 5: RNA polymerase sigma factor RpoD



- Molecule 6: Salinamide A



- Molecule 6: Salinamide A



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 185.80Å 208.19Å 308.18Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 49.87 – 3.90<br>49.87 – 3.90                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.0 (49.87-3.90)<br>97.6 (49.87-3.90)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.12                                                        | Depositor        |
| $R_{sym}$                                                               | 0.12                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.89 (at 3.88Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine: 1.8_1069)                            | Depositor        |
| R, $R_{free}$                                                           | 0.286 , 0.325<br>0.285 , 0.323                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2174 reflections (1.99%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 151.0                                                       | Xtriage          |
| Anisotropy                                                              | 0.330                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 201.3                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.89                                                        | EDS              |
| Total number of atoms                                                   | 50018                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 155.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 28J, 2TL, 28H, 28K, ZN, D4P, MEA

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     | 0.34         | 0/2263         | 0.88        | 2/3073 (0.1%)    |
| 1   | B     | 0.35         | 0/2185         | 0.90        | 3/2967 (0.1%)    |
| 1   | G     | 0.34         | 0/1636         | 0.89        | 3/2221 (0.1%)    |
| 1   | H     | 0.34         | 0/1623         | 0.86        | 1/2205 (0.0%)    |
| 2   | C     | 0.32         | 0/9653         | 0.85        | 18/13062 (0.1%)  |
| 2   | I     | 0.32         | 0/9676         | 0.85        | 15/13089 (0.1%)  |
| 3   | D     | 0.35         | 0/7667         | 0.98        | 32/10416 (0.3%)  |
| 3   | J     | 0.35         | 0/7630         | 0.95        | 22/10365 (0.2%)  |
| 4   | E     | 0.41         | 0/482          | 1.43        | 4/662 (0.6%)     |
| 4   | K     | 0.44         | 0/407          | 1.18        | 3/558 (0.5%)     |
| 5   | F     | 0.35         | 0/3636         | 0.95        | 10/4892 (0.2%)   |
| 5   | L     | 0.34         | 0/3636         | 0.96        | 13/4892 (0.3%)   |
| 6   | M     | 3.13         | 3/14 (21.4%)   | 0.59        | 0/14             |
| 6   | N     | 3.13         | 3/14 (21.4%)   | 0.60        | 0/14             |
| All | All   | 0.35         | 6/50522 (0.0%) | 0.91        | 126/68430 (0.2%) |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 6   | M     | 8   | GLY  | CA-C  | -7.00 | 1.39        | 1.52     |
| 6   | N     | 8   | GLY  | CA-C  | -6.99 | 1.39        | 1.52     |
| 6   | M     | 2   | THR  | CA-C  | -6.40 | 1.39        | 1.52     |
| 6   | N     | 2   | THR  | CA-C  | -6.40 | 1.39        | 1.52     |
| 6   | M     | 7   | SER  | CA-C  | -6.39 | 1.39        | 1.52     |
| 6   | N     | 7   | SER  | CA-C  | -6.39 | 1.39        | 1.52     |

All (126) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | I     | 109 | ALA  | CA-C-N | 13.69 | 136.95      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 2   | I     | 109  | ALA  | C-N-CA | 13.69 | 136.95      | 119.84   |
| 3   | D     | 587  | LEU  | CA-C-N | 13.61 | 136.86      | 119.84   |
| 3   | D     | 587  | LEU  | C-N-CA | 13.61 | 136.86      | 119.84   |
| 5   | F     | 489  | MET  | CA-C-N | 13.38 | 136.57      | 119.84   |
| 5   | F     | 489  | MET  | C-N-CA | 13.38 | 136.57      | 119.84   |
| 5   | L     | 489  | MET  | CA-C-N | 13.36 | 136.53      | 119.84   |
| 5   | L     | 489  | MET  | C-N-CA | 13.36 | 136.53      | 119.84   |
| 3   | J     | 1213 | GLY  | CA-C-N | 12.97 | 136.05      | 119.84   |
| 3   | J     | 1213 | GLY  | C-N-CA | 12.97 | 136.05      | 119.84   |
| 4   | E     | 36   | ASP  | CA-C-N | 12.01 | 134.85      | 119.84   |
| 4   | E     | 36   | ASP  | C-N-CA | 12.01 | 134.85      | 119.84   |
| 4   | E     | 39   | VAL  | CA-C-N | 11.65 | 154.96      | 127.00   |
| 4   | E     | 39   | VAL  | C-N-CA | 11.65 | 154.96      | 127.00   |
| 3   | D     | 850  | LYS  | CA-C-N | 11.25 | 133.90      | 119.84   |
| 3   | D     | 850  | LYS  | C-N-CA | 11.25 | 133.90      | 119.84   |
| 2   | C     | 42   | ASP  | CA-C-N | 10.69 | 130.92      | 119.05   |
| 2   | C     | 42   | ASP  | C-N-CA | 10.69 | 130.92      | 119.05   |
| 3   | D     | 858  | VAL  | CA-C-N | -9.50 | 107.96      | 119.84   |
| 3   | D     | 858  | VAL  | C-N-CA | -9.50 | 107.96      | 119.84   |
| 3   | D     | 1149 | ARG  | CA-C-N | 8.26  | 130.17      | 119.84   |
| 3   | D     | 1149 | ARG  | C-N-CA | 8.26  | 130.17      | 119.84   |
| 3   | J     | 858  | VAL  | CA-C-N | 8.06  | 129.92      | 119.84   |
| 3   | J     | 858  | VAL  | C-N-CA | 8.06  | 129.92      | 119.84   |
| 5   | L     | 600  | HIS  | CA-C-N | 8.03  | 127.96      | 119.05   |
| 5   | L     | 600  | HIS  | C-N-CA | 8.03  | 127.96      | 119.05   |
| 3   | D     | 1213 | GLY  | CA-C-N | 7.85  | 128.33      | 119.93   |
| 3   | D     | 1213 | GLY  | C-N-CA | 7.85  | 128.33      | 119.93   |
| 4   | K     | 36   | ASP  | CA-C-N | 7.64  | 129.40      | 119.84   |
| 4   | K     | 36   | ASP  | C-N-CA | 7.64  | 129.40      | 119.84   |
| 1   | A     | 322  | PRO  | CA-C-N | -7.47 | 110.51      | 119.84   |
| 1   | A     | 322  | PRO  | C-N-CA | -7.47 | 110.51      | 119.84   |
| 3   | D     | 1152 | GLU  | CA-C-N | 7.42  | 129.11      | 119.84   |
| 3   | D     | 1152 | GLU  | C-N-CA | 7.42  | 129.11      | 119.84   |
| 3   | J     | 1149 | ARG  | CA-C-N | 7.41  | 129.10      | 119.84   |
| 3   | J     | 1149 | ARG  | C-N-CA | 7.41  | 129.10      | 119.84   |
| 3   | D     | 823  | THR  | CA-C-N | 7.25  | 126.96      | 119.56   |
| 3   | D     | 823  | THR  | C-N-CA | 7.25  | 126.96      | 119.56   |
| 3   | J     | 1152 | GLU  | CA-C-N | 7.17  | 128.80      | 119.84   |
| 3   | J     | 1152 | GLU  | C-N-CA | 7.17  | 128.80      | 119.84   |
| 5   | F     | 150  | ARG  | N-CA-C | -7.10 | 105.80      | 114.75   |
| 2   | C     | 1151 | LEU  | N-CA-C | -6.97 | 103.68      | 111.28   |
| 3   | J     | 850  | LYS  | CA-C-N | 6.75  | 128.28      | 119.84   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | J     | 850  | LYS  | C-N-CA  | 6.75  | 128.28      | 119.84   |
| 3   | J     | 902  | ASP  | N-CA-C  | -6.67 | 99.78       | 109.59   |
| 5   | L     | 155  | GLU  | N-CA-C  | -6.61 | 105.84      | 114.04   |
| 2   | C     | 566  | GLY  | CA-C-N  | 6.59  | 126.36      | 119.05   |
| 2   | C     | 566  | GLY  | C-N-CA  | 6.59  | 126.36      | 119.05   |
| 2   | I     | 628  | HIS  | N-CA-C  | 6.49  | 118.93      | 110.43   |
| 5   | L     | 150  | ARG  | N-CA-C  | -6.40 | 106.68      | 114.75   |
| 3   | D     | 831  | VAL  | N-CA-C  | 6.39  | 116.87      | 110.23   |
| 3   | D     | 554  | GLU  | CB-CA-C | -6.35 | 109.23      | 116.54   |
| 5   | L     | 96   | ASP  | CA-C-N  | 6.32  | 126.23      | 119.28   |
| 5   | L     | 96   | ASP  | C-N-CA  | 6.32  | 126.23      | 119.28   |
| 5   | L     | 446  | GLN  | N-CA-C  | 6.29  | 118.22      | 111.36   |
| 5   | L     | 452  | ILE  | CA-C-N  | 6.27  | 126.30      | 119.90   |
| 5   | L     | 452  | ILE  | C-N-CA  | 6.27  | 126.30      | 119.90   |
| 5   | F     | 155  | GLU  | N-CA-C  | -6.25 | 106.29      | 114.04   |
| 2   | C     | 61   | SER  | N-CA-C  | 6.21  | 117.72      | 111.07   |
| 3   | J     | 529  | GLY  | CA-C-N  | 6.14  | 125.86      | 119.05   |
| 3   | J     | 529  | GLY  | C-N-CA  | 6.14  | 125.86      | 119.05   |
| 3   | D     | 1184 | ASP  | N-CA-C  | 6.13  | 113.52      | 108.07   |
| 2   | C     | 891  | GLY  | N-CA-C  | -6.07 | 106.22      | 113.99   |
| 3   | J     | 173  | GLY  | N-CA-C  | -6.05 | 105.48      | 112.50   |
| 3   | D     | 1315 | ALA  | N-CA-C  | 5.99  | 117.89      | 111.36   |
| 3   | J     | 853  | THR  | CB-CA-C | -5.92 | 109.18      | 117.23   |
| 2   | C     | 1318 | GLY  | N-CA-C  | -5.92 | 101.74      | 111.38   |
| 3   | D     | 1226 | VAL  | N-CA-C  | 5.89  | 116.63      | 110.62   |
| 3   | J     | 555  | TYR  | N-CA-C  | 5.88  | 123.20      | 114.09   |
| 3   | D     | 853  | THR  | CB-CA-C | -5.87 | 109.25      | 117.23   |
| 2   | C     | 113  | THR  | N-CA-C  | 5.82  | 117.72      | 110.91   |
| 3   | J     | 1184 | ASP  | N-CA-C  | 5.80  | 113.23      | 108.07   |
| 3   | J     | 745  | GLY  | N-CA-C  | 5.77  | 117.95      | 110.45   |
| 2   | I     | 61   | SER  | CB-CA-C | -5.76 | 109.95      | 116.63   |
| 3   | D     | 615  | LYS  | CA-C-N  | 5.75  | 125.43      | 119.05   |
| 3   | D     | 615  | LYS  | C-N-CA  | 5.75  | 125.43      | 119.05   |
| 5   | F     | 600  | HIS  | CA-C-N  | 5.69  | 125.36      | 119.05   |
| 5   | F     | 600  | HIS  | C-N-CA  | 5.69  | 125.36      | 119.05   |
| 1   | G     | 178  | SER  | CA-C-N  | 5.64  | 125.48      | 119.28   |
| 1   | G     | 178  | SER  | C-N-CA  | 5.64  | 125.48      | 119.28   |
| 2   | I     | 168  | GLY  | N-CA-C  | -5.63 | 105.67      | 112.49   |
| 1   | B     | 210  | THR  | N-CA-C  | -5.61 | 105.25      | 111.36   |
| 2   | C     | 559  | CYS  | CA-C-N  | 5.59  | 125.21      | 119.56   |
| 2   | C     | 559  | CYS  | C-N-CA  | 5.59  | 125.21      | 119.56   |
| 2   | C     | 1204 | LEU  | CA-C-N  | 5.59  | 140.43      | 127.00   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | C     | 1204 | LEU  | C-N-CA  | 5.59  | 140.43      | 127.00   |
| 2   | C     | 1312 | ASN  | N-CA-C  | 5.54  | 116.69      | 108.60   |
| 2   | I     | 566  | GLY  | CA-C-N  | 5.49  | 125.15      | 119.05   |
| 2   | I     | 566  | GLY  | C-N-CA  | 5.49  | 125.15      | 119.05   |
| 1   | B     | 10   | LYS  | CA-C-N  | 5.48  | 126.69      | 119.84   |
| 1   | B     | 10   | LYS  | C-N-CA  | 5.48  | 126.69      | 119.84   |
| 3   | D     | 855  | ASP  | CB-CA-C | -5.47 | 110.28      | 116.63   |
| 5   | F     | 153  | ALA  | N-CA-C  | -5.46 | 105.84      | 112.88   |
| 5   | F     | 116  | GLU  | N-CA-C  | -5.39 | 106.66      | 113.18   |
| 5   | F     | 530  | LEU  | CA-C-N  | 5.38  | 125.02      | 119.05   |
| 5   | F     | 530  | LEU  | C-N-CA  | 5.38  | 125.02      | 119.05   |
| 3   | J     | 492  | SER  | CA-C-N  | 5.38  | 124.99      | 119.56   |
| 3   | J     | 492  | SER  | C-N-CA  | 5.38  | 124.99      | 119.56   |
| 3   | D     | 504  | GLN  | CB-CA-C | -5.37 | 110.40      | 116.63   |
| 2   | I     | 1265 | PHE  | N-CA-C  | 5.36  | 117.87      | 111.71   |
| 3   | D     | 1163 | VAL  | N-CA-C  | 5.32  | 115.56      | 108.27   |
| 3   | D     | 1317 | GLU  | N-CA-C  | 5.30  | 117.14      | 111.36   |
| 3   | D     | 882  | VAL  | N-CA-C  | 5.28  | 114.82      | 108.06   |
| 2   | I     | 152  | SER  | CA-C-N  | -5.28 | 114.52      | 119.85   |
| 2   | I     | 152  | SER  | C-N-CA  | -5.28 | 114.52      | 119.85   |
| 3   | J     | 855  | ASP  | CB-CA-C | -5.25 | 110.09      | 117.23   |
| 5   | L     | 116  | GLU  | N-CA-C  | -5.24 | 106.84      | 113.18   |
| 2   | I     | 1316 | GLU  | CA-C-N  | 5.23  | 125.21      | 120.03   |
| 2   | I     | 1316 | GLU  | C-N-CA  | 5.23  | 125.21      | 120.03   |
| 2   | I     | 42   | ASP  | CA-C-N  | -5.20 | 113.34      | 119.84   |
| 2   | I     | 42   | ASP  | C-N-CA  | -5.20 | 113.34      | 119.84   |
| 2   | C     | 1147 | ARG  | N-CA-C  | 5.18  | 116.73      | 111.14   |
| 3   | D     | 827  | GLU  | N-CA-C  | 5.16  | 116.91      | 111.28   |
| 5   | L     | 153  | ALA  | N-CA-C  | -5.16 | 106.22      | 112.88   |
| 2   | C     | 1180 | MET  | CA-C-N  | -5.15 | 113.40      | 119.84   |
| 2   | C     | 1180 | MET  | C-N-CA  | -5.15 | 113.40      | 119.84   |
| 3   | D     | 15   | GLU  | CB-CA-C | -5.15 | 110.62      | 116.54   |
| 4   | K     | 49   | ILE  | N-CA-C  | -5.14 | 105.53      | 110.72   |
| 3   | J     | 882  | VAL  | N-CA-C  | 5.12  | 114.61      | 108.06   |
| 1   | G     | 30   | PRO  | CA-N-CD | -5.12 | 104.84      | 112.00   |
| 3   | D     | 529  | GLY  | CA-C-N  | 5.11  | 125.14      | 119.32   |
| 3   | D     | 529  | GLY  | C-N-CA  | 5.11  | 125.14      | 119.32   |
| 3   | D     | 82   | GLY  | N-CA-C  | -5.10 | 108.62      | 114.69   |
| 2   | I     | 616  | ILE  | N-CA-C  | 5.05  | 114.85      | 107.37   |
| 2   | C     | 1150 | ASP  | N-CA-C  | -5.04 | 107.20      | 113.55   |
| 1   | H     | 30   | PRO  | CA-N-CD | -5.04 | 104.95      | 112.00   |

There are no chirality outliers.

There are no planarity outliers.

## 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     | 2236  | 0        | 2254     | 52      | 0            |
| 1   | B     | 2160  | 0        | 2184     | 62      | 1            |
| 1   | G     | 1618  | 0        | 1622     | 42      | 0            |
| 1   | H     | 1605  | 0        | 1599     | 44      | 1            |
| 2   | C     | 9522  | 0        | 8569     | 150     | 0            |
| 2   | I     | 9544  | 0        | 8601     | 162     | 0            |
| 3   | D     | 7572  | 0        | 6293     | 161     | 0            |
| 3   | J     | 7535  | 0        | 6272     | 169     | 0            |
| 4   | E     | 482   | 0        | 301      | 7       | 0            |
| 4   | K     | 408   | 0        | 255      | 4       | 0            |
| 5   | F     | 3592  | 0        | 3433     | 95      | 1            |
| 5   | L     | 3592  | 0        | 3433     | 102     | 1            |
| 6   | M     | 73    | 0        | 64       | 33      | 0            |
| 6   | N     | 73    | 0        | 64       | 30      | 0            |
| 7   | D     | 1     | 0        | 0        | 0       | 0            |
| 7   | J     | 1     | 0        | 0        | 0       | 0            |
| 8   | D     | 2     | 0        | 0        | 0       | 0            |
| 8   | J     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 50018 | 0        | 44944    | 990     | 2            |

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 10.

All (990) 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) |
|------------------|-----------------|--------------------------|-------------------|
| 6:N:4:D4P:C4     | 6:N:9:28K:H46   | 1.64                     | 1.26              |
| 6:M:4:D4P:C4     | 6:M:9:28K:H46   | 1.64                     | 1.25              |
| 6:N:4:D4P:C3     | 6:N:9:28K:H46   | 1.68                     | 1.22              |
| 6:M:4:D4P:C5     | 6:M:9:28K:H46   | 1.68                     | 1.22              |
| 6:M:4:D4P:C4     | 6:M:9:28K:CAF   | 2.37                     | 0.99              |
| 2:C:936:ARG:HH21 | 2:C:936:ARG:HG3 | 1.29                     | 0.98              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:936:ARG:HH21 | 2:I:936:ARG:HG3  | 1.27                     | 0.96              |
| 6:N:4:D4P:C3     | 6:N:9:28K:CAF    | 2.45                     | 0.95              |
| 6:M:4:D4P:C5     | 6:M:9:28K:CAF    | 2.45                     | 0.94              |
| 6:N:4:D4P:C4     | 6:N:9:28K:CAF    | 2.37                     | 0.92              |
| 3:D:745:GLY:HA3  | 6:M:1:28H:H11    | 1.56                     | 0.88              |
| 3:J:744:ARG:NH2  | 3:J:767:LEU:HD21 | 1.89                     | 0.87              |
| 3:J:745:GLY:HA3  | 6:N:1:28H:H11    | 1.56                     | 0.87              |
| 1:G:44:ARG:NH2   | 2:I:1087:TYR:OH  | 2.07                     | 0.85              |
| 6:M:1:28H:H5     | 6:M:3:28J:H22    | 1.58                     | 0.84              |
| 1:H:29:GLU:HG3   | 1:H:30:PRO:HD2   | 1.61                     | 0.83              |
| 6:N:1:28H:H5     | 6:N:3:28J:H22    | 1.58                     | 0.83              |
| 1:B:10:LYS:HB3   | 1:B:11:PRO:HD2   | 1.61                     | 0.83              |
| 1:H:51:MET:HB3   | 1:H:179:PRO:HD2  | 1.60                     | 0.83              |
| 1:B:182:ARG:HD3  | 3:D:531:LYS:HA   | 1.59                     | 0.82              |
| 5:L:587:ILE:HD12 | 5:L:590:ILE:HD11 | 1.63                     | 0.81              |
| 3:J:527:LEU:O    | 3:J:529:GLY:N    | 2.14                     | 0.80              |
| 3:J:118:LYS:HE3  | 3:J:312:ARG:HG3  | 1.63                     | 0.80              |
| 5:F:587:ILE:HD12 | 5:F:590:ILE:HD11 | 1.63                     | 0.80              |
| 1:G:14:VAL:HG11  | 1:G:29:GLU:HG3   | 1.65                     | 0.79              |
| 2:C:808:ASN:H    | 3:D:633:ALA:HB2  | 1.48                     | 0.79              |
| 1:A:228:LEU:O    | 1:A:230:ALA:N    | 2.14                     | 0.78              |
| 3:D:781:LYS:HB3  | 6:M:5:MEA:CE1    | 2.14                     | 0.78              |
| 3:J:739:GLN:OE1  | 3:J:739:GLN:HA   | 1.84                     | 0.77              |
| 5:F:218:ARG:HG2  | 5:F:218:ARG:HH11 | 1.50                     | 0.77              |
| 2:I:345:PRO:O    | 2:I:347:ILE:N    | 2.17                     | 0.77              |
| 2:C:345:PRO:O    | 2:C:347:ILE:N    | 2.18                     | 0.77              |
| 3:J:744:ARG:HH21 | 3:J:767:LEU:HD21 | 1.50                     | 0.76              |
| 6:N:2:THR:HG21   | 6:N:6:2TL:O      | 1.86                     | 0.76              |
| 2:I:637:ARG:HG3  | 2:I:641:GLU:HA   | 1.69                     | 0.75              |
| 5:L:399:LEU:HD13 | 5:L:446:GLN:HG2  | 1.68                     | 0.75              |
| 6:M:2:THR:HG21   | 6:M:6:2TL:O      | 1.86                     | 0.75              |
| 3:D:738:ARG:HH22 | 6:M:1:28H:H6     | 1.51                     | 0.74              |
| 3:D:739:GLN:HA   | 3:D:739:GLN:OE1  | 1.87                     | 0.74              |
| 3:D:746:LEU:HD22 | 3:D:758:PRO:HB3  | 1.68                     | 0.74              |
| 3:J:738:ARG:HH22 | 6:N:1:28H:H6     | 1.52                     | 0.74              |
| 3:J:262:THR:HG22 | 5:L:504:PRO:HB2  | 1.69                     | 0.74              |
| 2:C:65:ASN:O     | 2:C:105:TYR:N    | 2.21                     | 0.73              |
| 1:G:60:GLU:HG3   | 1:G:170:ARG:HD2  | 1.69                     | 0.73              |
| 3:D:781:LYS:HB3  | 6:M:5:MEA:CD1    | 2.19                     | 0.73              |
| 1:B:110:VAL:HG21 | 1:B:140:ILE:HD11 | 1.71                     | 0.73              |
| 5:L:277:MET:HE1  | 5:L:359:LYS:HG2  | 1.70                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:885:GLY:HA2  | 2:I:917:SER:HB3  | 1.71                     | 0.72              |
| 1:A:208:ASN:OD1  | 1:A:210:THR:OG1  | 2.06                     | 0.72              |
| 1:B:302:GLU:HB2  | 2:C:943:LYS:HZ1  | 1.55                     | 0.72              |
| 1:H:91:ARG:NH2   | 1:H:210:THR:O    | 2.22                     | 0.72              |
| 2:C:885:GLY:HA2  | 2:C:917:SER:HB3  | 1.72                     | 0.71              |
| 3:D:262:THR:HG22 | 5:F:504:PRO:HB2  | 1.73                     | 0.71              |
| 1:H:110:VAL:HG21 | 1:H:140:ILE:HD11 | 1.73                     | 0.71              |
| 3:J:288:PRO:HA   | 5:L:377:LYS:HE3  | 1.73                     | 0.71              |
| 1:A:91:ARG:NH2   | 1:A:209:GLY:O    | 2.24                     | 0.70              |
| 3:D:367:GLY:HA3  | 3:D:448:GLN:HB2  | 1.74                     | 0.70              |
| 2:I:222:ASP:OD1  | 2:I:227:LYS:NZ   | 2.23                     | 0.70              |
| 1:H:86:LYS:HG2   | 1:H:173:VAL:HG23 | 1.74                     | 0.70              |
| 1:G:110:VAL:HG21 | 1:G:140:ILE:HD11 | 1.74                     | 0.69              |
| 1:B:30:PRO:HD3   | 1:B:190:ALA:HB1  | 1.72                     | 0.69              |
| 1:A:150:ARG:HH21 | 1:B:6:THR:HA     | 1.57                     | 0.69              |
| 3:D:744:ARG:HB3  | 3:D:759:ILE:HB   | 1.76                     | 0.68              |
| 5:F:134:VAL:HG11 | 5:F:266:PHE:HE1  | 1.58                     | 0.68              |
| 5:L:152:GLU:OE2  | 5:L:218:ARG:NH1  | 2.26                     | 0.68              |
| 2:C:1099:ASN:ND2 | 3:D:505:ASP:OD2  | 2.25                     | 0.68              |
| 3:J:245:LEU:O    | 3:J:250:ARG:NH1  | 2.26                     | 0.68              |
| 3:J:118:LYS:HB3  | 3:J:311:ARG:HD2  | 1.75                     | 0.68              |
| 3:D:118:LYS:HE3  | 3:D:312:ARG:HG3  | 1.75                     | 0.68              |
| 3:J:781:LYS:HB3  | 6:N:5:MEA:CE1    | 2.23                     | 0.68              |
| 3:D:781:LYS:HB3  | 6:M:5:MEA:HE1    | 1.75                     | 0.67              |
| 2:C:221:LEU:HD11 | 2:C:314:ASN:HB2  | 1.75                     | 0.67              |
| 2:I:548:ARG:NH2  | 2:I:567:PRO:O    | 2.26                     | 0.67              |
| 1:H:59:VAL:HG21  | 1:H:85:LEU:HD13  | 1.76                     | 0.67              |
| 2:I:1099:ASN:ND2 | 3:J:505:ASP:OD2  | 2.26                     | 0.67              |
| 3:J:744:ARG:HB3  | 3:J:759:ILE:HB   | 1.76                     | 0.67              |
| 5:L:218:ARG:HH11 | 5:L:218:ARG:HG2  | 1.58                     | 0.67              |
| 1:A:110:VAL:HG21 | 1:A:140:ILE:HD11 | 1.76                     | 0.67              |
| 6:M:4:D4P:C3     | 6:M:9:28K:H46    | 2.23                     | 0.67              |
| 2:I:915:ASP:OD1  | 2:I:917:SER:OG   | 2.12                     | 0.67              |
| 2:I:915:ASP:OD2  | 2:I:919:ARG:NH2  | 2.27                     | 0.67              |
| 3:J:114:ILE:HD12 | 3:J:114:ILE:H    | 1.60                     | 0.67              |
| 2:I:30:ILE:HD12  | 2:I:575:LEU:HD22 | 1.77                     | 0.66              |
| 2:I:86:GLN:HA    | 2:I:140:GLY:HA2  | 1.77                     | 0.66              |
| 2:C:890:LYS:HG2  | 2:C:914:LYS:HG3  | 1.78                     | 0.66              |
| 3:D:57:PHE:O     | 3:D:98:ARG:NH2   | 2.28                     | 0.66              |
| 2:C:344:GLY:H    | 2:C:437:ASN:ND2  | 1.92                     | 0.66              |
| 2:C:915:ASP:OD1  | 2:C:917:SER:OG   | 2.14                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:133:LEU:HD21  | 1:G:140:ILE:HG12  | 1.78                     | 0.65              |
| 2:C:548:ARG:NH2   | 2:C:567:PRO:O     | 2.30                     | 0.65              |
| 2:C:694:ARG:HG3   | 2:C:694:ARG:HH11  | 1.60                     | 0.65              |
| 5:F:98:VAL:HG22   | 5:F:402:LEU:HD13  | 1.79                     | 0.65              |
| 2:I:26:TYR:HB2    | 2:I:29:SER:HB3    | 1.77                     | 0.65              |
| 5:F:162:ILE:HG22  | 5:F:261:LEU:HD23  | 1.79                     | 0.65              |
| 1:G:91:ARG:NH2    | 1:G:209:GLY:O     | 2.30                     | 0.65              |
| 2:I:621:SER:HB2   | 2:I:629:PHE:CE1   | 2.32                     | 0.65              |
| 1:H:78:ILE:HD13   | 1:H:81:ILE:HD12   | 1.78                     | 0.64              |
| 2:C:796:LEU:N     | 2:C:1231:TYR:OH   | 2.29                     | 0.64              |
| 3:D:865:HIS:HB3   | 3:D:868:TRP:HD1   | 1.61                     | 0.64              |
| 6:M:1:28H:H6      | 6:M:1:28H:OCD     | 1.97                     | 0.64              |
| 6:N:4:D4P:C5      | 6:N:9:28K:H46     | 2.23                     | 0.64              |
| 1:B:59:VAL:HG21   | 1:B:85:LEU:HD13   | 1.80                     | 0.64              |
| 2:I:444:ASP:O     | 2:I:450:ASN:ND2   | 2.28                     | 0.64              |
| 2:I:1196:LYS:NZ   | 3:J:642:ASP:OD2   | 2.30                     | 0.64              |
| 3:J:370:LYS:HB3   | 3:J:409:TRP:CZ3   | 2.33                     | 0.64              |
| 2:C:86:GLN:HA     | 2:C:140:GLY:HA2   | 1.79                     | 0.64              |
| 5:F:405:ILE:HD12  | 5:F:406:GLN:HE21  | 1.61                     | 0.64              |
| 6:N:1:28H:H6      | 6:N:1:28H:OCD     | 1.97                     | 0.64              |
| 2:C:21:VAL:HG21   | 2:C:592:ARG:HD3   | 1.79                     | 0.64              |
| 2:I:890:LYS:HG2   | 2:I:914:LYS:HB2   | 1.80                     | 0.64              |
| 2:C:1186:VAL:HG13 | 2:C:1187:PHE:HD1  | 1.63                     | 0.64              |
| 2:I:936:ARG:HG3   | 2:I:936:ARG:NH2   | 2.03                     | 0.64              |
| 2:I:1186:VAL:HG13 | 2:I:1187:PHE:HD1  | 1.63                     | 0.64              |
| 3:D:288:PRO:HA    | 5:F:377:LYS:HE3   | 1.80                     | 0.63              |
| 4:E:26:ARG:NH1    | 4:E:29:GLN:OE1    | 2.31                     | 0.63              |
| 3:J:1146:GLU:OE2  | 3:J:1310:THR:OG1  | 2.17                     | 0.63              |
| 1:A:287:VAL:HG12  | 1:A:291:LYS:HE3   | 1.78                     | 0.63              |
| 2:I:897:PRO:HB3   | 5:L:563:PHE:O     | 1.98                     | 0.63              |
| 2:I:28:LEU:O      | 2:I:32:LEU:N      | 2.28                     | 0.63              |
| 3:J:932:MET:HE3   | 3:J:1138:LEU:HD23 | 1.79                     | 0.63              |
| 4:E:3:ARG:O       | 4:E:5:THR:N       | 2.31                     | 0.63              |
| 3:J:686:TRP:HB3   | 3:J:746:LEU:HD21  | 1.81                     | 0.63              |
| 5:L:124:GLU:OE1   | 5:L:422:ARG:NH1   | 2.29                     | 0.63              |
| 3:D:250:ARG:O     | 3:D:266:ASN:ND2   | 2.30                     | 0.62              |
| 1:G:59:VAL:HG21   | 1:G:85:LEU:HD13   | 1.79                     | 0.62              |
| 1:G:66:HIS:HB3    | 2:I:874:GLY:HA2   | 1.80                     | 0.62              |
| 3:J:1157:ALA:HB3  | 3:J:1208:ASP:HA   | 1.80                     | 0.62              |
| 5:L:422:ARG:HH11  | 5:L:422:ARG:CG    | 2.12                     | 0.62              |
| 6:M:4:D4P:C6      | 6:M:9:28K:H46     | 2.29                     | 0.62              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:I:344:GLY:H    | 2:I:437:ASN:HD21  | 1.45                     | 0.62              |
| 2:C:463:GLN:HG3  | 2:C:505:PHE:HB2   | 1.82                     | 0.62              |
| 2:C:1268:GLN:NE2 | 3:D:352:ARG:HB3   | 2.14                     | 0.62              |
| 1:H:37:HIS:CE1   | 1:H:187:VAL:HG21  | 2.34                     | 0.62              |
| 2:I:629:PHE:CE2  | 2:I:634:VAL:HG12  | 2.33                     | 0.62              |
| 3:J:114:ILE:HD13 | 3:J:307:LEU:HB2   | 1.80                     | 0.62              |
| 3:D:102:MET:HG2  | 3:D:246:PRO:HD3   | 1.80                     | 0.62              |
| 3:D:739:GLN:HE22 | 3:D:744:ARG:HG3   | 1.65                     | 0.62              |
| 3:J:781:LYS:HB3  | 6:N:5:MEA:HE1     | 1.81                     | 0.62              |
| 3:J:367:GLY:HA3  | 3:J:448:GLN:HB2   | 1.79                     | 0.62              |
| 2:C:56:VAL:HG21  | 2:C:468:LEU:HB3   | 1.82                     | 0.62              |
| 3:J:317:THR:HA   | 3:J:323:PRO:HA    | 1.81                     | 0.62              |
| 6:M:2:THR:HG23   | 6:M:6:2TL:HB      | 1.82                     | 0.62              |
| 1:B:29:GLU:HB3   | 1:B:30:PRO:HD2    | 1.82                     | 0.62              |
| 1:G:51:MET:HB3   | 1:G:179:PRO:HG2   | 1.82                     | 0.62              |
| 3:J:739:GLN:HE22 | 3:J:744:ARG:HG3   | 1.65                     | 0.62              |
| 3:J:1162:ILE:O   | 3:J:1180:VAL:N    | 2.26                     | 0.62              |
| 2:C:542:ARG:HG2  | 2:C:542:ARG:HH21  | 1.65                     | 0.62              |
| 1:A:133:LEU:HD21 | 1:A:140:ILE:HG12  | 1.80                     | 0.61              |
| 2:C:677:ASN:HD22 | 2:C:677:ASN:H     | 1.46                     | 0.61              |
| 1:H:208:ASN:HB3  | 1:H:210:THR:HG23  | 1.82                     | 0.61              |
| 1:B:37:HIS:CE1   | 1:B:187:VAL:HG21  | 2.35                     | 0.61              |
| 2:C:931:VAL:HB   | 2:C:944:ARG:HH22  | 1.64                     | 0.61              |
| 3:D:370:LYS:HB3  | 3:D:409:TRP:CZ3   | 2.35                     | 0.61              |
| 3:J:1162:ILE:HA  | 3:J:1203:ARG:HA   | 1.82                     | 0.61              |
| 1:B:184:ALA:HB3  | 1:B:204:GLU:HB3   | 1.82                     | 0.61              |
| 3:D:930:LEU:HA   | 3:D:1244:GLN:HG3  | 1.81                     | 0.61              |
| 2:I:614:TYR:HB3  | 2:I:651:ASP:HB2   | 1.82                     | 0.61              |
| 2:C:344:GLY:H    | 2:C:437:ASN:HD21  | 1.48                     | 0.61              |
| 1:H:211:ILE:HD11 | 1:H:216:ALA:HB2   | 1.82                     | 0.61              |
| 2:I:1304:MET:HA  | 2:I:1315:MET:HB3  | 1.81                     | 0.61              |
| 6:N:4:D4P:C2     | 6:N:9:28K:H46     | 2.29                     | 0.61              |
| 1:B:41:ASN:HD21  | 2:C:1217:THR:HG22 | 1.66                     | 0.61              |
| 5:L:354:THR:HG22 | 5:L:357:GLN:HE21  | 1.64                     | 0.61              |
| 6:N:2:THR:HG23   | 6:N:6:2TL:CB      | 2.31                     | 0.61              |
| 1:B:29:GLU:CB    | 1:B:30:PRO:HD2    | 2.31                     | 0.61              |
| 2:C:933:VAL:HG13 | 2:C:1050:VAL:HG22 | 1.83                     | 0.61              |
| 3:D:1238:GLN:NE2 | 3:D:1248:ILE:O    | 2.31                     | 0.61              |
| 6:N:2:THR:HG23   | 6:N:6:2TL:HB      | 1.82                     | 0.61              |
| 1:A:71:LYS:NZ    | 1:A:139:SER:O     | 2.34                     | 0.60              |
| 3:D:118:LYS:HB3  | 3:D:311:ARG:HD2   | 1.82                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:102:LEU:HG   | 1:G:115:ILE:HG12 | 1.83                     | 0.60              |
| 2:I:147:SER:HB2  | 2:I:530:ILE:HG22 | 1.81                     | 0.60              |
| 4:K:9:ALA:HB1    | 4:K:19:LEU:HD21  | 1.83                     | 0.60              |
| 2:C:151:ARG:HH21 | 2:C:445:ILE:HD13 | 1.66                     | 0.60              |
| 3:D:747:MET:HE1  | 3:D:771:GLN:HA   | 1.83                     | 0.60              |
| 1:B:287:VAL:HG12 | 1:B:291:LYS:HE3  | 1.82                     | 0.60              |
| 3:D:745:GLY:CA   | 6:M:1:28H:H11    | 2.31                     | 0.60              |
| 5:L:211:SER:OG   | 5:L:212:ILE:N    | 2.33                     | 0.60              |
| 3:J:650:LYS:NZ   | 3:J:765:GLU:OE2  | 2.33                     | 0.60              |
| 3:J:57:PHE:O     | 3:J:98:ARG:NH2   | 2.35                     | 0.60              |
| 6:M:2:THR:HG23   | 6:M:6:2TL:CB     | 2.31                     | 0.60              |
| 2:C:148:GLN:NE2  | 2:C:533:LEU:O    | 2.35                     | 0.60              |
| 2:I:796:LEU:N    | 2:I:1231:TYR:OH  | 2.33                     | 0.60              |
| 6:N:5:MEA:C      | 6:N:7:SER:N      | 2.65                     | 0.60              |
| 5:L:428:SER:O    | 5:L:432:THR:OG1  | 2.17                     | 0.59              |
| 3:J:232:ASN:OD1  | 3:J:232:ASN:N    | 2.34                     | 0.59              |
| 3:J:245:LEU:HD23 | 3:J:250:ARG:HG2  | 1.83                     | 0.59              |
| 3:D:232:ASN:N    | 3:D:232:ASN:OD1  | 2.32                     | 0.59              |
| 3:D:370:LYS:HB3  | 3:D:409:TRP:HZ3  | 1.66                     | 0.59              |
| 1:G:71:LYS:NZ    | 1:G:139:SER:O    | 2.34                     | 0.59              |
| 2:I:1070:HIS:NE2 | 2:I:1114:GLU:OE2 | 2.35                     | 0.59              |
| 5:F:354:THR:HG22 | 5:F:357:GLN:HE21 | 1.66                     | 0.59              |
| 3:J:301:GLU:CD   | 3:J:312:ARG:HH11 | 2.10                     | 0.59              |
| 2:C:338:THR:HG21 | 2:C:345:PRO:HB3  | 1.84                     | 0.59              |
| 2:I:185:ASP:HB2  | 2:I:197:ARG:HB2  | 1.84                     | 0.59              |
| 5:L:354:THR:H    | 5:L:357:GLN:HE21 | 1.48                     | 0.59              |
| 3:D:245:LEU:O    | 3:D:250:ARG:NH1  | 2.33                     | 0.59              |
| 2:I:246:LEU:HB3  | 2:I:269:ILE:HD13 | 1.85                     | 0.59              |
| 3:J:781:LYS:HB3  | 6:N:5:MEA:CD1    | 2.31                     | 0.59              |
| 1:A:78:ILE:HD13  | 1:A:81:ILE:HD12  | 1.84                     | 0.59              |
| 3:D:113:HIS:CD2  | 3:D:115:TRP:HB2  | 2.37                     | 0.59              |
| 2:I:611:GLU:OE1  | 2:I:637:ARG:NH1  | 2.35                     | 0.59              |
| 1:A:59:VAL:HG21  | 1:A:85:LEU:HD13  | 1.85                     | 0.59              |
| 1:G:78:ILE:HD13  | 1:G:81:ILE:HD12  | 1.84                     | 0.59              |
| 2:I:926:GLY:HA3  | 2:I:1055:ALA:O   | 2.02                     | 0.59              |
| 3:J:708:ASN:N    | 3:J:712:GLN:O    | 2.28                     | 0.59              |
| 3:D:746:LEU:CD2  | 3:D:758:PRO:HB3  | 2.33                     | 0.58              |
| 5:F:151:VAL:HG11 | 5:F:158:LEU:HG   | 1.83                     | 0.58              |
| 1:G:66:HIS:HD2   | 1:G:68:TYR:HB2   | 1.68                     | 0.58              |
| 2:C:227:LYS:NZ   | 2:C:334:GLU:OE2  | 2.29                     | 0.58              |
| 4:E:15:ASN:O     | 4:E:17:PHE:N     | 2.36                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:H:29:GLU:CG    | 1:H:30:PRO:HD2    | 2.30                     | 0.58              |
| 5:L:277:MET:HE3  | 5:L:281:ARG:HG3   | 1.85                     | 0.58              |
| 1:H:100:LEU:HD21 | 1:H:121:VAL:HG21  | 1.84                     | 0.58              |
| 6:M:5:MEA:C      | 6:M:7:SER:N       | 2.65                     | 0.58              |
| 2:I:1257:GLN:HG2 | 2:I:1296:ASP:HB3  | 1.85                     | 0.58              |
| 2:C:246:LEU:HB3  | 2:C:269:ILE:HD13  | 1.85                     | 0.58              |
| 1:H:71:LYS:NZ    | 1:H:139:SER:O     | 2.37                     | 0.58              |
| 1:H:133:LEU:HD21 | 1:H:140:ILE:HG12  | 1.85                     | 0.58              |
| 5:L:422:ARG:HH11 | 5:L:422:ARG:HG2   | 1.68                     | 0.58              |
| 2:I:979:LEU:HD21 | 2:I:1000:LEU:HD23 | 1.85                     | 0.58              |
| 5:L:435:ILE:O    | 5:L:439:ILE:HG13  | 2.04                     | 0.58              |
| 3:J:847:ASP:HA   | 3:J:860:ARG:HB2   | 1.85                     | 0.57              |
| 1:A:100:LEU:HD21 | 1:A:121:VAL:HG21  | 1.84                     | 0.57              |
| 2:C:975:ILE:HD11 | 2:C:997:TRP:HE3   | 1.69                     | 0.57              |
| 5:F:412:LEU:HD13 | 5:F:435:ILE:HD11  | 1.87                     | 0.57              |
| 2:I:1192:GLU:OE2 | 3:J:764:ARG:HD3   | 2.03                     | 0.57              |
| 2:C:221:LEU:HD12 | 2:C:313:ALA:HB1   | 1.86                     | 0.57              |
| 1:A:319:GLU:O    | 1:A:320:ASN:ND2   | 2.38                     | 0.57              |
| 2:C:444:ASP:O    | 2:C:450:ASN:ND2   | 2.36                     | 0.57              |
| 2:C:979:LEU:HD21 | 2:C:1000:LEU:HD23 | 1.85                     | 0.57              |
| 2:I:150:HIS:CE1  | 2:I:454:ARG:HD2   | 2.40                     | 0.57              |
| 2:I:463:GLN:HG3  | 2:I:505:PHE:HB2   | 1.86                     | 0.57              |
| 1:B:100:LEU:HD21 | 1:B:121:VAL:HG21  | 1.86                     | 0.57              |
| 2:C:1336:ASN:N   | 3:D:23:ALA:O      | 2.36                     | 0.57              |
| 3:D:514:THR:HB   | 3:D:595:ALA:HA    | 1.87                     | 0.57              |
| 5:L:462:LYS:HG2  | 5:L:487:MET:HE1   | 1.85                     | 0.57              |
| 5:L:151:VAL:HG11 | 5:L:158:LEU:HG    | 1.87                     | 0.57              |
| 3:D:775:SER:O    | 3:D:777:HIS:N     | 2.38                     | 0.57              |
| 3:D:781:LYS:HB3  | 6:M:5:MEA:HD1     | 1.85                     | 0.57              |
| 1:B:71:LYS:NZ    | 1:B:139:SER:O     | 2.38                     | 0.57              |
| 3:J:1225:GLY:O   | 3:J:1229:VAL:HG23 | 2.05                     | 0.56              |
| 2:C:185:ASP:HB2  | 2:C:197:ARG:HB2   | 1.87                     | 0.56              |
| 5:F:213:ASP:OD1  | 5:F:213:ASP:N     | 2.37                     | 0.56              |
| 5:F:218:ARG:HH11 | 5:F:218:ARG:CG    | 2.18                     | 0.56              |
| 2:C:578:TYR:CD2  | 2:C:659:GLN:HG2   | 2.41                     | 0.56              |
| 1:G:230:ALA:O    | 1:G:232:VAL:N     | 2.39                     | 0.56              |
| 3:J:520:ALA:HB2  | 3:J:707:ILE:O     | 2.06                     | 0.56              |
| 2:C:1243:MET:O   | 2:C:1244:HIS:ND1  | 2.39                     | 0.56              |
| 1:A:319:GLU:C    | 1:A:320:ASN:HD22  | 2.14                     | 0.56              |
| 5:F:262:VAL:HG12 | 5:F:263:PRO:HD2   | 1.86                     | 0.56              |
| 2:I:180:ARG:NH2  | 2:I:392:GLU:O     | 2.38                     | 0.56              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:1255:THR:HB   | 2:C:1257:GLN:HG3 | 1.88                     | 0.56              |
| 3:J:102:MET:HG2   | 3:J:246:PRO:HD3  | 1.88                     | 0.56              |
| 2:C:915:ASP:OD2   | 2:C:919:ARG:NH2  | 2.39                     | 0.56              |
| 2:C:1340:GLU:HB2  | 3:D:19:ALA:HB3   | 1.87                     | 0.56              |
| 1:G:52:PRO:HG3    | 1:G:150:ARG:NH1  | 2.20                     | 0.56              |
| 3:J:46:TYR:CZ     | 3:J:47:ARG:HG3   | 2.41                     | 0.56              |
| 2:C:805:MET:HE1   | 2:C:1221:PHE:CE1 | 2.41                     | 0.56              |
| 2:I:1075:VAL:HG21 | 3:J:354:VAL:HG11 | 1.86                     | 0.56              |
| 2:C:812:PHE:HB3   | 3:D:357:VAL:HG21 | 1.88                     | 0.55              |
| 1:B:102:LEU:HG    | 1:B:115:ILE:HG12 | 1.88                     | 0.55              |
| 3:D:46:TYR:CZ     | 3:D:47:ARG:HG3   | 2.41                     | 0.55              |
| 5:F:251:LYS:O     | 5:F:255:VAL:HG23 | 2.06                     | 0.55              |
| 2:C:404:LYS:HE2   | 2:C:586:PHE:CZ   | 2.41                     | 0.55              |
| 3:J:816:THR:HG21  | 3:J:889:ASP:HB3  | 1.88                     | 0.55              |
| 1:B:25:LYS:HE2    | 1:B:204:GLU:HG3  | 1.88                     | 0.55              |
| 3:D:879:ALA:O     | 3:D:880:VAL:HG12 | 2.07                     | 0.55              |
| 2:I:1244:HIS:HB2  | 2:I:1265:PHE:CG  | 2.42                     | 0.55              |
| 2:C:1254:VAL:O    | 3:D:99:ARG:NH1   | 2.34                     | 0.55              |
| 3:J:805:GLN:HE21  | 3:J:1347:LEU:HB2 | 1.71                     | 0.55              |
| 2:I:237:LEU:HD13  | 2:I:292:ILE:HD12 | 1.89                     | 0.55              |
| 2:I:674:ASP:O     | 3:J:772:TYR:OH   | 2.21                     | 0.55              |
| 2:I:444:ASP:OD1   | 2:I:447:HIS:N    | 2.33                     | 0.54              |
| 2:C:677:ASN:H     | 2:C:677:ASN:ND2  | 2.05                     | 0.54              |
| 2:C:1070:HIS:NE2  | 2:C:1114:GLU:OE2 | 2.39                     | 0.54              |
| 2:C:1259:LEU:HD12 | 2:C:1260:GLY:N   | 2.22                     | 0.54              |
| 1:G:100:LEU:HD21  | 1:G:121:VAL:HG21 | 1.89                     | 0.54              |
| 3:J:491:LEU:HA    | 3:J:499:ILE:H    | 1.72                     | 0.54              |
| 3:J:556:GLU:O     | 3:J:558:ASP:N    | 2.40                     | 0.54              |
| 3:D:298:MET:HG2   | 5:F:402:LEU:HD23 | 1.89                     | 0.54              |
| 2:C:901:LEU:O     | 2:C:905:ILE:HG13 | 2.07                     | 0.54              |
| 2:I:342:ASP:HA    | 2:I:437:ASN:HB3  | 1.89                     | 0.54              |
| 5:L:251:LYS:O     | 5:L:255:VAL:HG23 | 2.07                     | 0.54              |
| 2:C:103:VAL:HG22  | 2:C:117:ILE:HG12 | 1.90                     | 0.54              |
| 2:C:726:TYR:HB2   | 2:C:733:VAL:HB   | 1.89                     | 0.54              |
| 5:F:250:LEU:O     | 5:F:254:GLU:HG2  | 2.07                     | 0.54              |
| 3:J:114:ILE:HD11  | 3:J:304:ASP:HA   | 1.89                     | 0.54              |
| 1:A:52:PRO:HG3    | 1:A:150:ARG:NH1  | 2.22                     | 0.54              |
| 1:A:168:ILE:HA    | 1:B:310:ARG:HA   | 1.89                     | 0.54              |
| 1:B:33:ARG:HB2    | 1:B:197:ASP:O    | 2.08                     | 0.54              |
| 1:B:322:PRO:HB2   | 1:B:323:PRO:CD   | 2.38                     | 0.54              |
| 2:C:785:ASP:OD2   | 2:C:791:LEU:N    | 2.38                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:728:ASP:HB2   | 2:I:731:ARG:NH1   | 2.23                     | 0.54              |
| 2:C:150:HIS:CE1   | 2:C:454:ARG:HD2   | 2.42                     | 0.54              |
| 2:C:804:PHE:HE2   | 2:C:1115:THR:HG21 | 1.71                     | 0.54              |
| 3:D:650:LYS:NZ    | 3:D:765:GLU:OE2   | 2.36                     | 0.54              |
| 3:D:750:PRO:HA    | 3:D:777:HIS:CE1   | 2.43                     | 0.54              |
| 2:I:805:MET:HE1   | 2:I:1221:PHE:CE1  | 2.42                     | 0.54              |
| 3:J:1329:THR:O    | 3:J:1333:THR:HG23 | 2.06                     | 0.54              |
| 2:C:868:SER:OG    | 2:C:944:ARG:HB2   | 2.08                     | 0.54              |
| 3:D:738:ARG:NH2   | 6:M:1:28H:H6      | 2.23                     | 0.54              |
| 2:I:621:SER:HB2   | 2:I:629:PHE:HE1   | 1.72                     | 0.54              |
| 3:D:1225:GLY:HA3  | 3:J:1295:ASN:O    | 2.08                     | 0.54              |
| 1:G:37:HIS:CE1    | 1:G:187:VAL:HG21  | 2.43                     | 0.54              |
| 3:J:481:ARG:HA    | 3:J:485:MET:HG2   | 1.89                     | 0.54              |
| 3:D:278:ARG:HD3   | 5:F:406:GLN:HB3   | 1.89                     | 0.53              |
| 1:G:29:GLU:CB     | 1:G:30:PRO:HD2    | 2.38                     | 0.53              |
| 2:I:801:ARG:HH21  | 2:I:1227:VAL:HG11 | 1.73                     | 0.53              |
| 2:C:1289:GLU:HB3  | 2:C:1294:LYS:HD2  | 1.90                     | 0.53              |
| 3:D:767:LEU:H     | 3:D:767:LEU:HD12  | 1.73                     | 0.53              |
| 3:D:1295:ASN:O    | 3:J:1225:GLY:HA3  | 2.08                     | 0.53              |
| 3:D:1296:GLY:HA3  | 3:J:1225:GLY:HA2  | 1.89                     | 0.53              |
| 5:F:277:MET:HE3   | 5:F:281:ARG:HG3   | 1.90                     | 0.53              |
| 3:J:1238:GLN:NE2  | 3:J:1248:ILE:O    | 2.36                     | 0.53              |
| 2:C:237:LEU:HD13  | 2:C:292:ILE:HD12  | 1.89                     | 0.53              |
| 3:J:297:ARG:NH2   | 5:L:104:GLU:OE2   | 2.42                     | 0.53              |
| 1:B:51:MET:HE1    | 1:B:219:ARG:HB3   | 1.90                     | 0.53              |
| 2:I:1226:THR:HG21 | 3:J:639:VAL:O     | 2.09                     | 0.53              |
| 6:N:5:MEA:O       | 6:N:7:SER:N       | 2.42                     | 0.53              |
| 3:D:1221:LEU:HD22 | 3:D:1306:LEU:HB2  | 1.90                     | 0.53              |
| 5:L:383:ASN:N     | 5:L:383:ASN:HD22  | 2.06                     | 0.53              |
| 2:C:962:GLU:O     | 2:C:966:ILE:HG13  | 2.09                     | 0.53              |
| 2:C:1276:TRP:CE2  | 3:D:801:VAL:HG11  | 2.43                     | 0.53              |
| 3:D:739:GLN:NE2   | 3:D:744:ARG:HG3   | 2.24                     | 0.53              |
| 2:I:404:LYS:HE2   | 2:I:586:PHE:CZ    | 2.44                     | 0.53              |
| 1:A:286:GLU:OE1   | 1:A:304:LYS:NZ    | 2.31                     | 0.53              |
| 3:J:1216:ALA:HB3  | 3:J:1219:ASP:HB2  | 1.89                     | 0.53              |
| 3:D:179:LYS:O     | 3:D:184:ALA:HB2   | 2.08                     | 0.53              |
| 3:D:1329:THR:O    | 3:D:1333:THR:HG23 | 2.09                     | 0.53              |
| 1:H:14:VAL:HG11   | 1:H:29:GLU:CD     | 2.33                     | 0.53              |
| 6:M:5:MEA:O       | 6:M:7:SER:N       | 2.42                     | 0.53              |
| 2:C:898:GLU:HG2   | 5:F:541:ARG:HA    | 1.89                     | 0.53              |
| 2:I:812:PHE:HB3   | 3:J:357:VAL:HG21  | 1.91                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:I:975:ILE:HD11 | 2:I:997:TRP:HE3   | 1.73                     | 0.53              |
| 2:C:905:ILE:HD11 | 5:F:598:LEU:HD13  | 1.91                     | 0.52              |
| 3:D:145:VAL:HA   | 3:D:159:ILE:HA    | 1.90                     | 0.52              |
| 3:D:704:GLU:O    | 3:D:715:LYS:HA    | 2.09                     | 0.52              |
| 2:I:144:VAL:HG23 | 2:I:515:MET:SD    | 2.49                     | 0.52              |
| 5:L:250:LEU:O    | 5:L:254:GLU:HG2   | 2.08                     | 0.52              |
| 5:L:406:GLN:HA   | 5:L:406:GLN:OE1   | 2.09                     | 0.52              |
| 2:I:1334:GLY:O   | 3:J:25:ALA:HB3    | 2.09                     | 0.52              |
| 1:B:302:GLU:HB2  | 2:C:943:LYS:NZ    | 2.24                     | 0.52              |
| 3:D:381:ILE:HA   | 3:D:415:VAL:HG21  | 1.91                     | 0.52              |
| 2:I:1173:ALA:O   | 2:I:1177:ARG:N    | 2.41                     | 0.52              |
| 1:A:14:VAL:HG11  | 1:A:29:GLU:HG2    | 1.92                     | 0.52              |
| 1:B:133:LEU:HD21 | 1:B:140:ILE:HG12  | 1.90                     | 0.52              |
| 2:I:808:ASN:H    | 3:J:633:ALA:HB2   | 1.75                     | 0.52              |
| 3:D:1225:GLY:O   | 3:D:1229:VAL:HG23 | 2.10                     | 0.52              |
| 3:D:814:CYS:HB3  | 3:D:890:THR:OG1   | 2.09                     | 0.52              |
| 2:I:1087:TYR:CZ  | 2:I:1213:TYR:HB2  | 2.45                     | 0.52              |
| 3:J:746:LEU:HD22 | 3:J:758:PRO:HB3   | 1.92                     | 0.52              |
| 6:M:5:MEA:O      | 6:M:6:2TL:C       | 2.57                     | 0.52              |
| 2:C:1192:GLU:OE2 | 3:D:764:ARG:HD3   | 2.10                     | 0.51              |
| 3:D:746:LEU:O    | 6:M:2:THR:HG22    | 2.10                     | 0.51              |
| 2:I:798:GLN:OE1  | 2:I:828:PHE:N     | 2.43                     | 0.51              |
| 3:J:108:ALA:HB2  | 3:J:280:LYS:HG3   | 1.91                     | 0.51              |
| 5:L:124:GLU:CD   | 5:L:422:ARG:HH12  | 2.16                     | 0.51              |
| 5:L:218:ARG:HH11 | 5:L:218:ARG:CG    | 2.20                     | 0.51              |
| 5:F:428:SER:O    | 5:F:432:THR:OG1   | 2.27                     | 0.51              |
| 1:H:51:MET:CB    | 1:H:179:PRO:HD2   | 2.37                     | 0.51              |
| 2:I:726:TYR:HB2  | 2:I:733:VAL:HB    | 1.90                     | 0.51              |
| 2:I:1222:GLU:OE2 | 3:J:512:TYR:OH    | 2.24                     | 0.51              |
| 2:C:1199:LEU:O   | 2:C:1204:LEU:N    | 2.40                     | 0.51              |
| 3:D:275:ARG:NH2  | 5:F:400:GLN:OE1   | 2.43                     | 0.51              |
| 3:D:510:LEU:O    | 3:D:514:THR:OG1   | 2.27                     | 0.51              |
| 1:G:44:ARG:HG3   | 1:G:183:ILE:HB    | 1.91                     | 0.51              |
| 5:L:344:LEU:HD12 | 5:L:347:ILE:HD12  | 1.93                     | 0.51              |
| 1:A:68:TYR:CE2   | 2:C:831:ILE:HD11  | 2.46                     | 0.51              |
| 1:A:285:THR:HG23 | 1:A:288:GLU:H     | 1.76                     | 0.51              |
| 1:G:214:GLU:O    | 1:G:218:ARG:HG3   | 2.10                     | 0.51              |
| 5:L:363:ARG:O    | 5:L:367:ILE:HG13  | 2.10                     | 0.51              |
| 6:N:5:MEA:O      | 6:N:6:2TL:C       | 2.57                     | 0.51              |
| 2:I:344:GLY:H    | 2:I:437:ASN:ND2   | 2.08                     | 0.51              |
| 2:C:48:GLY:O     | 2:C:50:GLU:N      | 2.37                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:134:VAL:HG11  | 5:F:266:PHE:CE1   | 2.44                     | 0.51              |
| 3:J:301:GLU:OE1   | 5:L:97:PRO:HG3    | 2.09                     | 0.51              |
| 5:L:226:ALA:HA    | 5:L:229:VAL:HG22  | 1.93                     | 0.51              |
| 5:L:270:VAL:HA    | 5:L:273:MET:HE3   | 1.93                     | 0.51              |
| 5:L:383:ASN:O     | 5:L:386:LEU:N     | 2.39                     | 0.51              |
| 1:A:44:ARG:NH1    | 2:C:1087:TYR:OH   | 2.43                     | 0.51              |
| 3:D:1257:VAL:HA   | 3:D:1260:MET:HE3  | 1.91                     | 0.51              |
| 5:L:145:LEU:HD12  | 5:L:228:TYR:HD2   | 1.74                     | 0.51              |
| 5:F:292:VAL:HA    | 5:F:297:MET:O     | 2.10                     | 0.51              |
| 3:J:56:LEU:HB3    | 3:J:250:ARG:NH2   | 2.25                     | 0.51              |
| 1:B:7:GLU:O       | 1:B:8:PHE:HB2     | 2.10                     | 0.50              |
| 3:D:245:LEU:HD23  | 3:D:250:ARG:HG2   | 1.93                     | 0.50              |
| 5:L:585:GLU:OE1   | 5:L:588:ARG:NH2   | 2.44                     | 0.50              |
| 5:F:383:ASN:HD22  | 5:F:383:ASN:N     | 2.09                     | 0.50              |
| 2:I:344:GLY:HA3   | 2:I:346:TYR:CZ    | 2.45                     | 0.50              |
| 3:J:879:ALA:O     | 3:J:880:VAL:HG12  | 2.11                     | 0.50              |
| 5:L:231:THR:HA    | 5:L:234:THR:HG23  | 1.92                     | 0.50              |
| 5:L:412:LEU:HD13  | 5:L:435:ILE:HD11  | 1.92                     | 0.50              |
| 1:A:29:GLU:CB     | 1:A:30:PRO:HD2    | 2.41                     | 0.50              |
| 1:B:286:GLU:OE1   | 1:B:304:LYS:NZ    | 2.35                     | 0.50              |
| 2:C:890:LYS:HD3   | 2:C:914:LYS:HE3   | 1.93                     | 0.50              |
| 3:D:746:LEU:CD2   | 3:D:746:LEU:N     | 2.74                     | 0.50              |
| 5:F:261:LEU:HB2   | 5:F:266:PHE:CE2   | 2.46                     | 0.50              |
| 2:I:533:LEU:HD21  | 2:I:571:LEU:HD13  | 1.93                     | 0.50              |
| 2:I:909:LYS:O     | 2:I:911:SER:N     | 2.44                     | 0.50              |
| 3:J:842:ARG:NH2   | 3:J:1254:GLU:OE1  | 2.44                     | 0.50              |
| 5:L:397:ARG:HB3   | 5:L:443:ILE:HD13  | 1.94                     | 0.50              |
| 3:D:317:THR:HB    | 3:D:319:SER:O     | 2.11                     | 0.50              |
| 3:D:932:MET:HE3   | 3:D:1138:LEU:HD23 | 1.92                     | 0.50              |
| 1:G:152:TYR:HD2   | 2:I:824:GLN:CG    | 2.25                     | 0.50              |
| 3:J:615:LYS:H     | 4:K:7:GLN:CG      | 2.24                     | 0.50              |
| 3:D:747:MET:HA    | 6:M:2:THR:HG21    | 1.93                     | 0.50              |
| 2:I:225:PHE:HE1   | 2:I:345:PRO:HA    | 1.77                     | 0.50              |
| 2:I:801:ARG:HE    | 2:I:1227:VAL:CG1  | 2.25                     | 0.50              |
| 2:I:1255:THR:HB   | 2:I:1257:GLN:HG3  | 1.92                     | 0.50              |
| 5:L:292:VAL:HA    | 5:L:297:MET:O     | 2.11                     | 0.50              |
| 2:C:404:LYS:HE2   | 2:C:586:PHE:HZ    | 1.76                     | 0.50              |
| 3:D:775:SER:O     | 3:D:778:GLY:N     | 2.43                     | 0.50              |
| 5:F:551:LEU:HB2   | 5:F:555:GLU:HG3   | 1.92                     | 0.50              |
| 2:I:1333:LEU:HD13 | 3:J:115:TRP:CZ3   | 2.47                     | 0.50              |
| 3:J:750:PRO:HA    | 3:J:777:HIS:CE1   | 2.46                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:703:GLY:N     | 2:I:705:GLU:OE2   | 2.44                     | 0.50              |
| 2:I:1192:GLU:O    | 2:I:1196:LYS:HG2  | 2.12                     | 0.50              |
| 3:J:647:PRO:HG3   | 3:J:697:MET:HA    | 1.93                     | 0.50              |
| 1:A:107:ILE:HG13  | 1:A:136:GLU:HG3   | 1.94                     | 0.50              |
| 1:B:182:ARG:HD3   | 3:D:531:LYS:CA    | 2.37                     | 0.50              |
| 1:H:41:ASN:ND2    | 2:I:1217:THR:HG22 | 2.27                     | 0.50              |
| 2:I:1087:TYR:HE1  | 2:I:1215:GLY:HA2  | 1.77                     | 0.50              |
| 3:J:370:LYS:HB3   | 3:J:409:TRP:HZ3   | 1.75                     | 0.50              |
| 5:L:469:GLN:O     | 5:L:473:GLU:HG2   | 2.12                     | 0.50              |
| 1:B:285:THR:HG23  | 1:B:288:GLU:H     | 1.77                     | 0.49              |
| 3:D:317:THR:HG22  | 3:D:323:PRO:HA    | 1.94                     | 0.49              |
| 3:J:452:LEU:HG    | 3:J:625:MET:HE3   | 1.94                     | 0.49              |
| 3:J:597:GLY:H     | 3:J:600:ALA:HB3   | 1.77                     | 0.49              |
| 3:J:739:GLN:NE2   | 3:J:744:ARG:HG3   | 2.25                     | 0.49              |
| 2:C:728:ASP:HB2   | 2:C:731:ARG:NH1   | 2.27                     | 0.49              |
| 2:C:1226:THR:HG23 | 3:D:638:SER:OG    | 2.11                     | 0.49              |
| 5:F:487:MET:HE2   | 5:F:487:MET:HA    | 1.94                     | 0.49              |
| 2:C:703:GLY:N     | 2:C:705:GLU:OE2   | 2.46                     | 0.49              |
| 5:F:276:MET:SD    | 5:F:279:ARG:NH2   | 2.85                     | 0.49              |
| 5:F:299:LYS:O     | 5:F:303:ILE:HG12  | 2.13                     | 0.49              |
| 3:J:1244:GLN:HA   | 3:J:1244:GLN:OE1  | 2.12                     | 0.49              |
| 1:B:78:ILE:HD13   | 1:B:81:ILE:HD12   | 1.94                     | 0.49              |
| 2:C:151:ARG:NH2   | 2:C:445:ILE:HD13  | 2.27                     | 0.49              |
| 2:C:1222:GLU:OE2  | 3:D:512:TYR:OH    | 2.19                     | 0.49              |
| 1:H:66:HIS:HD2    | 1:H:68:TYR:HB3    | 1.77                     | 0.49              |
| 5:L:231:THR:O     | 5:L:235:ILE:HG12  | 2.12                     | 0.49              |
| 2:C:1253:LEU:HA   | 5:F:525:ASP:HB2   | 1.93                     | 0.49              |
| 3:J:738:ARG:NH2   | 6:N:1:28H:H6      | 2.24                     | 0.49              |
| 5:L:306:PHE:O     | 5:L:308:GLY:N     | 2.44                     | 0.49              |
| 3:D:382:TYR:HB3   | 3:D:394:ILE:HG23  | 1.94                     | 0.49              |
| 3:D:435:GLN:HB2   | 3:D:457:TYR:OH    | 2.13                     | 0.49              |
| 3:J:382:TYR:HB3   | 3:J:394:ILE:HG23  | 1.95                     | 0.49              |
| 3:D:647:PRO:HG3   | 3:D:697:MET:HA    | 1.95                     | 0.49              |
| 5:F:148:TYR:C     | 5:F:150:ARG:H     | 2.21                     | 0.49              |
| 2:I:40:GLU:O      | 2:I:73:TYR:OH     | 2.27                     | 0.49              |
| 1:A:29:GLU:CG     | 1:A:30:PRO:HD2    | 2.43                     | 0.49              |
| 1:B:301:THR:HG22  | 2:C:867:GLU:OE2   | 2.12                     | 0.49              |
| 2:C:736:VAL:O     | 2:C:737:ASN:HB2   | 2.13                     | 0.49              |
| 3:D:686:TRP:HB3   | 3:D:746:LEU:HD21  | 1.95                     | 0.49              |
| 1:H:42:ALA:O      | 1:H:46:ILE:HG12   | 2.13                     | 0.49              |
| 2:I:804:PHE:HE2   | 2:I:1115:THR:HG21 | 1.76                     | 0.49              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:J:145:VAL:O     | 3:J:178:ALA:HA   | 2.13                     | 0.49              |
| 4:K:27:ALA:HB2    | 4:K:47:THR:HA    | 1.95                     | 0.49              |
| 5:L:590:ILE:HA    | 5:L:593:LYS:HG2  | 1.95                     | 0.49              |
| 1:A:42:ALA:O      | 1:A:46:ILE:HG12  | 2.13                     | 0.49              |
| 2:C:1268:GLN:HE22 | 3:D:352:ARG:HB3  | 1.77                     | 0.49              |
| 3:D:113:HIS:CE1   | 3:D:307:LEU:HD13 | 2.47                     | 0.49              |
| 3:D:767:LEU:HD11  | 3:D:772:TYR:HD2  | 1.78                     | 0.49              |
| 1:H:180:VAL:HG11  | 1:H:183:ILE:HD11 | 1.95                     | 0.49              |
| 1:B:17:GLU:HB3    | 1:B:25:LYS:HB2   | 1.94                     | 0.49              |
| 2:C:48:GLY:C      | 2:C:50:GLU:H     | 2.18                     | 0.49              |
| 2:C:103:VAL:HG12  | 2:C:104:ILE:O    | 2.13                     | 0.49              |
| 2:C:1209:GLN:HA   | 2:C:1226:THR:HA  | 1.95                     | 0.48              |
| 2:I:756:TYR:H     | 2:I:766:ASN:HB3  | 1.77                     | 0.48              |
| 2:C:542:ARG:HG2   | 2:C:542:ARG:NH2  | 2.27                     | 0.48              |
| 2:I:27:LEU:HD23   | 2:I:711:ASP:OD2  | 2.14                     | 0.48              |
| 5:L:299:LYS:O     | 5:L:303:ILE:HG12 | 2.13                     | 0.48              |
| 2:C:796:LEU:H     | 2:C:1231:TYR:HH  | 1.58                     | 0.48              |
| 3:D:775:SER:O     | 3:D:776:THR:C    | 2.56                     | 0.48              |
| 1:G:29:GLU:CG     | 1:G:30:PRO:HD2   | 2.43                     | 0.48              |
| 1:G:134:THR:OG1   | 1:G:135:ASP:N    | 2.46                     | 0.48              |
| 1:H:86:LYS:HG2    | 1:H:173:VAL:CG2  | 2.42                     | 0.48              |
| 2:I:150:HIS:CE1   | 2:I:152:SER:HA   | 2.48                     | 0.48              |
| 5:L:394:TYR:OH    | 5:L:436:ARG:HG3  | 2.13                     | 0.48              |
| 2:C:694:ARG:HH11  | 2:C:694:ARG:CG   | 2.26                     | 0.48              |
| 1:H:102:LEU:HG    | 1:H:115:ILE:HG12 | 1.96                     | 0.48              |
| 3:J:550:VAL:O     | 3:J:569:LEU:HA   | 2.14                     | 0.48              |
| 5:L:383:ASN:HD22  | 5:L:383:ASN:H    | 1.62                     | 0.48              |
| 1:B:42:ALA:O      | 1:B:46:ILE:HG12  | 2.14                     | 0.48              |
| 3:D:127:LEU:HD12  | 3:D:237:MET:HE1  | 1.96                     | 0.48              |
| 5:F:226:ALA:HA    | 5:F:229:VAL:HG22 | 1.95                     | 0.48              |
| 5:F:231:THR:O     | 5:F:235:ILE:HG12 | 2.13                     | 0.48              |
| 5:L:344:LEU:HG    | 5:L:355:ILE:HD12 | 1.94                     | 0.48              |
| 3:D:550:VAL:O     | 3:D:569:LEU:HA   | 2.14                     | 0.48              |
| 2:I:930:ASP:HB2   | 2:I:1053:TYR:HB2 | 1.95                     | 0.48              |
| 5:L:148:TYR:C     | 5:L:150:ARG:H    | 2.22                     | 0.48              |
| 5:L:324:LYS:HB3   | 5:L:325:PRO:HD2  | 1.95                     | 0.48              |
| 2:C:542:ARG:HH21  | 2:C:542:ARG:CG   | 2.27                     | 0.48              |
| 3:D:507:VAL:HG21  | 3:D:598:LYS:HB2  | 1.96                     | 0.48              |
| 5:F:216:LEU:O     | 5:F:219:GLU:HB3  | 2.14                     | 0.48              |
| 3:J:410:ASP:O     | 3:J:414:GLU:HG3  | 2.13                     | 0.48              |
| 5:L:98:VAL:HG22   | 5:L:402:LEU:HD13 | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:C:14:ASP:HB3    | 2:C:1158:LYS:CB   | 2.44                     | 0.48              |
| 3:D:1146:GLU:OE2  | 3:D:1310:THR:OG1  | 2.32                     | 0.48              |
| 3:J:113:HIS:HB3   | 3:J:116:PHE:HD2   | 1.79                     | 0.48              |
| 5:L:383:ASN:N     | 5:L:383:ASN:ND2   | 2.62                     | 0.48              |
| 2:C:145:ILE:HB    | 2:C:456:VAL:HG13  | 1.95                     | 0.47              |
| 2:C:890:LYS:HE3   | 2:C:911:SER:O     | 2.14                     | 0.47              |
| 5:F:324:LYS:HB3   | 5:F:325:PRO:HD2   | 1.95                     | 0.47              |
| 1:B:95:LYS:HE2    | 1:B:95:LYS:HA     | 1.96                     | 0.47              |
| 2:C:560:PRO:HB2   | 3:D:776:THR:CB    | 2.44                     | 0.47              |
| 3:D:1346:GLY:O    | 3:D:1350:ASN:ND2  | 2.45                     | 0.47              |
| 5:F:355:ILE:H     | 5:F:355:ILE:HG13  | 1.41                     | 0.47              |
| 2:I:225:PHE:CE1   | 2:I:345:PRO:HA    | 2.49                     | 0.47              |
| 3:J:260:PHE:HB3   | 5:L:504:PRO:HB3   | 1.96                     | 0.47              |
| 3:D:893:GLY:C     | 3:D:1258:ARG:HH12 | 2.23                     | 0.47              |
| 5:F:407:GLU:HG3   | 5:F:442:SER:OG    | 2.14                     | 0.47              |
| 5:F:433:TRP:O     | 5:F:437:GLN:HB3   | 2.15                     | 0.47              |
| 3:J:745:GLY:CA    | 6:N:1:28H:H11     | 2.35                     | 0.47              |
| 3:J:1163:VAL:N    | 3:J:1202:GLU:O    | 2.47                     | 0.47              |
| 2:C:533:LEU:HD21  | 2:C:571:LEU:HD13  | 1.97                     | 0.47              |
| 2:I:25:PRO:HD3    | 2:I:578:TYR:CD1   | 2.48                     | 0.47              |
| 3:J:821:MET:HA    | 3:J:881:LYS:HA    | 1.96                     | 0.47              |
| 3:J:1161:GLY:O    | 3:J:1204:VAL:N    | 2.48                     | 0.47              |
| 2:C:801:ARG:HE    | 2:C:1227:VAL:HG11 | 1.79                     | 0.47              |
| 2:I:1239:VAL:HG13 | 3:J:354:VAL:HB    | 1.97                     | 0.47              |
| 1:B:107:ILE:HG13  | 1:B:136:GLU:HG3   | 1.96                     | 0.47              |
| 2:C:1192:GLU:O    | 2:C:1196:LYS:HG2  | 2.14                     | 0.47              |
| 3:D:301:GLU:CD    | 3:D:312:ARG:HH11  | 2.19                     | 0.47              |
| 1:H:95:LYS:HA     | 1:H:95:LYS:HE2    | 1.97                     | 0.47              |
| 3:J:733:SER:O     | 3:J:737:ILE:HG12  | 2.14                     | 0.47              |
| 3:D:56:LEU:HB3    | 3:D:250:ARG:NH2   | 2.29                     | 0.47              |
| 1:G:42:ALA:O      | 1:G:46:ILE:HG12   | 2.15                     | 0.47              |
| 1:H:155:ALA:HB1   | 1:H:172:LEU:HB2   | 1.96                     | 0.47              |
| 2:I:1099:ASN:HD21 | 3:J:505:ASP:CG    | 2.21                     | 0.47              |
| 3:J:553:THR:HA    | 3:J:567:THR:HA    | 1.95                     | 0.47              |
| 3:J:865:HIS:O     | 3:J:869:CYS:N     | 2.36                     | 0.47              |
| 3:J:1257:VAL:HA   | 3:J:1260:MET:HE3  | 1.95                     | 0.47              |
| 3:J:1346:GLY:O    | 3:J:1350:ASN:ND2  | 2.45                     | 0.47              |
| 6:M:4:D4P:HA      | 6:M:5:MEA:HC1     | 1.57                     | 0.47              |
| 3:D:108:ALA:HB2   | 3:D:280:LYS:HG3   | 1.96                     | 0.47              |
| 5:F:277:MET:HE1   | 5:F:359:LYS:HG2   | 1.97                     | 0.47              |
| 1:H:30:PRO:HB3    | 1:H:198:LEU:HD13  | 1.96                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:H:82:LEU:HD21  | 1:H:171:LEU:HD12  | 1.96                     | 0.47              |
| 2:I:944:ARG:HH21 | 2:I:1050:VAL:HG13 | 1.80                     | 0.47              |
| 3:D:894:VAL:HG13 | 3:D:895:CYS:N     | 2.30                     | 0.47              |
| 5:F:306:PHE:O    | 5:F:308:GLY:N     | 2.48                     | 0.47              |
| 2:I:160:ASP:C    | 2:I:162:GLY:H     | 2.23                     | 0.47              |
| 3:J:893:GLY:O    | 3:J:1258:ARG:NH2  | 2.38                     | 0.47              |
| 3:J:894:VAL:HG13 | 3:J:895:CYS:N     | 2.30                     | 0.47              |
| 3:D:1244:GLN:OE1 | 3:D:1244:GLN:HA   | 2.14                     | 0.47              |
| 5:F:383:ASN:N    | 5:F:383:ASN:ND2   | 2.62                     | 0.47              |
| 5:F:520:GLY:HA2  | 5:F:523:ILE:HD12  | 1.97                     | 0.47              |
| 5:F:590:ILE:HA   | 5:F:593:LYS:HG2   | 1.96                     | 0.47              |
| 1:G:31:LEU:HD13  | 1:G:36:GLY:HA2    | 1.96                     | 0.47              |
| 1:G:95:LYS:HE2   | 1:G:95:LYS:HA     | 1.97                     | 0.47              |
| 1:H:212:ASP:HB2  | 1:H:215:GLU:HG2   | 1.97                     | 0.47              |
| 1:A:30:PRO:HB3   | 1:A:198:LEU:HD13  | 1.97                     | 0.46              |
| 1:A:95:LYS:HA    | 1:A:95:LYS:HE2    | 1.97                     | 0.46              |
| 2:C:1314:GLN:HB2 | 3:D:473:THR:CB    | 2.45                     | 0.46              |
| 5:F:363:ARG:O    | 5:F:367:ILE:HG13  | 2.15                     | 0.46              |
| 2:I:716:ALA:HB3  | 2:I:784:ALA:HB3   | 1.96                     | 0.46              |
| 3:J:857:LEU:HA   | 3:J:858:VAL:HA    | 1.70                     | 0.46              |
| 5:L:387:VAL:HG23 | 5:L:412:LEU:HD22  | 1.97                     | 0.46              |
| 1:A:38:THR:HG23  | 1:B:42:ALA:HA     | 1.97                     | 0.46              |
| 1:B:56:VAL:HG12  | 1:B:173:VAL:HG11  | 1.96                     | 0.46              |
| 3:D:271:ARG:NH1  | 5:F:400:GLN:OE1   | 2.48                     | 0.46              |
| 3:D:410:ASP:O    | 3:D:414:GLU:HG3   | 2.15                     | 0.46              |
| 3:D:452:LEU:HG   | 3:D:625:MET:HE3   | 1.97                     | 0.46              |
| 3:D:811:GLU:OE2  | 3:D:890:THR:OG1   | 2.32                     | 0.46              |
| 5:F:270:VAL:HA   | 5:F:273:MET:HE3   | 1.97                     | 0.46              |
| 2:I:1297:ASP:OD1 | 2:I:1300:GLY:N    | 2.23                     | 0.46              |
| 3:J:510:LEU:O    | 3:J:514:THR:OG1   | 2.33                     | 0.46              |
| 3:J:834:PRO:O    | 3:J:835:LEU:HB2   | 2.15                     | 0.46              |
| 3:J:930:LEU:O    | 3:J:931:THR:HB    | 2.16                     | 0.46              |
| 1:A:152:TYR:CE2  | 2:C:824:GLN:HA    | 2.50                     | 0.46              |
| 1:B:52:PRO:HG3   | 1:B:150:ARG:HH12  | 1.80                     | 0.46              |
| 3:D:210:SER:O    | 3:D:214:ARG:NH2   | 2.47                     | 0.46              |
| 5:F:97:PRO:HB2   | 5:F:402:LEU:HD21  | 1.96                     | 0.46              |
| 5:F:132:CYS:O    | 5:F:136:GLU:HG3   | 2.15                     | 0.46              |
| 1:B:260:LEU:HD23 | 1:B:310:ARG:HH11  | 1.80                     | 0.46              |
| 1:B:321:TRP:HA   | 1:B:321:TRP:CE3   | 2.51                     | 0.46              |
| 3:D:491:LEU:HD21 | 3:D:609:TYR:CZ    | 2.50                     | 0.46              |
| 3:D:546:ALA:O    | 3:D:573:THR:HA    | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1259:LEU:HD12 | 2:I:1260:GLY:N    | 2.30                     | 0.46              |
| 5:L:311:THR:HG21  | 5:L:348:GLU:CD    | 2.40                     | 0.46              |
| 2:C:903:ARG:NH1   | 2:C:908:GLU:OE1   | 2.36                     | 0.46              |
| 1:G:107:ILE:HG13  | 1:G:136:GLU:HG3   | 1.97                     | 0.46              |
| 3:J:298:MET:HG2   | 5:L:402:LEU:HD23  | 1.96                     | 0.46              |
| 4:K:40:PRO:C      | 4:K:42:GLU:H      | 2.23                     | 0.46              |
| 1:A:102:LEU:HG    | 1:A:115:ILE:HG12  | 1.97                     | 0.46              |
| 3:D:297:ARG:HG2   | 5:F:97:PRO:HB3    | 1.97                     | 0.46              |
| 1:H:107:ILE:HG13  | 1:H:136:GLU:HG3   | 1.97                     | 0.46              |
| 3:J:650:LYS:HE3   | 3:J:743:MET:HB2   | 1.98                     | 0.46              |
| 1:A:143:ARG:N     | 1:A:143:ARG:HD2   | 2.31                     | 0.46              |
| 2:C:645:PHE:CG    | 2:C:649:GLN:HB2   | 2.51                     | 0.46              |
| 2:C:867:GLU:OE1   | 2:C:867:GLU:N     | 2.48                     | 0.46              |
| 3:D:816:THR:HG21  | 3:D:889:ASP:HB3   | 1.97                     | 0.46              |
| 2:I:905:ILE:HD11  | 5:L:598:LEU:HD13  | 1.98                     | 0.46              |
| 5:L:557:LYS:HB3   | 5:L:580:PHE:HZ    | 1.81                     | 0.46              |
| 1:A:134:THR:HG21  | 2:C:727:VAL:O     | 2.16                     | 0.46              |
| 2:C:539:THR:O     | 2:C:540:ARG:HB2   | 2.16                     | 0.46              |
| 3:D:141:PHE:CD2   | 3:D:293:ARG:HG3   | 2.50                     | 0.46              |
| 3:D:901:ARG:O     | 3:D:1251:LYS:NZ   | 2.49                     | 0.46              |
| 5:F:383:ASN:HD22  | 5:F:383:ASN:H     | 1.64                     | 0.46              |
| 5:F:437:GLN:HG3   | 5:F:438:ALA:N     | 2.28                     | 0.46              |
| 5:L:134:VAL:HG11  | 5:L:266:PHE:HE1   | 1.81                     | 0.46              |
| 5:L:437:GLN:HG3   | 5:L:438:ALA:N     | 2.30                     | 0.46              |
| 3:D:127:LEU:HD11  | 3:D:227:PHE:CE2   | 2.51                     | 0.46              |
| 3:D:746:LEU:N     | 6:M:1:28H:H11     | 2.31                     | 0.46              |
| 2:I:819:SER:HA    | 2:I:1085:MET:HE3  | 1.97                     | 0.46              |
| 5:L:420:GLU:O     | 5:L:423:ARG:HB2   | 2.15                     | 0.46              |
| 2:C:890:LYS:O     | 2:C:892:GLU:HG3   | 2.16                     | 0.46              |
| 2:I:1328:LYS:HA   | 2:I:1328:LYS:HD3  | 1.80                     | 0.46              |
| 1:A:62:ASP:OD2    | 1:A:143:ARG:NH2   | 2.49                     | 0.45              |
| 3:D:1172:LYS:HA   | 3:D:1192:LYS:H    | 1.81                     | 0.45              |
| 1:G:76:GLU:HB2    | 1:G:80:GLU:HB2    | 1.97                     | 0.45              |
| 3:J:842:ARG:HD2   | 3:J:842:ARG:HA    | 1.57                     | 0.45              |
| 1:A:46:ILE:HG21   | 1:A:220:ALA:HA    | 1.98                     | 0.45              |
| 1:A:321:TRP:HA    | 1:A:321:TRP:CE3   | 2.51                     | 0.45              |
| 2:C:474:ALA:HB1   | 2:C:478:ARG:NH2   | 2.31                     | 0.45              |
| 2:C:1150:ASP:HA   | 2:C:1153:ALA:HB3  | 1.97                     | 0.45              |
| 1:G:86:LYS:NZ     | 2:I:826:ASP:OD2   | 2.49                     | 0.45              |
| 2:I:745:GLU:HA    | 2:I:1014:LEU:HD21 | 1.97                     | 0.45              |
| 2:I:887:VAL:HB    | 2:I:913:VAL:HB    | 1.99                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:J:686:TRP:CD2  | 3:J:758:PRO:HG3   | 2.51                     | 0.45              |
| 6:M:5:MEA:C      | 6:M:7:SER:H       | 2.29                     | 0.45              |
| 1:A:42:ALA:HA    | 1:B:38:THR:HG23   | 1.98                     | 0.45              |
| 2:C:85:CYS:HB3   | 2:C:90:VAL:O      | 2.17                     | 0.45              |
| 3:D:660:GLU:O    | 3:D:664:ILE:HG13  | 2.15                     | 0.45              |
| 3:D:730:ALA:O    | 3:D:731:ARG:HG2   | 2.16                     | 0.45              |
| 3:D:265:LEU:HD23 | 3:D:268:LEU:HD12  | 1.98                     | 0.45              |
| 3:J:374:LEU:O    | 3:J:378:LYS:HG3   | 2.17                     | 0.45              |
| 5:L:584:ARG:O    | 5:L:587:ILE:HG22  | 2.16                     | 0.45              |
| 5:F:462:LYS:HG2  | 5:F:487:MET:HE1   | 1.97                     | 0.45              |
| 1:H:41:ASN:HD21  | 2:I:1217:THR:HG22 | 1.80                     | 0.45              |
| 2:I:67:GLU:N     | 2:I:103:VAL:O     | 2.29                     | 0.45              |
| 2:I:85:CYS:HB3   | 2:I:90:VAL:O      | 2.15                     | 0.45              |
| 5:L:117:ILE:O    | 5:L:121:LYS:HG3   | 2.15                     | 0.45              |
| 2:C:559:CYS:HB2  | 2:C:662:SER:HB3   | 1.98                     | 0.45              |
| 1:A:322:PRO:HB2  | 1:A:323:PRO:CD    | 2.46                     | 0.45              |
| 3:D:37:GLU:HB2   | 3:D:104:HIS:CE1   | 2.51                     | 0.45              |
| 3:D:744:ARG:HE   | 6:M:2:THR:HA      | 1.82                     | 0.45              |
| 5:F:225:ARG:O    | 5:F:229:VAL:HG13  | 2.16                     | 0.45              |
| 5:F:311:THR:HG21 | 5:F:348:GLU:CD    | 2.41                     | 0.45              |
| 5:F:344:LEU:HD12 | 5:F:347:ILE:HD12  | 1.98                     | 0.45              |
| 2:I:933:VAL:HG13 | 2:I:1050:VAL:HG22 | 1.99                     | 0.45              |
| 6:N:1:28H:H6     | 6:N:1:28H:CBX     | 2.46                     | 0.45              |
| 3:D:504:GLN:HB2  | 3:D:505:ASP:H     | 1.56                     | 0.45              |
| 3:D:733:SER:O    | 3:D:737:ILE:HG12  | 2.17                     | 0.45              |
| 1:G:51:MET:HA    | 1:G:52:PRO:HD3    | 1.62                     | 0.45              |
| 2:I:785:ASP:OD2  | 2:I:791:LEU:N     | 2.45                     | 0.45              |
| 2:I:1087:TYR:CE2 | 2:I:1213:TYR:HB2  | 2.51                     | 0.45              |
| 3:J:435:GLN:HB2  | 3:J:457:TYR:OH    | 2.16                     | 0.45              |
| 1:A:62:ASP:CG    | 1:A:143:ARG:HH22  | 2.25                     | 0.45              |
| 2:C:682:GLY:O    | 2:C:686:GLN:HG3   | 2.17                     | 0.45              |
| 1:H:180:VAL:HA   | 1:H:207:THR:HA    | 1.98                     | 0.45              |
| 2:I:562:GLU:OE1  | 2:I:662:SER:OG    | 2.21                     | 0.45              |
| 1:B:195:ARG:O    | 1:B:196:THR:HG22  | 2.17                     | 0.44              |
| 3:D:609:TYR:HA   | 3:D:617:THR:OG1   | 2.16                     | 0.44              |
| 3:D:762:ASN:O    | 3:D:765:GLU:N     | 2.50                     | 0.44              |
| 3:D:930:LEU:O    | 3:D:931:THR:HB    | 2.16                     | 0.44              |
| 2:I:52:ALA:O     | 2:I:56:VAL:HG23   | 2.17                     | 0.44              |
| 2:I:142:GLU:O    | 2:I:515:MET:HB2   | 2.17                     | 0.44              |
| 2:I:338:THR:HG21 | 2:I:345:PRO:HB3   | 2.00                     | 0.44              |
| 2:I:539:THR:O    | 2:I:540:ARG:HB2   | 2.16                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1212:LEU:HB3  | 2:I:1221:PHE:HD2  | 1.81                     | 0.44              |
| 2:I:1246:ARG:NE   | 3:J:348:ASP:OD1   | 2.48                     | 0.44              |
| 3:J:425:ARG:HB2   | 3:J:466:MET:HG2   | 1.98                     | 0.44              |
| 1:A:51:MET:HA     | 1:A:52:PRO:HD3    | 1.67                     | 0.44              |
| 2:I:15:PHE:HE2    | 2:I:1198:LEU:HD11 | 1.82                     | 0.44              |
| 2:I:84:GLU:OE2    | 2:I:1035:LYS:HD2  | 2.17                     | 0.44              |
| 2:I:801:ARG:HE    | 2:I:1227:VAL:HG11 | 1.82                     | 0.44              |
| 2:I:844:LYS:HE3   | 3:J:49:PHE:CZ     | 2.51                     | 0.44              |
| 5:L:513:ASP:CG    | 5:L:515:GLU:H     | 2.24                     | 0.44              |
| 6:M:2:THR:CG2     | 6:M:6:2TL:O       | 2.63                     | 0.44              |
| 6:N:5:MEA:C       | 6:N:7:SER:H       | 2.29                     | 0.44              |
| 1:A:279:GLY:O     | 1:A:283:GLN:HG3   | 2.18                     | 0.44              |
| 2:C:756:TYR:H     | 2:C:766:ASN:HB3   | 1.82                     | 0.44              |
| 2:I:101:ARG:HB2   | 2:I:117:ILE:HD12  | 1.99                     | 0.44              |
| 2:I:1077:SER:HA   | 3:J:356:THR:HB    | 1.99                     | 0.44              |
| 5:L:487:MET:HA    | 5:L:487:MET:HE2   | 2.00                     | 0.44              |
| 4:E:79:GLU:O      | 4:E:82:ALA:N      | 2.50                     | 0.44              |
| 5:F:117:ILE:O     | 5:F:121:LYS:HG3   | 2.17                     | 0.44              |
| 3:J:781:LYS:HB3   | 6:N:5:MEA:HD1     | 1.99                     | 0.44              |
| 5:L:509:THR:HA    | 5:L:510:PRO:HD3   | 1.87                     | 0.44              |
| 5:L:559:LEU:HG    | 5:L:563:PHE:HE2   | 1.83                     | 0.44              |
| 1:A:22:THR:HB     | 1:A:207:THR:O     | 2.17                     | 0.44              |
| 3:D:502:PRO:HB3   | 3:D:506:VAL:HG11  | 2.00                     | 0.44              |
| 3:D:1164:SER:N    | 3:D:1178:THR:O    | 2.39                     | 0.44              |
| 1:H:51:MET:HA     | 1:H:52:PRO:HD3    | 1.78                     | 0.44              |
| 5:L:407:GLU:HG3   | 5:L:442:SER:OG    | 2.17                     | 0.44              |
| 6:M:2:THR:HG23    | 6:M:6:2TL:OG1     | 2.17                     | 0.44              |
| 1:B:321:TRP:HA    | 1:B:322:PRO:HA    | 1.69                     | 0.44              |
| 2:C:344:GLY:HA3   | 2:C:346:TYR:CZ    | 2.53                     | 0.44              |
| 2:C:930:ASP:HB2   | 2:C:1053:TYR:HB2  | 2.00                     | 0.44              |
| 1:G:68:TYR:CG     | 2:I:929:ILE:HG21  | 2.53                     | 0.44              |
| 1:H:124:VAL:HG21  | 1:H:210:THR:HB    | 2.00                     | 0.44              |
| 2:I:1226:THR:HG23 | 3:J:638:SER:OG    | 2.17                     | 0.44              |
| 3:J:288:PRO:HG3   | 5:L:377:LYS:HG3   | 1.99                     | 0.44              |
| 3:J:377:PHE:HE1   | 3:J:419:HIS:ND1   | 2.16                     | 0.44              |
| 5:L:261:LEU:HB2   | 5:L:266:PHE:CE2   | 2.53                     | 0.44              |
| 2:C:960:LEU:HD22  | 2:C:1029:LEU:HD12 | 2.00                     | 0.44              |
| 3:D:650:LYS:HE3   | 3:D:743:MET:HB2   | 1.99                     | 0.44              |
| 5:F:137:TYR:O     | 5:F:141:ILE:HG12  | 2.18                     | 0.44              |
| 2:I:176:ILE:HD12  | 2:I:184:LEU:HD23  | 2.00                     | 0.44              |
| 3:J:179:LYS:HB2   | 3:J:184:ALA:HB2   | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:124:VAL:HG21 | 1:B:210:THR:HG22 | 2.00                     | 0.44              |
| 5:F:137:TYR:HE2  | 5:F:273:MET:HB3  | 1.82                     | 0.44              |
| 2:I:1243:MET:SD  | 3:J:445:LYS:HB3  | 2.57                     | 0.44              |
| 2:I:1330:ILE:O   | 2:I:1333:LEU:HB2 | 2.18                     | 0.44              |
| 3:J:730:ALA:O    | 3:J:731:ARG:HG2  | 2.17                     | 0.44              |
| 3:J:787:ALA:O    | 3:J:790:THR:HG23 | 2.17                     | 0.44              |
| 5:L:132:CYS:O    | 5:L:136:GLU:HG3  | 2.18                     | 0.44              |
| 5:L:145:LEU:HB3  | 5:L:225:ARG:HH21 | 1.82                     | 0.44              |
| 5:L:433:TRP:O    | 5:L:437:GLN:HB3  | 2.17                     | 0.44              |
| 1:A:82:LEU:O     | 1:A:86:LYS:HG3   | 2.18                     | 0.44              |
| 2:C:901:LEU:HD13 | 5:F:563:PHE:CE2  | 2.53                     | 0.44              |
| 2:C:936:ARG:HG3  | 2:C:936:ARG:NH2  | 2.06                     | 0.44              |
| 3:D:746:LEU:O    | 6:M:1:28H:H12    | 2.18                     | 0.44              |
| 1:H:76:GLU:HB2   | 1:H:80:GLU:HB2   | 2.00                     | 0.44              |
| 5:L:354:THR:HG22 | 5:L:357:GLN:NE2  | 2.31                     | 0.44              |
| 1:A:287:VAL:O    | 1:A:291:LYS:HG3  | 2.17                     | 0.43              |
| 1:B:82:LEU:O     | 1:B:86:LYS:HG3   | 2.18                     | 0.43              |
| 2:C:903:ARG:O    | 2:C:907:GLY:N    | 2.52                     | 0.43              |
| 3:D:481:ARG:HA   | 3:D:485:MET:HG2  | 2.00                     | 0.43              |
| 1:H:152:TYR:CD1  | 1:H:176:CYS:HA   | 2.52                     | 0.43              |
| 2:I:677:ASN:HD22 | 2:I:677:ASN:H    | 1.66                     | 0.43              |
| 3:J:212:THR:O    | 3:J:216:LYS:HG2  | 2.18                     | 0.43              |
| 1:A:143:ARG:HE   | 1:B:254:LEU:HD11 | 1.82                     | 0.43              |
| 5:F:420:GLU:O    | 5:F:423:ARG:HB2  | 2.18                     | 0.43              |
| 3:J:189:LEU:HD12 | 3:J:238:ILE:HD13 | 2.00                     | 0.43              |
| 6:N:2:THR:HG23   | 6:N:6:2TL:OG1    | 2.17                     | 0.43              |
| 1:B:180:VAL:HG11 | 1:B:183:ILE:HD11 | 2.00                     | 0.43              |
| 2:C:155:VAL:HG12 | 2:C:405:PHE:HA   | 2.00                     | 0.43              |
| 2:C:890:LYS:HE2  | 2:C:914:LYS:HG3  | 1.99                     | 0.43              |
| 3:D:232:ASN:ND2  | 3:D:1337:VAL:O   | 2.51                     | 0.43              |
| 2:I:221:LEU:HD22 | 2:I:336:LEU:HD11 | 2.01                     | 0.43              |
| 3:D:781:LYS:CB   | 6:M:5:MEA:HD1    | 2.48                     | 0.43              |
| 3:D:792:ASN:CG   | 3:D:932:MET:HE1  | 2.44                     | 0.43              |
| 1:H:82:LEU:O     | 1:H:86:LYS:HG3   | 2.18                     | 0.43              |
| 5:L:137:TYR:O    | 5:L:141:ILE:HG12 | 2.18                     | 0.43              |
| 1:B:51:MET:HB3   | 1:B:179:PRO:HD2  | 1.99                     | 0.43              |
| 3:D:109:SER:OG   | 3:D:296:LYS:HE2  | 2.17                     | 0.43              |
| 5:F:440:THR:HA   | 5:F:443:ILE:HD11 | 2.00                     | 0.43              |
| 2:I:392:GLU:HA   | 2:I:395:TYR:O    | 2.19                     | 0.43              |
| 3:J:190:LYS:HG3  | 3:J:235:GLU:CD   | 2.44                     | 0.43              |
| 6:M:1:28H:H6     | 6:M:1:28H:CBX    | 2.46                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:279:GLY:O    | 1:B:283:GLN:HG3   | 2.19                     | 0.43              |
| 3:D:554:GLU:HA   | 3:D:580:TRP:CZ2   | 2.53                     | 0.43              |
| 3:D:646:ILE:HG12 | 3:D:741:ALA:O     | 2.18                     | 0.43              |
| 1:G:41:ASN:ND2   | 1:G:44:ARG:NH2    | 2.67                     | 0.43              |
| 3:J:452:LEU:HG   | 3:J:625:MET:CE    | 2.48                     | 0.43              |
| 5:L:344:LEU:HD12 | 5:L:344:LEU:HA    | 1.86                     | 0.43              |
| 1:B:273:GLU:OE2  | 1:B:293:PRO:HD2   | 2.19                     | 0.43              |
| 3:D:763:PHE:HD1  | 3:D:763:PHE:HA    | 1.71                     | 0.43              |
| 1:G:68:TYR:CZ    | 2:I:1055:ALA:HB1  | 2.54                     | 0.43              |
| 1:G:74:VAL:HG11  | 1:G:81:ILE:HD11   | 1.99                     | 0.43              |
| 3:J:109:SER:OG   | 3:J:296:LYS:HE2   | 2.19                     | 0.43              |
| 3:J:1319:PHE:CE2 | 3:J:1342:ASP:HB2  | 2.54                     | 0.43              |
| 5:L:134:VAL:HA   | 5:L:273:MET:HE1   | 2.01                     | 0.43              |
| 1:B:27:THR:HG22  | 1:B:202:VAL:HG13  | 2.00                     | 0.43              |
| 2:C:478:ARG:HE   | 2:C:478:ARG:HB2   | 1.62                     | 0.43              |
| 2:C:870:ILE:HG21 | 2:C:944:ARG:NH2   | 2.34                     | 0.43              |
| 2:I:1214:ASP:OD2 | 2:I:1216:ARG:NH1  | 2.52                     | 0.43              |
| 3:J:762:ASN:O    | 3:J:765:GLU:N     | 2.51                     | 0.43              |
| 3:J:1318:SER:OG  | 3:J:1342:ASP:OD2  | 2.35                     | 0.43              |
| 5:L:306:PHE:C    | 5:L:308:GLY:H     | 2.27                     | 0.43              |
| 5:L:499:LYS:O    | 5:L:501:ALA:N     | 2.51                     | 0.43              |
| 1:A:319:GLU:O    | 1:A:319:GLU:HG3   | 2.18                     | 0.43              |
| 3:J:188:LEU:O    | 3:J:192:MET:HB3   | 2.19                     | 0.43              |
| 3:J:492:SER:HA   | 3:J:493:PRO:HD3   | 1.84                     | 0.43              |
| 3:J:899:TYR:CZ   | 3:J:1251:LYS:HD2  | 2.54                     | 0.43              |
| 1:A:56:VAL:HG12  | 1:A:173:VAL:HG11  | 1.99                     | 0.43              |
| 3:D:678:ARG:NH2  | 3:D:756:GLU:OE1   | 2.51                     | 0.43              |
| 3:D:865:HIS:HB3  | 3:D:868:TRP:CD1   | 2.48                     | 0.43              |
| 5:F:270:VAL:HA   | 5:F:273:MET:HG3   | 2.00                     | 0.43              |
| 5:F:509:THR:HA   | 5:F:510:PRO:HD3   | 1.89                     | 0.43              |
| 2:I:906:PHE:HB3  | 2:I:907:GLY:H     | 1.54                     | 0.43              |
| 5:L:253:SER:O    | 5:L:257:LYS:HG3   | 2.19                     | 0.43              |
| 2:C:590:PRO:HG2  | 2:C:659:GLN:NE2   | 2.34                     | 0.42              |
| 2:I:844:LYS:HE3  | 3:J:49:PHE:CE2    | 2.54                     | 0.42              |
| 1:B:214:GLU:O    | 1:B:218:ARG:HG3   | 2.20                     | 0.42              |
| 2:C:213:LEU:HD13 | 2:C:422:LYS:HB2   | 2.01                     | 0.42              |
| 1:G:28:LEU:HD12  | 1:G:201:LEU:HD23  | 2.01                     | 0.42              |
| 1:H:47:LEU:HA    | 1:H:51:MET:HG2    | 1.99                     | 0.42              |
| 1:H:52:PRO:HG3   | 1:H:150:ARG:NH1   | 2.34                     | 0.42              |
| 2:I:957:LYS:HA   | 2:I:1029:LEU:HD11 | 2.01                     | 0.42              |
| 1:A:224:LEU:HD23 | 1:B:228:LEU:HD11  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:69:GLU:HG3   | 3:D:76:LYS:HG2    | 2.00                     | 0.42              |
| 3:D:612:LEU:HD22 | 3:D:612:LEU:O     | 2.18                     | 0.42              |
| 3:D:761:ALA:HB3  | 3:D:767:LEU:HB3   | 2.01                     | 0.42              |
| 4:E:39:VAL:HA    | 4:E:40:PRO:CB     | 2.49                     | 0.42              |
| 5:F:101:TYR:CE2  | 5:F:405:ILE:HD13  | 2.54                     | 0.42              |
| 1:H:211:ILE:HD12 | 1:H:215:GLU:HG3   | 2.01                     | 0.42              |
| 3:J:514:THR:O    | 3:J:595:ALA:HA    | 2.19                     | 0.42              |
| 5:L:259:PHE:O    | 5:L:261:LEU:HD12  | 2.19                     | 0.42              |
| 5:L:296:LYS:HD3  | 5:L:296:LYS:HA    | 1.78                     | 0.42              |
| 5:L:402:LEU:HD12 | 5:L:402:LEU:HA    | 1.84                     | 0.42              |
| 1:B:263:THR:HG22 | 2:C:947:GLU:HG2   | 2.00                     | 0.42              |
| 1:B:322:PRO:HB2  | 1:B:323:PRO:HD3   | 2.01                     | 0.42              |
| 2:C:180:ARG:NH2  | 2:C:392:GLU:O     | 2.52                     | 0.42              |
| 2:C:802:VAL:HG12 | 2:C:1228:GLY:O    | 2.19                     | 0.42              |
| 2:C:972:PHE:HB3  | 2:C:994:ARG:HH21  | 1.83                     | 0.42              |
| 5:F:300:LYS:HB3  | 5:F:300:LYS:HE3   | 1.80                     | 0.42              |
| 1:H:29:GLU:CB    | 1:H:30:PRO:HD2    | 2.48                     | 0.42              |
| 2:I:890:LYS:HG2  | 2:I:914:LYS:HE3   | 2.00                     | 0.42              |
| 3:J:836:ARG:O    | 3:J:840:LEU:N     | 2.49                     | 0.42              |
| 5:L:383:ASN:O    | 5:L:385:ARG:N     | 2.52                     | 0.42              |
| 5:L:598:LEU:HD23 | 5:L:598:LEU:HA    | 1.93                     | 0.42              |
| 2:C:619:ALA:HA   | 2:C:653:MET:HE3   | 2.00                     | 0.42              |
| 3:D:113:HIS:CD2  | 3:D:115:TRP:H     | 2.37                     | 0.42              |
| 3:D:506:VAL:HG13 | 3:D:628:GLY:HA3   | 2.01                     | 0.42              |
| 5:F:397:ARG:HH12 | 5:F:461:ASN:ND2   | 2.17                     | 0.42              |
| 1:H:74:VAL:HG11  | 1:H:81:ILE:HD11   | 2.02                     | 0.42              |
| 2:I:1125:GLY:HA3 | 2:I:1179:GLY:HA2  | 2.01                     | 0.42              |
| 3:J:50:LYS:HA    | 3:J:50:LYS:HD3    | 1.84                     | 0.42              |
| 3:J:814:CYS:HB3  | 3:J:890:THR:OG1   | 2.19                     | 0.42              |
| 6:N:1:28H:H3     | 6:N:1:28H:H10     | 1.81                     | 0.42              |
| 1:B:9:LEU:HD23   | 1:B:9:LEU:HA      | 1.81                     | 0.42              |
| 2:C:714:VAL:O    | 2:C:767:GLN:NE2   | 2.46                     | 0.42              |
| 3:D:16:GLU:HG2   | 3:D:16:GLU:O      | 2.20                     | 0.42              |
| 3:D:1272:SER:HB3 | 3:D:1292:LEU:HD11 | 2.00                     | 0.42              |
| 2:I:933:VAL:HG11 | 2:I:944:ARG:HG3   | 2.00                     | 0.42              |
| 3:J:744:ARG:HE   | 6:N:2:THR:HA      | 1.84                     | 0.42              |
| 5:L:121:LYS:HE2  | 5:L:421:TYR:OH    | 2.20                     | 0.42              |
| 1:A:190:ALA:H    | 1:A:199:ASP:HA    | 1.85                     | 0.42              |
| 3:D:787:ALA:O    | 3:D:790:THR:HG23  | 2.20                     | 0.42              |
| 1:G:76:GLU:CD    | 1:G:76:GLU:H      | 2.28                     | 0.42              |
| 2:I:1336:ASN:HB2 | 3:J:25:ALA:HB2    | 2.02                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:J:660:GLU:O    | 3:J:664:ILE:HG13  | 2.20                     | 0.42              |
| 3:J:749:LYS:HB2  | 3:J:753:SER:O     | 2.20                     | 0.42              |
| 1:A:33:ARG:C     | 1:A:35:PHE:H      | 2.28                     | 0.42              |
| 1:B:29:GLU:CD    | 1:B:30:PRO:HD2    | 2.45                     | 0.42              |
| 2:C:152:SER:OG   | 2:C:452:ARG:HG2   | 2.19                     | 0.42              |
| 2:C:728:ASP:HB3  | 2:C:731:ARG:H     | 1.84                     | 0.42              |
| 2:C:1328:LYS:HA  | 2:C:1328:LYS:HD3  | 1.82                     | 0.42              |
| 5:F:97:PRO:HB2   | 5:F:402:LEU:CD2   | 2.50                     | 0.42              |
| 5:F:306:PHE:C    | 5:F:308:GLY:H     | 2.28                     | 0.42              |
| 2:I:346:TYR:O    | 2:I:350:THR:N     | 2.49                     | 0.42              |
| 2:I:589:THR:OG1  | 2:I:659:GLN:NE2   | 2.53                     | 0.42              |
| 3:J:796:LEU:HD22 | 3:J:1138:LEU:HD11 | 2.01                     | 0.42              |
| 6:N:2:THR:CG2    | 6:N:6:2TL:O       | 2.63                     | 0.42              |
| 1:B:10:LYS:CB    | 1:B:11:PRO:HD2    | 2.35                     | 0.42              |
| 2:C:367:TYR:CD1  | 2:C:376:PRO:HB3   | 2.55                     | 0.42              |
| 2:C:626:GLU:HA   | 2:C:627:GLY:C     | 2.45                     | 0.42              |
| 2:C:677:ASN:ND2  | 2:C:677:ASN:N     | 2.68                     | 0.42              |
| 2:C:890:LYS:HG2  | 2:C:914:LYS:CG    | 2.49                     | 0.42              |
| 5:F:584:ARG:O    | 5:F:587:ILE:HG22  | 2.20                     | 0.42              |
| 2:I:227:LYS:NZ   | 2:I:334:GLU:OE2   | 2.53                     | 0.42              |
| 2:I:674:ASP:OD2  | 2:I:1070:HIS:ND1  | 2.39                     | 0.42              |
| 5:L:228:TYR:C    | 5:L:228:TYR:CD1   | 2.98                     | 0.42              |
| 5:L:409:ASN:O    | 5:L:413:MET:HG3   | 2.20                     | 0.42              |
| 1:A:76:GLU:HB2   | 1:A:80:GLU:HB2    | 2.01                     | 0.42              |
| 1:B:101:THR:OG1  | 1:B:116:THR:OG1   | 2.30                     | 0.42              |
| 3:J:597:GLY:O    | 3:J:601:ILE:N     | 2.44                     | 0.42              |
| 3:J:907:HIS:CG   | 3:J:908:ILE:N     | 2.88                     | 0.42              |
| 3:J:930:LEU:HA   | 3:J:1244:GLN:HG3  | 2.01                     | 0.42              |
| 5:L:316:PHE:CE2  | 5:L:334:SER:HA    | 2.55                     | 0.42              |
| 1:B:83:LEU:CD1   | 3:D:528:THR:HA    | 2.48                     | 0.41              |
| 2:C:1085:MET:HG2 | 2:C:1094:VAL:O    | 2.20                     | 0.41              |
| 2:C:1307:ASN:O   | 2:C:1311:GLY:N    | 2.53                     | 0.41              |
| 3:D:195:GLU:HA   | 3:D:198:CYS:SG    | 2.60                     | 0.41              |
| 3:D:242:LEU:HA   | 3:D:243:PRO:HD3   | 1.92                     | 0.41              |
| 3:D:1360:GLY:HA2 | 4:E:17:PHE:CE1    | 2.56                     | 0.41              |
| 5:F:316:PHE:CE2  | 5:F:334:SER:HA    | 2.55                     | 0.41              |
| 2:I:130:MET:SD   | 2:I:134:GLY:HA2   | 2.60                     | 0.41              |
| 2:I:675:ASP:HA   | 3:J:763:PHE:HZ    | 1.84                     | 0.41              |
| 5:L:300:LYS:HB3  | 5:L:300:LYS:HE3   | 1.81                     | 0.41              |
| 1:A:207:THR:HG23 | 1:A:209:GLY:H     | 1.86                     | 0.41              |
| 1:B:37:HIS:CD2   | 2:C:1216:ARG:HG2  | 2.55                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:176:ILE:HD12  | 2:C:184:LEU:HD23 | 2.02                     | 0.41              |
| 3:D:22:ILE:O      | 3:D:1339:GLY:HA2 | 2.19                     | 0.41              |
| 3:D:46:TYR:HB3    | 5:F:451:ARG:O    | 2.20                     | 0.41              |
| 3:D:573:THR:O     | 3:D:577:ALA:N    | 2.42                     | 0.41              |
| 1:G:179:PRO:HA    | 1:G:208:ASN:ND2  | 2.36                     | 0.41              |
| 2:I:151:ARG:H     | 2:I:151:ARG:HG2  | 1.34                     | 0.41              |
| 2:I:1187:PHE:HZ   | 3:J:772:TYR:CG   | 2.37                     | 0.41              |
| 2:I:1244:HIS:HB2  | 2:I:1265:PHE:CD1 | 2.55                     | 0.41              |
| 5:F:354:THR:CG2   | 5:F:357:GLN:HE21 | 2.33                     | 0.41              |
| 5:F:548:LEU:HA    | 5:F:551:LEU:HD21 | 2.03                     | 0.41              |
| 2:I:145:ILE:HB    | 2:I:456:VAL:HG13 | 2.02                     | 0.41              |
| 2:I:1186:VAL:HG13 | 2:I:1187:PHE:CD1 | 2.50                     | 0.41              |
| 3:J:419:HIS:O     | 3:J:439:PRO:HD2  | 2.21                     | 0.41              |
| 3:J:527:LEU:C     | 3:J:529:GLY:H    | 2.19                     | 0.41              |
| 5:L:276:MET:SD    | 5:L:279:ARG:NH2  | 2.93                     | 0.41              |
| 3:D:597:GLY:O     | 3:D:601:ILE:N    | 2.46                     | 0.41              |
| 3:D:1169:THR:HA   | 3:D:1174:ARG:CB  | 2.50                     | 0.41              |
| 5:F:228:TYR:C     | 5:F:228:TYR:CD1  | 2.99                     | 0.41              |
| 5:F:234:THR:HG21  | 5:F:248:GLU:OE2  | 2.19                     | 0.41              |
| 5:F:530:LEU:HA    | 5:F:531:PRO:HD3  | 1.88                     | 0.41              |
| 2:I:474:ALA:HB1   | 2:I:478:ARG:NH2  | 2.34                     | 0.41              |
| 3:J:451:PRO:HB2   | 3:J:625:MET:HE2  | 2.03                     | 0.41              |
| 5:L:277:MET:CE    | 5:L:359:LYS:HG2  | 2.45                     | 0.41              |
| 1:A:29:GLU:HG3    | 1:A:30:PRO:HD2   | 2.03                     | 0.41              |
| 3:D:187:ALA:O     | 3:D:191:SER:HB2  | 2.21                     | 0.41              |
| 5:F:559:LEU:O     | 5:F:563:PHE:HD2  | 2.04                     | 0.41              |
| 1:G:75:GLN:HB3    | 1:G:132:HIS:HB2  | 2.02                     | 0.41              |
| 1:H:129:VAL:HG11  | 1:H:132:HIS:CE1  | 2.56                     | 0.41              |
| 2:I:27:LEU:HD11   | 2:I:663:VAL:HG21 | 2.03                     | 0.41              |
| 2:I:1289:GLU:HB3  | 2:I:1294:LYS:HD2 | 2.01                     | 0.41              |
| 3:J:746:LEU:HD22  | 3:J:746:LEU:N    | 2.35                     | 0.41              |
| 1:H:88:LEU:HD23   | 1:H:88:LEU:HA    | 1.91                     | 0.41              |
| 2:I:448:LEU:HD23  | 2:I:448:LEU:HA   | 1.88                     | 0.41              |
| 2:I:690:VAL:HA    | 2:I:691:PRO:HD3  | 1.96                     | 0.41              |
| 3:J:775:SER:O     | 3:J:778:GLY:N    | 2.54                     | 0.41              |
| 6:N:4:D4P:HA      | 6:N:5:MEA:HC1    | 1.57                     | 0.41              |
| 3:D:261:ALA:HA    | 5:F:505:ILE:O    | 2.21                     | 0.41              |
| 5:F:344:LEU:HD12  | 5:F:344:LEU:HA   | 1.90                     | 0.41              |
| 5:F:440:THR:O     | 5:F:443:ILE:HG12 | 2.21                     | 0.41              |
| 3:J:738:ARG:NH2   | 6:N:1:28H:OCD    | 2.53                     | 0.41              |
| 3:J:775:SER:O     | 3:J:776:THR:C    | 2.64                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:J:816:THR:CG2  | 3:J:889:ASP:HB3   | 2.51                     | 0.41              |
| 5:L:337:VAL:O    | 5:L:341:LEU:HG    | 2.21                     | 0.41              |
| 5:L:379:MET:HG2  | 5:L:416:VAL:HG13  | 2.03                     | 0.41              |
| 1:B:287:VAL:O    | 1:B:291:LYS:HG3   | 2.21                     | 0.41              |
| 3:D:527:LEU:CB   | 3:D:533:ALA:HB2   | 2.51                     | 0.41              |
| 5:F:143:TYR:OH   | 5:F:265:GLN:OE1   | 2.18                     | 0.41              |
| 5:F:269:LEU:O    | 5:F:272:SER:HB3   | 2.21                     | 0.41              |
| 5:F:352:GLY:O    | 5:F:353:LEU:HD23  | 2.21                     | 0.41              |
| 5:F:355:ILE:HD12 | 5:F:356:GLU:H     | 1.85                     | 0.41              |
| 5:F:585:GLU:OE1  | 5:F:588:ARG:NH2   | 2.54                     | 0.41              |
| 1:G:179:PRO:HA   | 1:G:208:ASN:HD21  | 1.86                     | 0.41              |
| 1:G:219:ARG:O    | 1:G:223:ILE:HG13  | 2.20                     | 0.41              |
| 1:H:56:VAL:HG12  | 1:H:173:VAL:HG11  | 2.02                     | 0.41              |
| 2:I:682:GLY:O    | 2:I:686:GLN:HG3   | 2.21                     | 0.41              |
| 3:J:233:LYS:HB2  | 3:J:236:TRP:CE2   | 2.56                     | 0.41              |
| 3:J:418:GLU:O    | 3:J:481:ARG:NH1   | 2.54                     | 0.41              |
| 3:J:813:ASP:HB2  | 3:J:897:HIS:HD2   | 1.86                     | 0.41              |
| 2:C:24:VAL:HA    | 2:C:25:PRO:HD3    | 1.93                     | 0.41              |
| 2:C:812:PHE:CE2  | 3:D:451:PRO:HB3   | 2.56                     | 0.41              |
| 3:D:739:GLN:OE1  | 3:D:739:GLN:CA    | 2.64                     | 0.41              |
| 5:F:355:ILE:HD12 | 5:F:356:GLU:HG3   | 2.03                     | 0.41              |
| 2:I:61:SER:OG    | 2:I:62:TYR:N      | 2.53                     | 0.41              |
| 2:I:972:PHE:HB3  | 2:I:994:ARG:HH21  | 1.86                     | 0.41              |
| 3:J:291:ILE:HD12 | 5:L:413:MET:HE3   | 2.03                     | 0.41              |
| 3:J:690:ASN:CG   | 3:J:743:MET:HE3   | 2.46                     | 0.41              |
| 5:L:120:ALA:HA   | 5:L:123:ILE:HD12  | 2.03                     | 0.41              |
| 5:L:134:VAL:HG11 | 5:L:266:PHE:CE1   | 2.56                     | 0.41              |
| 5:L:245:ALA:O    | 5:L:249:ILE:HG13  | 2.20                     | 0.41              |
| 2:C:38:PHE:HA    | 2:C:48:GLY:HA2    | 2.04                     | 0.40              |
| 2:C:373:GLY:HA3  | 5:F:99:ARG:NH1    | 2.37                     | 0.40              |
| 2:C:957:LYS:HA   | 2:C:1029:LEU:HD11 | 2.03                     | 0.40              |
| 1:H:68:TYR:O     | 1:H:68:TYR:CG     | 2.73                     | 0.40              |
| 2:I:205:PRO:O    | 2:I:208:ILE:HG22  | 2.21                     | 0.40              |
| 2:I:213:LEU:HD13 | 2:I:422:LYS:HB2   | 2.03                     | 0.40              |
| 2:I:677:ASN:H    | 2:I:677:ASN:ND2   | 2.18                     | 0.40              |
| 2:I:836:LEU:HB3  | 2:I:918:LEU:HD21  | 2.02                     | 0.40              |
| 2:I:960:LEU:HD22 | 2:I:1029:LEU:HD12 | 2.03                     | 0.40              |
| 2:I:1246:ARG:CZ  | 2:I:1258:PRO:HB3  | 2.51                     | 0.40              |
| 3:J:141:PHE:HB3  | 3:J:293:ARG:HD3   | 2.02                     | 0.40              |
| 3:J:261:ALA:HA   | 5:L:505:ILE:O     | 2.21                     | 0.40              |
| 3:J:704:GLU:O    | 3:J:715:LYS:HA    | 2.21                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:L:420:GLU:HB2   | 5:L:423:ARG:HH11 | 1.86                     | 0.40              |
| 2:C:52:ALA:O      | 2:C:56:VAL:HG23  | 2.20                     | 0.40              |
| 2:C:392:GLU:HA    | 2:C:395:TYR:O    | 2.21                     | 0.40              |
| 2:C:821:ARG:HA    | 2:C:824:GLN:HB2  | 2.04                     | 0.40              |
| 5:F:337:VAL:O     | 5:F:341:LEU:HG   | 2.22                     | 0.40              |
| 5:F:551:LEU:HD23  | 5:F:556:ALA:HB2  | 2.03                     | 0.40              |
| 2:I:802:VAL:HG12  | 2:I:1228:GLY:O   | 2.22                     | 0.40              |
| 3:J:1196:LEU:CB   | 3:J:1211:SER:HA  | 2.51                     | 0.40              |
| 1:A:63:GLY:H      | 1:B:259:ASP:CG   | 2.29                     | 0.40              |
| 1:B:32:GLU:HA     | 1:B:198:LEU:HD22 | 2.03                     | 0.40              |
| 2:C:374:GLU:HA    | 2:C:375:PRO:HD3  | 1.89                     | 0.40              |
| 2:C:623:LEU:C     | 2:C:625:GLU:H    | 2.28                     | 0.40              |
| 2:C:1247:SER:HB3  | 3:D:375:GLU:O    | 2.21                     | 0.40              |
| 5:F:598:LEU:HD23  | 5:F:598:LEU:HA   | 1.90                     | 0.40              |
| 2:I:61:SER:C      | 2:I:64:GLY:H     | 2.29                     | 0.40              |
| 2:I:797:GLY:N     | 2:I:1231:TYR:OH  | 2.54                     | 0.40              |
| 3:J:706:VAL:O     | 3:J:714:GLU:N    | 2.30                     | 0.40              |
| 5:L:101:TYR:CE2   | 5:L:405:ILE:HD13 | 2.56                     | 0.40              |
| 5:L:271:ASN:O     | 5:L:275:VAL:HG23 | 2.22                     | 0.40              |
| 2:C:225:PHE:CB    | 2:C:336:LEU:HD22 | 2.51                     | 0.40              |
| 2:C:948:ILE:O     | 2:C:952:GLN:HG3  | 2.21                     | 0.40              |
| 3:D:801:VAL:O     | 3:D:805:GLN:HB2  | 2.22                     | 0.40              |
| 5:F:138:PRO:O     | 5:F:142:THR:HG23 | 2.21                     | 0.40              |
| 5:F:253:SER:O     | 5:F:257:LYS:HG3  | 2.21                     | 0.40              |
| 2:I:1297:ASP:OD1  | 2:I:1297:ASP:C   | 2.64                     | 0.40              |
| 3:J:264:ASP:HB3   | 3:J:324:LEU:HB3  | 2.03                     | 0.40              |
| 3:J:265:LEU:HD23  | 3:J:265:LEU:HA   | 1.87                     | 0.40              |
| 3:J:278:ARG:HD3   | 5:L:406:GLN:HB3  | 2.03                     | 0.40              |
| 3:J:738:ARG:O     | 3:J:742:GLY:N    | 2.54                     | 0.40              |
| 3:J:1224:ARG:HB3  | 3:J:1228:ALA:CB  | 2.51                     | 0.40              |
| 5:L:415:ALA:HB2   | 5:L:434:TRP:HB2  | 2.04                     | 0.40              |
| 2:C:1150:ASP:HA   | 2:C:1153:ALA:CB  | 2.51                     | 0.40              |
| 3:D:50:LYS:HA     | 3:D:50:LYS:HD3   | 1.84                     | 0.40              |
| 3:D:740:LEU:O     | 3:D:764:ARG:HB2  | 2.21                     | 0.40              |
| 3:D:910:ASN:HB3   | 4:E:15:ASN:HA    | 2.03                     | 0.40              |
| 5:F:513:ASP:CG    | 5:F:514:ASP:N    | 2.80                     | 0.40              |
| 1:G:151:GLY:O     | 1:G:177:TYR:HB2  | 2.21                     | 0.40              |
| 1:G:170:ARG:NE    | 1:G:170:ARG:HA   | 2.37                     | 0.40              |
| 2:I:805:MET:HE1   | 2:I:1221:PHE:CD1 | 2.57                     | 0.40              |
| 2:I:1101:LEU:HD23 | 3:J:725:MET:SD   | 2.61                     | 0.40              |
| 3:J:1291:GLU:O    | 3:J:1295:ASN:HB2 | 2.22                     | 0.40              |

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

| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 5:F:218:ARG:NH2 | 5:L:149:ASP:OD1[1_545] | 2.05                     | 0.15              |
| 1:B:292:THR:O   | 1:H:68:TYR:OH[4_555]   | 2.19                     | 0.01              |

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|----------|-------------|----|
| 1   | A     | 292/335 (87%)    | 261 (89%)  | 19 (6%)  | 12 (4%)  | 2           | 20 |
| 1   | B     | 281/335 (84%)    | 252 (90%)  | 13 (5%)  | 16 (6%)  | 1           | 16 |
| 1   | G     | 212/335 (63%)    | 193 (91%)  | 14 (7%)  | 5 (2%)   | 4           | 29 |
| 1   | H     | 211/335 (63%)    | 193 (92%)  | 13 (6%)  | 5 (2%)   | 4           | 29 |
| 2   | C     | 1338/1342 (100%) | 1265 (94%) | 55 (4%)  | 18 (1%)  | 9           | 40 |
| 2   | I     | 1338/1342 (100%) | 1265 (94%) | 54 (4%)  | 19 (1%)  | 9           | 38 |
| 3   | D     | 1144/1407 (81%)  | 1027 (90%) | 77 (7%)  | 40 (4%)  | 3           | 23 |
| 3   | J     | 1137/1407 (81%)  | 1029 (90%) | 60 (5%)  | 48 (4%)  | 2           | 20 |
| 4   | E     | 87/91 (96%)      | 70 (80%)   | 8 (9%)   | 9 (10%)  | 0           | 7  |
| 4   | K     | 73/91 (80%)      | 58 (80%)   | 10 (14%) | 5 (7%)   | 1           | 14 |
| 5   | F     | 456/613 (74%)    | 431 (94%)  | 19 (4%)  | 6 (1%)   | 9           | 40 |
| 5   | L     | 456/613 (74%)    | 430 (94%)  | 18 (4%)  | 8 (2%)   | 6           | 34 |
| All | All   | 7025/8246 (85%)  | 6474 (92%) | 360 (5%) | 191 (3%) | 4           | 28 |

All (191) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 30  | PRO  |
| 1   | A     | 93  | GLN  |
| 1   | A     | 188 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 229  | GLU  |
| 1   | A     | 320  | ASN  |
| 1   | A     | 322  | PRO  |
| 1   | A     | 323  | PRO  |
| 1   | B     | 8    | PHE  |
| 1   | B     | 11   | PRO  |
| 1   | B     | 13   | LEU  |
| 1   | B     | 30   | PRO  |
| 1   | B     | 93   | GLN  |
| 1   | B     | 188  | GLU  |
| 1   | B     | 195  | ARG  |
| 1   | B     | 320  | ASN  |
| 1   | B     | 322  | PRO  |
| 2   | C     | 63   | SER  |
| 2   | C     | 110  | PRO  |
| 2   | C     | 214  | ASN  |
| 2   | C     | 346  | TYR  |
| 2   | C     | 748  | ILE  |
| 3   | D     | 151  | MET  |
| 3   | D     | 407  | VAL  |
| 3   | D     | 539  | SER  |
| 3   | D     | 559  | ALA  |
| 3   | D     | 588  | PRO  |
| 3   | D     | 744  | ARG  |
| 3   | D     | 825  | VAL  |
| 3   | D     | 833  | GLU  |
| 3   | D     | 834  | PRO  |
| 3   | D     | 851  | PRO  |
| 3   | D     | 880  | VAL  |
| 3   | D     | 1149 | ARG  |
| 3   | D     | 1153 | PRO  |
| 3   | D     | 1168 | GLU  |
| 3   | D     | 1169 | THR  |
| 3   | D     | 1177 | ILE  |
| 3   | D     | 1185 | PRO  |
| 3   | D     | 1191 | PRO  |
| 4   | E     | 4    | VAL  |
| 4   | E     | 16   | ARG  |
| 4   | E     | 34   | GLY  |
| 4   | E     | 36   | ASP  |
| 4   | E     | 37   | PRO  |
| 4   | E     | 40   | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | F     | 488  | LEU  |
| 5   | F     | 490  | PRO  |
| 1   | G     | 30   | PRO  |
| 1   | G     | 93   | GLN  |
| 1   | G     | 188  | GLU  |
| 1   | G     | 231  | PHE  |
| 1   | H     | 30   | PRO  |
| 1   | H     | 93   | GLN  |
| 1   | H     | 188  | GLU  |
| 2   | I     | 106  | GLU  |
| 2   | I     | 110  | PRO  |
| 2   | I     | 214  | ASN  |
| 2   | I     | 346  | TYR  |
| 2   | I     | 748  | ILE  |
| 3   | J     | 407  | VAL  |
| 3   | J     | 528  | THR  |
| 3   | J     | 539  | SER  |
| 3   | J     | 564  | VAL  |
| 3   | J     | 587  | LEU  |
| 3   | J     | 588  | PRO  |
| 3   | J     | 744  | ARG  |
| 3   | J     | 833  | GLU  |
| 3   | J     | 835  | LEU  |
| 3   | J     | 851  | PRO  |
| 3   | J     | 859  | PRO  |
| 3   | J     | 880  | VAL  |
| 3   | J     | 1149 | ARG  |
| 3   | J     | 1153 | PRO  |
| 3   | J     | 1168 | GLU  |
| 3   | J     | 1176 | VAL  |
| 3   | J     | 1185 | PRO  |
| 3   | J     | 1191 | PRO  |
| 3   | J     | 1202 | GLU  |
| 3   | J     | 1209 | VAL  |
| 3   | J     | 1214 | PRO  |
| 3   | J     | 1215 | GLU  |
| 4   | K     | 34   | GLY  |
| 4   | K     | 36   | ASP  |
| 4   | K     | 37   | PRO  |
| 4   | K     | 39   | VAL  |
| 5   | L     | 488  | LEU  |
| 5   | L     | 490  | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 319  | GLU  |
| 1   | B     | 7    | GLU  |
| 1   | B     | 191  | ARG  |
| 1   | B     | 192  | VAL  |
| 1   | B     | 319  | GLU  |
| 2   | C     | 109  | ALA  |
| 2   | C     | 746  | ALA  |
| 2   | C     | 909  | LYS  |
| 2   | C     | 1040 | ASP  |
| 3   | D     | 420  | PRO  |
| 3   | D     | 564  | VAL  |
| 3   | D     | 587  | LEU  |
| 3   | D     | 776  | THR  |
| 3   | D     | 906  | GLY  |
| 3   | D     | 1155 | ILE  |
| 3   | D     | 1190 | ILE  |
| 5   | F     | 307  | THR  |
| 5   | F     | 606  | VAL  |
| 2   | I     | 746  | ALA  |
| 2   | I     | 891  | GLY  |
| 2   | I     | 910  | ALA  |
| 2   | I     | 941  | LYS  |
| 3   | J     | 151  | MET  |
| 3   | J     | 179  | LYS  |
| 3   | J     | 420  | PRO  |
| 3   | J     | 556  | GLU  |
| 3   | J     | 560  | ASN  |
| 3   | J     | 593  | ASN  |
| 3   | J     | 776  | THR  |
| 3   | J     | 906  | GLY  |
| 3   | J     | 1213 | GLY  |
| 5   | L     | 307  | THR  |
| 5   | L     | 384  | LEU  |
| 5   | L     | 606  | VAL  |
| 1   | A     | 33   | ARG  |
| 1   | A     | 192  | VAL  |
| 1   | B     | 193  | GLU  |
| 1   | B     | 229  | GLU  |
| 2   | C     | 925  | SER  |
| 2   | C     | 1204 | LEU  |
| 3   | D     | 718  | SER  |
| 3   | D     | 859  | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 1150 | PRO  |
| 4   | E     | 60   | ASN  |
| 5   | F     | 384  | LEU  |
| 2   | I     | 925  | SER  |
| 3   | J     | 557  | LYS  |
| 3   | J     | 596  | LEU  |
| 3   | J     | 718  | SER  |
| 3   | J     | 1160 | SER  |
| 3   | J     | 1203 | ARG  |
| 5   | L     | 212  | ILE  |
| 5   | L     | 611  | LEU  |
| 1   | A     | 248  | GLU  |
| 2   | C     | 49   | LEU  |
| 2   | C     | 1155 | VAL  |
| 2   | C     | 1164 | PHE  |
| 3   | D     | 818  | GLU  |
| 3   | D     | 1176 | VAL  |
| 4   | E     | 79   | GLU  |
| 4   | E     | 80   | LEU  |
| 2   | I     | 43   | PRO  |
| 2   | I     | 162  | GLY  |
| 2   | I     | 908  | GLU  |
| 2   | I     | 1203 | ASP  |
| 2   | I     | 1204 | LEU  |
| 3   | J     | 145  | VAL  |
| 3   | J     | 818  | GLU  |
| 3   | J     | 1150 | PRO  |
| 3   | J     | 1190 | ILE  |
| 4   | K     | 45   | LYS  |
| 2   | C     | 152  | SER  |
| 2   | C     | 1041 | ASP  |
| 2   | C     | 1181 | PRO  |
| 2   | C     | 1203 | ASP  |
| 3   | D     | 555  | TYR  |
| 3   | D     | 828  | GLY  |
| 3   | D     | 858  | VAL  |
| 3   | D     | 1208 | ASP  |
| 3   | D     | 1212 | ASP  |
| 1   | G     | 49   | SER  |
| 1   | H     | 49   | SER  |
| 2   | I     | 152  | SER  |
| 2   | I     | 1164 | PHE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | I     | 1181 | PRO  |
| 1   | A     | 49   | SER  |
| 1   | B     | 49   | SER  |
| 3   | D     | 1213 | GLY  |
| 5   | F     | 214  | PRO  |
| 2   | I     | 1179 | GLY  |
| 3   | J     | 322  | ARG  |
| 3   | D     | 856  | ILE  |
| 3   | J     | 823  | THR  |
| 3   | J     | 834  | PRO  |
| 3   | J     | 856  | ILE  |
| 1   | H     | 52   | PRO  |
| 3   | J     | 647  | PRO  |
| 3   | J     | 1159 | ILE  |
| 3   | J     | 1177 | ILE  |
| 3   | D     | 582  | ILE  |
| 3   | D     | 909  | ILE  |
| 5   | L     | 500  | ILE  |
| 3   | D     | 647  | PRO  |
| 3   | J     | 582  | ILE  |

### 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     | 239/292 (82%)  | 218 (91%) | 21 (9%)  | 9           | 32 |
| 1   | B     | 233/292 (80%)  | 212 (91%) | 21 (9%)  | 9           | 31 |
| 1   | G     | 173/292 (59%)  | 157 (91%) | 16 (9%)  | 8           | 30 |
| 1   | H     | 171/292 (59%)  | 157 (92%) | 14 (8%)  | 10          | 34 |
| 2   | C     | 822/1157 (71%) | 761 (93%) | 61 (7%)  | 13          | 38 |
| 2   | I     | 828/1157 (72%) | 758 (92%) | 70 (8%)  | 10          | 33 |
| 3   | D     | 520/1168 (44%) | 452 (87%) | 68 (13%) | 4           | 19 |
| 3   | J     | 518/1168 (44%) | 447 (86%) | 71 (14%) | 3           | 18 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 4   | E     | 10/75 (13%)     | 9 (90%)    | 1 (10%)   | 7           | 27 |
| 4   | K     | 9/75 (12%)      | 7 (78%)    | 2 (22%)   | 1           | 6  |
| 5   | F     | 348/540 (64%)   | 309 (89%)  | 39 (11%)  | 6           | 23 |
| 5   | L     | 348/540 (64%)   | 304 (87%)  | 44 (13%)  | 4           | 20 |
| 6   | M     | 2/2 (100%)      | 1 (50%)    | 1 (50%)   | 0           | 0  |
| 6   | N     | 2/2 (100%)      | 1 (50%)    | 1 (50%)   | 0           | 0  |
| All | All   | 4223/7052 (60%) | 3793 (90%) | 430 (10%) | 7           | 26 |

All (430) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 14  | VAL  |
| 1   | A     | 29  | GLU  |
| 1   | A     | 30  | PRO  |
| 1   | A     | 31  | LEU  |
| 1   | A     | 32  | GLU  |
| 1   | A     | 67  | GLU  |
| 1   | A     | 88  | LEU  |
| 1   | A     | 95  | LYS  |
| 1   | A     | 102 | LEU  |
| 1   | A     | 104 | LYS  |
| 1   | A     | 117 | HIS  |
| 1   | A     | 131 | CYS  |
| 1   | A     | 140 | ILE  |
| 1   | A     | 171 | LEU  |
| 1   | A     | 173 | VAL  |
| 1   | A     | 178 | SER  |
| 1   | A     | 210 | THR  |
| 1   | A     | 287 | VAL  |
| 1   | A     | 318 | LEU  |
| 1   | A     | 319 | GLU  |
| 1   | A     | 321 | TRP  |
| 1   | B     | 14  | VAL  |
| 1   | B     | 28  | LEU  |
| 1   | B     | 29  | GLU  |
| 1   | B     | 30  | PRO  |
| 1   | B     | 31  | LEU  |
| 1   | B     | 32  | GLU  |
| 1   | B     | 88  | LEU  |
| 1   | B     | 95  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 102 | LEU  |
| 1   | B     | 104 | LYS  |
| 1   | B     | 117 | HIS  |
| 1   | B     | 131 | CYS  |
| 1   | B     | 140 | ILE  |
| 1   | B     | 171 | LEU  |
| 1   | B     | 173 | VAL  |
| 1   | B     | 178 | SER  |
| 1   | B     | 196 | THR  |
| 1   | B     | 287 | VAL  |
| 1   | B     | 318 | LEU  |
| 1   | B     | 319 | GLU  |
| 1   | B     | 321 | TRP  |
| 2   | C     | 15  | PHE  |
| 2   | C     | 24  | VAL  |
| 2   | C     | 55  | SER  |
| 2   | C     | 66  | SER  |
| 2   | C     | 79  | VAL  |
| 2   | C     | 90  | VAL  |
| 2   | C     | 151 | ARG  |
| 2   | C     | 374 | GLU  |
| 2   | C     | 378 | ARG  |
| 2   | C     | 456 | VAL  |
| 2   | C     | 478 | ARG  |
| 2   | C     | 525 | THR  |
| 2   | C     | 529 | ARG  |
| 2   | C     | 538 | LEU  |
| 2   | C     | 542 | ARG  |
| 2   | C     | 547 | VAL  |
| 2   | C     | 552 | PRO  |
| 2   | C     | 574 | SER  |
| 2   | C     | 581 | THR  |
| 2   | C     | 595 | THR  |
| 2   | C     | 600 | THR  |
| 2   | C     | 602 | GLU  |
| 2   | C     | 610 | GLU  |
| 2   | C     | 634 | VAL  |
| 2   | C     | 635 | THR  |
| 2   | C     | 643 | SER  |
| 2   | C     | 677 | ASN  |
| 2   | C     | 692 | THR  |
| 2   | C     | 694 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 705  | GLU  |
| 2   | C     | 761  | GLN  |
| 2   | C     | 776  | PRO  |
| 2   | C     | 818  | VAL  |
| 2   | C     | 822  | VAL  |
| 2   | C     | 845  | LEU  |
| 2   | C     | 888  | THR  |
| 2   | C     | 893  | THR  |
| 2   | C     | 896  | THR  |
| 2   | C     | 902  | LEU  |
| 2   | C     | 903  | ARG  |
| 2   | C     | 911  | SER  |
| 2   | C     | 914  | LYS  |
| 2   | C     | 917  | SER  |
| 2   | C     | 935  | THR  |
| 2   | C     | 936  | ARG  |
| 2   | C     | 1029 | LEU  |
| 2   | C     | 1042 | LEU  |
| 2   | C     | 1056 | VAL  |
| 2   | C     | 1075 | VAL  |
| 2   | C     | 1079 | ILE  |
| 2   | C     | 1186 | VAL  |
| 2   | C     | 1191 | LYS  |
| 2   | C     | 1197 | GLU  |
| 2   | C     | 1216 | ARG  |
| 2   | C     | 1226 | THR  |
| 2   | C     | 1239 | VAL  |
| 2   | C     | 1243 | MET  |
| 2   | C     | 1250 | SER  |
| 2   | C     | 1259 | LEU  |
| 2   | C     | 1298 | VAL  |
| 2   | C     | 1341 | ASP  |
| 3   | D     | 26   | SER  |
| 3   | D     | 34   | SER  |
| 3   | D     | 42   | GLU  |
| 3   | D     | 58   | CYS  |
| 3   | D     | 92   | VAL  |
| 3   | D     | 93   | THR  |
| 3   | D     | 118  | LYS  |
| 3   | D     | 167  | ASP  |
| 3   | D     | 191  | SER  |
| 3   | D     | 232  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 250 | ARG  |
| 3   | D     | 254 | PRO  |
| 3   | D     | 262 | THR  |
| 3   | D     | 273 | ILE  |
| 3   | D     | 301 | GLU  |
| 3   | D     | 311 | ARG  |
| 3   | D     | 319 | SER  |
| 3   | D     | 352 | ARG  |
| 3   | D     | 378 | LYS  |
| 3   | D     | 392 | THR  |
| 3   | D     | 419 | HIS  |
| 3   | D     | 420 | PRO  |
| 3   | D     | 430 | HIS  |
| 3   | D     | 491 | LEU  |
| 3   | D     | 514 | THR  |
| 3   | D     | 612 | LEU  |
| 3   | D     | 616 | PRO  |
| 3   | D     | 635 | SER  |
| 3   | D     | 646 | ILE  |
| 3   | D     | 648 | GLU  |
| 3   | D     | 661 | VAL  |
| 3   | D     | 673 | VAL  |
| 3   | D     | 674 | THR  |
| 3   | D     | 690 | ASN  |
| 3   | D     | 721 | SER  |
| 3   | D     | 733 | SER  |
| 3   | D     | 739 | GLN  |
| 3   | D     | 740 | LEU  |
| 3   | D     | 746 | LEU  |
| 3   | D     | 753 | SER  |
| 3   | D     | 763 | PHE  |
| 3   | D     | 764 | ARG  |
| 3   | D     | 767 | LEU  |
| 3   | D     | 769 | VAL  |
| 3   | D     | 781 | LYS  |
| 3   | D     | 783 | LEU  |
| 3   | D     | 785 | ASP  |
| 3   | D     | 786 | THR  |
| 3   | D     | 790 | THR  |
| 3   | D     | 810 | THR  |
| 3   | D     | 816 | THR  |
| 3   | D     | 842 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | D     | 862  | THR  |
| 3   | D     | 869  | CYS  |
| 3   | D     | 877  | VAL  |
| 3   | D     | 880  | VAL  |
| 3   | D     | 882  | VAL  |
| 3   | D     | 885  | VAL  |
| 3   | D     | 894  | VAL  |
| 3   | D     | 913  | GLU  |
| 3   | D     | 931  | THR  |
| 3   | D     | 1226 | VAL  |
| 3   | D     | 1247 | LYS  |
| 3   | D     | 1282 | TYR  |
| 3   | D     | 1316 | THR  |
| 3   | D     | 1353 | VAL  |
| 3   | D     | 1355 | ARG  |
| 3   | D     | 1361 | THR  |
| 4   | E     | 4    | VAL  |
| 5   | F     | 158  | LEU  |
| 5   | F     | 159  | SER  |
| 5   | F     | 162  | ILE  |
| 5   | F     | 218  | ARG  |
| 5   | F     | 250  | LEU  |
| 5   | F     | 262  | VAL  |
| 5   | F     | 264  | LYS  |
| 5   | F     | 273  | MET  |
| 5   | F     | 311  | THR  |
| 5   | F     | 333  | VAL  |
| 5   | F     | 336  | GLU  |
| 5   | F     | 354  | THR  |
| 5   | F     | 355  | ILE  |
| 5   | F     | 360  | ASP  |
| 5   | F     | 374  | ARG  |
| 5   | F     | 383  | ASN  |
| 5   | F     | 395  | THR  |
| 5   | F     | 397  | ARG  |
| 5   | F     | 420  | GLU  |
| 5   | F     | 421  | TYR  |
| 5   | F     | 425  | TYR  |
| 5   | F     | 426  | LYS  |
| 5   | F     | 428  | SER  |
| 5   | F     | 437  | GLN  |
| 5   | F     | 443  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | F     | 479 | THR  |
| 5   | F     | 480 | PRO  |
| 5   | F     | 513 | ASP  |
| 5   | F     | 537 | THR  |
| 5   | F     | 544 | THR  |
| 5   | F     | 551 | LEU  |
| 5   | F     | 552 | THR  |
| 5   | F     | 554 | ARG  |
| 5   | F     | 569 | THR  |
| 5   | F     | 583 | THR  |
| 5   | F     | 584 | ARG  |
| 5   | F     | 586 | ARG  |
| 5   | F     | 589 | GLN  |
| 5   | F     | 597 | LYS  |
| 1   | G     | 13  | LEU  |
| 1   | G     | 14  | VAL  |
| 1   | G     | 29  | GLU  |
| 1   | G     | 30  | PRO  |
| 1   | G     | 88  | LEU  |
| 1   | G     | 95  | LYS  |
| 1   | G     | 102 | LEU  |
| 1   | G     | 104 | LYS  |
| 1   | G     | 117 | HIS  |
| 1   | G     | 131 | CYS  |
| 1   | G     | 140 | ILE  |
| 1   | G     | 170 | ARG  |
| 1   | G     | 171 | LEU  |
| 1   | G     | 173 | VAL  |
| 1   | G     | 181 | GLU  |
| 1   | G     | 210 | THR  |
| 1   | H     | 14  | VAL  |
| 1   | H     | 29  | GLU  |
| 1   | H     | 30  | PRO  |
| 1   | H     | 88  | LEU  |
| 1   | H     | 95  | LYS  |
| 1   | H     | 102 | LEU  |
| 1   | H     | 104 | LYS  |
| 1   | H     | 117 | HIS  |
| 1   | H     | 131 | CYS  |
| 1   | H     | 140 | ILE  |
| 1   | H     | 171 | LEU  |
| 1   | H     | 173 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 208 | ASN  |
| 1   | H     | 211 | ILE  |
| 2   | I     | 15  | PHE  |
| 2   | I     | 24  | VAL  |
| 2   | I     | 27  | LEU  |
| 2   | I     | 55  | SER  |
| 2   | I     | 79  | VAL  |
| 2   | I     | 90  | VAL  |
| 2   | I     | 117 | ILE  |
| 2   | I     | 135 | THR  |
| 2   | I     | 151 | ARG  |
| 2   | I     | 374 | GLU  |
| 2   | I     | 378 | ARG  |
| 2   | I     | 451 | ARG  |
| 2   | I     | 456 | VAL  |
| 2   | I     | 478 | ARG  |
| 2   | I     | 525 | THR  |
| 2   | I     | 529 | ARG  |
| 2   | I     | 530 | ILE  |
| 2   | I     | 538 | LEU  |
| 2   | I     | 541 | GLU  |
| 2   | I     | 542 | ARG  |
| 2   | I     | 547 | VAL  |
| 2   | I     | 552 | PRO  |
| 2   | I     | 574 | SER  |
| 2   | I     | 581 | THR  |
| 2   | I     | 595 | THR  |
| 2   | I     | 600 | THR  |
| 2   | I     | 602 | GLU  |
| 2   | I     | 610 | GLU  |
| 2   | I     | 634 | VAL  |
| 2   | I     | 635 | THR  |
| 2   | I     | 637 | ARG  |
| 2   | I     | 657 | THR  |
| 2   | I     | 694 | ARG  |
| 2   | I     | 705 | GLU  |
| 2   | I     | 736 | VAL  |
| 2   | I     | 761 | GLN  |
| 2   | I     | 770 | CYS  |
| 2   | I     | 776 | PRO  |
| 2   | I     | 818 | VAL  |
| 2   | I     | 822 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | I     | 845  | LEU  |
| 2   | I     | 893  | THR  |
| 2   | I     | 896  | THR  |
| 2   | I     | 902  | LEU  |
| 2   | I     | 903  | ARG  |
| 2   | I     | 906  | PHE  |
| 2   | I     | 914  | LYS  |
| 2   | I     | 917  | SER  |
| 2   | I     | 936  | ARG  |
| 2   | I     | 942  | ASP  |
| 2   | I     | 1029 | LEU  |
| 2   | I     | 1042 | LEU  |
| 2   | I     | 1056 | VAL  |
| 2   | I     | 1075 | VAL  |
| 2   | I     | 1079 | ILE  |
| 2   | I     | 1184 | THR  |
| 2   | I     | 1186 | VAL  |
| 2   | I     | 1191 | LYS  |
| 2   | I     | 1197 | GLU  |
| 2   | I     | 1216 | ARG  |
| 2   | I     | 1226 | THR  |
| 2   | I     | 1227 | VAL  |
| 2   | I     | 1239 | VAL  |
| 2   | I     | 1243 | MET  |
| 2   | I     | 1250 | SER  |
| 2   | I     | 1259 | LEU  |
| 2   | I     | 1262 | LYS  |
| 2   | I     | 1293 | VAL  |
| 2   | I     | 1298 | VAL  |
| 2   | I     | 1341 | ASP  |
| 3   | J     | 26   | SER  |
| 3   | J     | 34   | SER  |
| 3   | J     | 42   | GLU  |
| 3   | J     | 58   | CYS  |
| 3   | J     | 92   | VAL  |
| 3   | J     | 93   | THR  |
| 3   | J     | 118  | LYS  |
| 3   | J     | 167  | ASP  |
| 3   | J     | 191  | SER  |
| 3   | J     | 193  | ASP  |
| 3   | J     | 210  | SER  |
| 3   | J     | 232  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | J     | 250 | ARG  |
| 3   | J     | 254 | PRO  |
| 3   | J     | 262 | THR  |
| 3   | J     | 273 | ILE  |
| 3   | J     | 301 | GLU  |
| 3   | J     | 311 | ARG  |
| 3   | J     | 319 | SER  |
| 3   | J     | 352 | ARG  |
| 3   | J     | 392 | THR  |
| 3   | J     | 400 | MET  |
| 3   | J     | 401 | VAL  |
| 3   | J     | 402 | GLU  |
| 3   | J     | 419 | HIS  |
| 3   | J     | 430 | HIS  |
| 3   | J     | 491 | LEU  |
| 3   | J     | 514 | THR  |
| 3   | J     | 598 | LYS  |
| 3   | J     | 612 | LEU  |
| 3   | J     | 616 | PRO  |
| 3   | J     | 627 | THR  |
| 3   | J     | 635 | SER  |
| 3   | J     | 646 | ILE  |
| 3   | J     | 648 | GLU  |
| 3   | J     | 661 | VAL  |
| 3   | J     | 673 | VAL  |
| 3   | J     | 674 | THR  |
| 3   | J     | 690 | ASN  |
| 3   | J     | 721 | SER  |
| 3   | J     | 733 | SER  |
| 3   | J     | 739 | GLN  |
| 3   | J     | 740 | LEU  |
| 3   | J     | 753 | SER  |
| 3   | J     | 763 | PHE  |
| 3   | J     | 764 | ARG  |
| 3   | J     | 767 | LEU  |
| 3   | J     | 769 | VAL  |
| 3   | J     | 781 | LYS  |
| 3   | J     | 783 | LEU  |
| 3   | J     | 785 | ASP  |
| 3   | J     | 786 | THR  |
| 3   | J     | 790 | THR  |
| 3   | J     | 816 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | J     | 842  | ARG  |
| 3   | J     | 862  | THR  |
| 3   | J     | 864  | LEU  |
| 3   | J     | 868  | TRP  |
| 3   | J     | 869  | CYS  |
| 3   | J     | 877  | VAL  |
| 3   | J     | 880  | VAL  |
| 3   | J     | 882  | VAL  |
| 3   | J     | 885  | VAL  |
| 3   | J     | 894  | VAL  |
| 3   | J     | 913  | GLU  |
| 3   | J     | 931  | THR  |
| 3   | J     | 1226 | VAL  |
| 3   | J     | 1247 | LYS  |
| 3   | J     | 1316 | THR  |
| 3   | J     | 1353 | VAL  |
| 3   | J     | 1355 | ARG  |
| 4   | K     | 4    | VAL  |
| 4   | K     | 6    | VAL  |
| 5   | L     | 137  | TYR  |
| 5   | L     | 158  | LEU  |
| 5   | L     | 159  | SER  |
| 5   | L     | 162  | ILE  |
| 5   | L     | 210  | ASN  |
| 5   | L     | 211  | SER  |
| 5   | L     | 212  | ILE  |
| 5   | L     | 218  | ARG  |
| 5   | L     | 230  | VAL  |
| 5   | L     | 234  | THR  |
| 5   | L     | 242  | HIS  |
| 5   | L     | 250  | LEU  |
| 5   | L     | 262  | VAL  |
| 5   | L     | 264  | LYS  |
| 5   | L     | 273  | MET  |
| 5   | L     | 311  | THR  |
| 5   | L     | 333  | VAL  |
| 5   | L     | 336  | GLU  |
| 5   | L     | 354  | THR  |
| 5   | L     | 355  | ILE  |
| 5   | L     | 360  | ASP  |
| 5   | L     | 383  | ASN  |
| 5   | L     | 395  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | L     | 397 | ARG  |
| 5   | L     | 420 | GLU  |
| 5   | L     | 421 | TYR  |
| 5   | L     | 422 | ARG  |
| 5   | L     | 425 | TYR  |
| 5   | L     | 426 | LYS  |
| 5   | L     | 428 | SER  |
| 5   | L     | 437 | GLN  |
| 5   | L     | 479 | THR  |
| 5   | L     | 480 | PRO  |
| 5   | L     | 513 | ASP  |
| 5   | L     | 537 | THR  |
| 5   | L     | 544 | THR  |
| 5   | L     | 552 | THR  |
| 5   | L     | 554 | ARG  |
| 5   | L     | 555 | GLU  |
| 5   | L     | 569 | THR  |
| 5   | L     | 584 | ARG  |
| 5   | L     | 589 | GLN  |
| 5   | L     | 590 | ILE  |
| 5   | L     | 597 | LYS  |
| 6   | M     | 2   | THR  |
| 6   | N     | 2   | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 18  | GLN  |
| 1   | A     | 37  | HIS  |
| 1   | A     | 41  | ASN  |
| 1   | A     | 75  | GLN  |
| 1   | A     | 128 | HIS  |
| 1   | A     | 227 | GLN  |
| 1   | A     | 283 | GLN  |
| 1   | A     | 320 | ASN  |
| 1   | B     | 37  | HIS  |
| 1   | B     | 41  | ASN  |
| 1   | B     | 75  | GLN  |
| 1   | B     | 128 | HIS  |
| 1   | B     | 283 | GLN  |
| 1   | B     | 294 | ASN  |
| 1   | B     | 320 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | C     | 437  | ASN  |
| 2   | C     | 618  | GLN  |
| 2   | C     | 659  | GLN  |
| 2   | C     | 955  | GLN  |
| 2   | C     | 1013 | GLN  |
| 2   | C     | 1023 | HIS  |
| 2   | C     | 1061 | GLN  |
| 3   | D     | 113  | HIS  |
| 3   | D     | 469  | HIS  |
| 3   | D     | 477  | GLN  |
| 3   | D     | 690  | ASN  |
| 3   | D     | 777  | HIS  |
| 3   | D     | 865  | HIS  |
| 3   | D     | 897  | HIS  |
| 3   | D     | 921  | GLN  |
| 3   | D     | 1326 | GLN  |
| 5   | F     | 128  | ASN  |
| 5   | F     | 129  | GLN  |
| 5   | F     | 131  | GLN  |
| 5   | F     | 227  | GLN  |
| 5   | F     | 283  | GLN  |
| 5   | F     | 294  | GLN  |
| 5   | F     | 309  | ASN  |
| 5   | F     | 342  | GLN  |
| 5   | F     | 357  | GLN  |
| 5   | F     | 383  | ASN  |
| 5   | F     | 406  | GLN  |
| 5   | F     | 437  | GLN  |
| 5   | F     | 461  | ASN  |
| 1   | G     | 37   | HIS  |
| 1   | G     | 41   | ASN  |
| 1   | G     | 128  | HIS  |
| 1   | G     | 147  | GLN  |
| 1   | G     | 227  | GLN  |
| 1   | H     | 66   | HIS  |
| 1   | H     | 75   | GLN  |
| 1   | H     | 128  | HIS  |
| 1   | H     | 186  | ASN  |
| 1   | H     | 208  | ASN  |
| 1   | H     | 227  | GLN  |
| 2   | I     | 437  | ASN  |
| 2   | I     | 659  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | I     | 955  | GLN  |
| 2   | I     | 1013 | GLN  |
| 2   | I     | 1017 | GLN  |
| 2   | I     | 1023 | HIS  |
| 2   | I     | 1061 | GLN  |
| 2   | I     | 1257 | GLN  |
| 3   | J     | 477  | GLN  |
| 3   | J     | 777  | HIS  |
| 3   | J     | 805  | GLN  |
| 3   | J     | 897  | HIS  |
| 3   | J     | 929  | GLN  |
| 3   | J     | 1326 | GLN  |
| 5   | L     | 128  | ASN  |
| 5   | L     | 129  | GLN  |
| 5   | L     | 131  | GLN  |
| 5   | L     | 227  | GLN  |
| 5   | L     | 283  | GLN  |
| 5   | L     | 294  | GLN  |
| 5   | L     | 309  | ASN  |
| 5   | L     | 357  | GLN  |
| 5   | L     | 383  | ASN  |
| 5   | L     | 437  | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 6   | MEA  | N     | 5   | 6    | 11,12,13     | 1.60 | 1 (9%)      | 13,14,16    | 1.19 | 2 (15%)     |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 6   | D4P  | N     | 4   | 6    | 10,11,12     | 4.69 | 2 (20%)  | 11,14,16    | 0.76 | 0        |
| 6   | 2TL  | N     | 6   | 6    | 5,6,7        | 0.50 | 0        | 5,7,9       | 0.92 | 0        |
| 6   | 28J  | N     | 3   | 6    | 6,7,8        | 0.46 | 0        | 4,8,10      | 1.10 | 0        |
| 6   | MEA  | M     | 5   | 6    | 11,12,13     | 1.59 | 1 (9%)   | 13,14,16    | 1.20 | 2 (15%)  |
| 6   | 2TL  | M     | 6   | 6    | 5,6,7        | 0.50 | 0        | 5,7,9       | 0.91 | 0        |
| 6   | D4P  | M     | 4   | 6    | 10,11,12     | 4.70 | 2 (20%)  | 11,14,16    | 0.74 | 0        |
| 6   | 28J  | M     | 3   | 6    | 6,7,8        | 0.46 | 0        | 4,8,10      | 1.10 | 0        |

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   |
|-----|------|-------|-----|------|---------|----------|---------|
| 6   | MEA  | N     | 5   | 6    | -       | 4/5/8/10 | 0/1/1/1 |
| 6   | D4P  | N     | 4   | 6    | -       | 0/4/6/8  | 0/1/1/1 |
| 6   | 2TL  | N     | 6   | 6    | -       | 2/5/6/8  | -       |
| 6   | 28J  | N     | 3   | 6    | -       | 6/7/8/10 | -       |
| 6   | MEA  | M     | 5   | 6    | -       | 4/5/8/10 | 0/1/1/1 |
| 6   | 2TL  | M     | 6   | 6    | -       | 2/5/6/8  | -       |
| 6   | D4P  | M     | 4   | 6    | -       | 0/4/6/8  | 0/1/1/1 |
| 6   | 28J  | M     | 3   | 6    | -       | 6/7/8/10 | -       |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 6   | M     | 4   | D4P  | C1-CA | -13.09 | 1.39        | 1.52     |
| 6   | N     | 4   | D4P  | C1-CA | -13.08 | 1.39        | 1.52     |
| 6   | M     | 4   | D4P  | CA-C  | -6.90  | 1.39        | 1.51     |
| 6   | N     | 4   | D4P  | CA-C  | -6.87  | 1.39        | 1.51     |
| 6   | N     | 5   | MEA  | CB-CG | -5.02  | 1.39        | 1.51     |
| 6   | M     | 5   | MEA  | CB-CG | -5.01  | 1.39        | 1.51     |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 6   | M     | 5   | MEA  | CG-CB-CA | -2.80 | 109.53      | 113.51   |
| 6   | N     | 5   | MEA  | CG-CB-CA | -2.78 | 109.55      | 113.51   |
| 6   | M     | 5   | MEA  | C1-N-CA  | 2.12  | 120.04      | 113.70   |
| 6   | N     | 5   | MEA  | C1-N-CA  | 2.12  | 120.03      | 113.70   |

There are no chirality outliers.

All (24) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 6   | M     | 5   | MEA  | N-CA-CB-CG     |
| 6   | N     | 5   | MEA  | N-CA-CB-CG     |
| 6   | M     | 3   | 28J  | N-CA-CB-CG2    |
| 6   | M     | 3   | 28J  | C-CA-CB-CG2    |
| 6   | M     | 3   | 28J  | C-CA-CB-CG1    |
| 6   | N     | 3   | 28J  | N-CA-CB-CG2    |
| 6   | N     | 3   | 28J  | C-CA-CB-CG2    |
| 6   | N     | 3   | 28J  | C-CA-CB-CG1    |
| 6   | M     | 6   | 2TL  | O-C-CA-CB      |
| 6   | N     | 6   | 2TL  | O-C-CA-CB      |
| 6   | M     | 3   | 28J  | CG2-CB-CG1-CD1 |
| 6   | N     | 3   | 28J  | CG2-CB-CG1-CD1 |
| 6   | M     | 3   | 28J  | CA-CB-CG1-CD1  |
| 6   | N     | 3   | 28J  | CA-CB-CG1-CD1  |
| 6   | M     | 3   | 28J  | N-CA-CB-CG1    |
| 6   | N     | 3   | 28J  | N-CA-CB-CG1    |
| 6   | M     | 5   | MEA  | CA-CB-CG-CD2   |
| 6   | N     | 5   | MEA  | CA-CB-CG-CD2   |
| 6   | M     | 5   | MEA  | CA-CB-CG-CD1   |
| 6   | N     | 5   | MEA  | CA-CB-CG-CD1   |
| 6   | M     | 6   | 2TL  | N-CA-CB-CG2    |
| 6   | N     | 6   | 2TL  | N-CA-CB-CG2    |
| 6   | M     | 5   | MEA  | C-CA-CB-CG     |
| 6   | N     | 5   | MEA  | C-CA-CB-CG     |

There are no ring outliers.

8 monomers are involved in 43 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 6   | N     | 5   | MEA  | 9       | 0            |
| 6   | N     | 4   | D4P  | 7       | 0            |
| 6   | N     | 6   | 2TL  | 6       | 0            |
| 6   | N     | 3   | 28J  | 1       | 0            |
| 6   | M     | 5   | MEA  | 10      | 0            |
| 6   | M     | 6   | 2TL  | 6       | 0            |
| 6   | M     | 4   | D4P  | 7       | 0            |
| 6   | M     | 3   | 28J  | 1       | 0            |



## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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     | 298/335 (88%)   | 0.17   | 17 (5%)   | 29  | 24  | 41, 129, 238, 393     | 0       |
| 1   | B     | 287/335 (85%)   | 0.28   | 22 (7%)   | 19  | 18  | 58, 173, 336, 460     | 0       |
| 1   | G     | 216/335 (64%)   | 0.23   | 11 (5%)   | 33  | 26  | 68, 183, 311, 358     | 0       |
| 1   | H     | 215/335 (64%)   | 0.29   | 10 (4%)   | 36  | 28  | 79, 191, 326, 488     | 0       |
| 2   | C     | 1340/1342 (99%) | 0.15   | 55 (4%)   | 41  | 31  | 16, 113, 346, 550     | 1 (0%)  |
| 2   | I     | 1340/1342 (99%) | 0.19   | 65 (4%)   | 35  | 27  | 37, 162, 408, 550     | 1 (0%)  |
| 3   | D     | 1150/1407 (81%) | 0.10   | 53 (4%)   | 37  | 28  | 19, 89, 227, 505      | 0       |
| 3   | J     | 1143/1407 (81%) | -0.01  | 34 (2%)   | 52  | 36  | 31, 110, 251, 550     | 0       |
| 4   | E     | 89/91 (97%)     | -0.00  | 5 (5%)    | 30  | 24  | 28, 105, 210, 326     | 0       |
| 4   | K     | 75/91 (82%)     | 0.17   | 4 (5%)    | 32  | 25  | 91, 185, 373, 403     | 0       |
| 5   | F     | 464/613 (75%)   | 0.05   | 19 (4%)   | 41  | 31  | 45, 151, 353, 550     | 0       |
| 5   | L     | 464/613 (75%)   | -0.00  | 11 (2%)   | 59  | 42  | 53, 167, 378, 550     | 0       |
| 6   | M     | 3/9 (33%)       | -0.38  | 0         | 100 | 100 | 107, 107, 108, 111    | 0       |
| 6   | N     | 3/9 (33%)       | -0.38  | 0         | 100 | 100 | 130, 130, 134, 138    | 0       |
| All | All   | 7087/8264 (85%) | 0.12   | 306 (4%)  | 40  | 30  | 16, 134, 326, 550     | 2 (0%)  |

All (306) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 4   | K     | 18   | ASP  | 8.5  |
| 2   | I     | 787  | PRO  | 6.3  |
| 1   | H     | 146  | VAL  | 6.0  |
| 2   | I     | 333  | ILE  | 5.9  |
| 1   | G     | 68   | TYR  | 5.5  |
| 3   | D     | 139  | LEU  | 5.4  |
| 2   | I     | 1312 | ASN  | 5.4  |
| 1   | H     | 26   | VAL  | 5.1  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | G            | 39         | LEU         | 5.0         |
| 1          | B            | 26         | VAL         | 4.9         |
| 5          | L            | 416        | VAL         | 4.9         |
| 1          | A            | 131        | CYS         | 4.8         |
| 2          | I            | 1313       | HIS         | 4.8         |
| 5          | L            | 420        | GLU         | 4.7         |
| 1          | G            | 43         | LEU         | 4.6         |
| 2          | C            | 9          | LYS         | 4.6         |
| 5          | F            | 412        | LEU         | 4.6         |
| 5          | L            | 412        | LEU         | 4.4         |
| 1          | A            | 270        | LEU         | 4.3         |
| 2          | C            | 42         | ASP         | 4.2         |
| 3          | J            | 345        | LYS         | 4.1         |
| 2          | C            | 1313       | HIS         | 4.1         |
| 2          | I            | 1295       | SER         | 4.1         |
| 2          | C            | 1179       | GLY         | 4.1         |
| 1          | H            | 144        | ILE         | 4.1         |
| 2          | C            | 686        | GLN         | 4.0         |
| 3          | D            | 394        | ILE         | 4.0         |
| 2          | I            | 667        | LEU         | 3.9         |
| 2          | I            | 1072       | ASN         | 3.9         |
| 4          | K            | 19         | LEU         | 3.9         |
| 2          | I            | 1060       | ILE         | 3.9         |
| 3          | J            | 289        | ASP         | 3.9         |
| 3          | J            | 1214       | PRO         | 3.8         |
| 2          | C            | 558        | VAL         | 3.8         |
| 2          | C            | 1040       | ASP         | 3.8         |
| 2          | C            | 944        | ARG         | 3.7         |
| 2          | I            | 596        | ASP         | 3.7         |
| 1          | H            | 39         | LEU         | 3.7         |
| 3          | D            | 1317       | GLU         | 3.7         |
| 1          | B            | 144        | ILE         | 3.7         |
| 3          | J            | 510        | LEU         | 3.7         |
| 1          | A            | 6          | THR         | 3.6         |
| 3          | D            | 505        | ASP         | 3.6         |
| 2          | I            | 796        | LEU         | 3.6         |
| 2          | I            | 334        | GLU         | 3.5         |
| 3          | J            | 1152       | GLU         | 3.5         |
| 2          | I            | 690        | VAL         | 3.5         |
| 2          | C            | 517        | GLN         | 3.5         |
| 3          | J            | 806        | ASP         | 3.4         |
| 2          | I            | 664        | GLY         | 3.4         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | J     | 228  | VAL  | 3.4  |
| 2   | I     | 792  | GLY  | 3.4  |
| 2   | C     | 565  | GLU  | 3.4  |
| 2   | I     | 663  | VAL  | 3.3  |
| 2   | C     | 942  | ASP  | 3.3  |
| 5   | F     | 381  | GLU  | 3.3  |
| 3   | J     | 1299 | GLY  | 3.3  |
| 3   | D     | 140  | TYR  | 3.3  |
| 2   | I     | 1314 | GLN  | 3.3  |
| 2   | C     | 209  | ILE  | 3.2  |
| 3   | J     | 502  | PRO  | 3.2  |
| 1   | A     | 205  | MET  | 3.2  |
| 1   | B     | 6    | THR  | 3.2  |
| 3   | J     | 650  | LYS  | 3.2  |
| 1   | B     | 261  | GLU  | 3.2  |
| 1   | A     | 247  | PRO  | 3.2  |
| 3   | D     | 1353 | VAL  | 3.2  |
| 3   | J     | 249  | LEU  | 3.2  |
| 4   | E     | 43   | ASN  | 3.2  |
| 1   | A     | 110  | VAL  | 3.1  |
| 3   | J     | 394  | ILE  | 3.1  |
| 2   | I     | 240  | GLU  | 3.1  |
| 2   | I     | 583  | GLU  | 3.1  |
| 3   | D     | 1352 | ILE  | 3.0  |
| 2   | C     | 813  | GLU  | 3.0  |
| 2   | C     | 560  | PRO  | 3.0  |
| 3   | D     | 406  | ALA  | 3.0  |
| 2   | I     | 1067 | ALA  | 3.0  |
| 1   | B     | 260  | LEU  | 3.0  |
| 5   | F     | 252  | LEU  | 3.0  |
| 2   | I     | 1321 | GLU  | 3.0  |
| 2   | C     | 506  | PHE  | 3.0  |
| 2   | C     | 812  | PHE  | 3.0  |
| 1   | G     | 205  | MET  | 3.0  |
| 2   | I     | 793  | GLU  | 3.0  |
| 3   | D     | 136  | GLU  | 3.0  |
| 3   | J     | 872  | LEU  | 3.0  |
| 2   | I     | 813  | GLU  | 2.9  |
| 3   | D     | 318  | GLY  | 2.9  |
| 2   | I     | 520  | PRO  | 2.9  |
| 3   | J     | 218  | THR  | 2.9  |
| 1   | H     | 28   | LEU  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 34   | GLY  | 2.9  |
| 2   | I     | 981  | ALA  | 2.9  |
| 3   | D     | 878  | ASP  | 2.9  |
| 2   | I     | 474  | ALA  | 2.9  |
| 2   | C     | 5    | TYR  | 2.9  |
| 2   | I     | 1325 | VAL  | 2.8  |
| 1   | B     | 78   | ILE  | 2.8  |
| 2   | C     | 184  | LEU  | 2.8  |
| 2   | I     | 1183 | ALA  | 2.8  |
| 2   | I     | 1190 | ALA  | 2.8  |
| 2   | I     | 922  | ASN  | 2.8  |
| 3   | D     | 1323 | ALA  | 2.8  |
| 2   | C     | 1049 | ILE  | 2.8  |
| 2   | C     | 502  | VAL  | 2.8  |
| 3   | J     | 1143 | ASP  | 2.8  |
| 1   | A     | 5    | VAL  | 2.8  |
| 5   | F     | 577  | GLY  | 2.8  |
| 2   | C     | 543  | ALA  | 2.7  |
| 2   | C     | 1190 | ALA  | 2.7  |
| 2   | I     | 833  | ILE  | 2.7  |
| 5   | F     | 431  | ALA  | 2.7  |
| 1   | G     | 168  | ILE  | 2.7  |
| 5   | F     | 590  | ILE  | 2.7  |
| 5   | L     | 447  | ALA  | 2.7  |
| 1   | H     | 98   | VAL  | 2.7  |
| 2   | I     | 1296 | ASP  | 2.7  |
| 3   | J     | 282  | LEU  | 2.7  |
| 2   | I     | 831  | ILE  | 2.7  |
| 3   | D     | 854  | ALA  | 2.7  |
| 3   | J     | 316  | ILE  | 2.7  |
| 1   | B     | 67   | GLU  | 2.7  |
| 2   | I     | 1180 | MET  | 2.7  |
| 1   | B     | 146  | VAL  | 2.6  |
| 2   | I     | 109  | ALA  | 2.6  |
| 2   | I     | 1234 | LYS  | 2.6  |
| 3   | J     | 1289 | ASN  | 2.6  |
| 1   | B     | 309  | SER  | 2.6  |
| 2   | C     | 288  | PRO  | 2.6  |
| 3   | D     | 1230 | THR  | 2.6  |
| 3   | D     | 1314 | LEU  | 2.6  |
| 3   | D     | 1234 | VAL  | 2.6  |
| 2   | C     | 764  | CYS  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | I     | 1256 | GLN  | 2.6  |
| 5   | F     | 140  | ALA  | 2.6  |
| 4   | E     | 24   | ALA  | 2.6  |
| 5   | F     | 580  | PHE  | 2.6  |
| 3   | J     | 1208 | ASP  | 2.6  |
| 2   | C     | 925  | SER  | 2.6  |
| 1   | A     | 121  | VAL  | 2.6  |
| 2   | C     | 547  | VAL  | 2.6  |
| 3   | D     | 512  | TYR  | 2.6  |
| 1   | G     | 47   | LEU  | 2.6  |
| 5   | L     | 501  | ALA  | 2.5  |
| 2   | C     | 250  | THR  | 2.5  |
| 5   | F     | 407  | GLU  | 2.5  |
| 3   | D     | 675  | ALA  | 2.5  |
| 2   | C     | 198  | ILE  | 2.5  |
| 5   | F     | 101  | TYR  | 2.5  |
| 1   | B     | 33   | ARG  | 2.5  |
| 1   | B     | 201  | LEU  | 2.5  |
| 3   | D     | 777  | HIS  | 2.5  |
| 2   | C     | 676  | ALA  | 2.5  |
| 2   | I     | 299  | LYS  | 2.5  |
| 3   | D     | 509  | GLY  | 2.5  |
| 2   | C     | 1265 | PHE  | 2.5  |
| 1   | G     | 203  | ILE  | 2.5  |
| 1   | G     | 26   | VAL  | 2.5  |
| 2   | I     | 1227 | VAL  | 2.5  |
| 3   | D     | 1141 | VAL  | 2.5  |
| 2   | I     | 987  | GLU  | 2.4  |
| 2   | I     | 827  | ARG  | 2.4  |
| 3   | D     | 502  | PRO  | 2.4  |
| 2   | C     | 464  | PHE  | 2.4  |
| 3   | D     | 176  | PHE  | 2.4  |
| 1   | G     | 85   | LEU  | 2.4  |
| 3   | D     | 857  | LEU  | 2.4  |
| 3   | D     | 1322 | ALA  | 2.4  |
| 5   | L     | 130  | VAL  | 2.4  |
| 3   | J     | 631  | TYR  | 2.4  |
| 2   | C     | 370  | MET  | 2.4  |
| 3   | D     | 461  | PHE  | 2.4  |
| 5   | F     | 384  | LEU  | 2.4  |
| 4   | K     | 20   | VAL  | 2.4  |
| 5   | F     | 583  | THR  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 3   | D     | 395  | LYS  | 2.4  |
| 2   | I     | 1322 | SER  | 2.4  |
| 2   | I     | 442  | VAL  | 2.4  |
| 3   | J     | 683  | ILE  | 2.4  |
| 2   | C     | 116  | ASP  | 2.4  |
| 1   | A     | 230  | ALA  | 2.4  |
| 2   | I     | 379  | GLU  | 2.4  |
| 3   | D     | 666  | GLU  | 2.4  |
| 5   | L     | 116  | GLU  | 2.4  |
| 1   | B     | 298  | LYS  | 2.4  |
| 3   | J     | 1244 | GLN  | 2.3  |
| 2   | I     | 311  | CYS  | 2.3  |
| 3   | D     | 593  | ASN  | 2.3  |
| 1   | B     | 85   | LEU  | 2.3  |
| 2   | I     | 822  | VAL  | 2.3  |
| 4   | K     | 16   | ARG  | 2.3  |
| 2   | I     | 641  | GLU  | 2.3  |
| 3   | D     | 1215 | GLU  | 2.3  |
| 4   | E     | 81   | GLN  | 2.3  |
| 3   | J     | 231  | GLY  | 2.3  |
| 1   | B     | 142  | MET  | 2.3  |
| 2   | I     | 1122 | LYS  | 2.3  |
| 2   | C     | 1342 | GLU  | 2.3  |
| 5   | F     | 261  | LEU  | 2.3  |
| 3   | J     | 808  | VAL  | 2.3  |
| 3   | D     | 1294 | ALA  | 2.3  |
| 3   | D     | 1332 | LEU  | 2.3  |
| 1   | A     | 140  | ILE  | 2.3  |
| 1   | A     | 211  | ILE  | 2.3  |
| 5   | F     | 570  | ASP  | 2.3  |
| 3   | D     | 1299 | GLY  | 2.3  |
| 2   | C     | 575  | LEU  | 2.3  |
| 5   | F     | 266  | PHE  | 2.3  |
| 5   | F     | 415  | ALA  | 2.3  |
| 2   | C     | 56   | VAL  | 2.3  |
| 2   | C     | 1205 | PRO  | 2.3  |
| 3   | D     | 1354 | GLY  | 2.3  |
| 3   | J     | 1246 | VAL  | 2.3  |
| 2   | C     | 856  | ASN  | 2.3  |
| 3   | J     | 232  | ASN  | 2.3  |
| 5   | L     | 234  | THR  | 2.3  |
| 2   | I     | 325  | LEU  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | C     | 251  | ALA  | 2.3  |
| 3   | D     | 1315 | ALA  | 2.3  |
| 2   | C     | 1046 | VAL  | 2.3  |
| 3   | J     | 267  | ASP  | 2.3  |
| 5   | L     | 521  | ASP  | 2.3  |
| 2   | C     | 1000 | LEU  | 2.2  |
| 2   | C     | 1173 | ALA  | 2.2  |
| 1   | A     | 30   | PRO  | 2.2  |
| 1   | A     | 16   | ILE  | 2.2  |
| 1   | A     | 86   | LYS  | 2.2  |
| 2   | I     | 686  | GLN  | 2.2  |
| 2   | I     | 1251 | TYR  | 2.2  |
| 1   | B     | 205  | MET  | 2.2  |
| 1   | B     | 12   | ARG  | 2.2  |
| 3   | J     | 891  | ASP  | 2.2  |
| 2   | I     | 649  | GLN  | 2.2  |
| 1   | B     | 172  | LEU  | 2.2  |
| 5   | F     | 280  | VAL  | 2.2  |
| 3   | D     | 575  | GLY  | 2.2  |
| 3   | J     | 575  | GLY  | 2.2  |
| 1   | B     | 217  | ILE  | 2.2  |
| 2   | I     | 450  | ASN  | 2.2  |
| 1   | H     | 51   | MET  | 2.2  |
| 2   | C     | 488  | MET  | 2.2  |
| 3   | D     | 1324 | SER  | 2.2  |
| 3   | D     | 43   | THR  | 2.2  |
| 3   | J     | 487  | THR  | 2.2  |
| 5   | L     | 235  | ILE  | 2.2  |
| 3   | D     | 1274 | PHE  | 2.2  |
| 2   | I     | 573  | ASN  | 2.2  |
| 2   | I     | 312  | ALA  | 2.1  |
| 5   | F     | 587  | ILE  | 2.1  |
| 1   | B     | 188  | GLU  | 2.1  |
| 5   | L     | 531  | PRO  | 2.1  |
| 3   | D     | 449  | LEU  | 2.1  |
| 3   | D     | 612  | LEU  | 2.1  |
| 3   | D     | 520  | ALA  | 2.1  |
| 3   | J     | 99   | ARG  | 2.1  |
| 2   | I     | 788  | SER  | 2.1  |
| 1   | B     | 305  | ASP  | 2.1  |
| 1   | G     | 217  | ILE  | 2.1  |
| 2   | I     | 978  | VAL  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 4   | E     | 4    | VAL  | 2.1  |
| 2   | I     | 230  | PHE  | 2.1  |
| 2   | I     | 231  | GLU  | 2.1  |
| 4   | E     | 5    | THR  | 2.1  |
| 3   | J     | 804  | ALA  | 2.1  |
| 1   | A     | 266  | SER  | 2.1  |
| 3   | D     | 858  | VAL  | 2.1  |
| 2   | C     | 14   | ASP  | 2.1  |
| 2   | C     | 739  | ASP  | 2.1  |
| 2   | C     | 1018 | TYR  | 2.1  |
| 2   | I     | 301  | TYR  | 2.1  |
| 1   | G     | 169  | GLY  | 2.1  |
| 3   | D     | 776  | THR  | 2.1  |
| 2   | I     | 944  | ARG  | 2.1  |
| 3   | D     | 481  | ARG  | 2.1  |
| 1   | B     | 81   | ILE  | 2.1  |
| 3   | D     | 670  | SER  | 2.1  |
| 2   | I     | 483  | ASP  | 2.1  |
| 2   | C     | 562  | GLU  | 2.1  |
| 5   | F     | 460  | ILE  | 2.1  |
| 2   | C     | 1073 | LYS  | 2.1  |
| 3   | D     | 639  | VAL  | 2.1  |
| 3   | J     | 579  | LEU  | 2.1  |
| 2   | C     | 626  | GLU  | 2.1  |
| 2   | C     | 12   | ARG  | 2.1  |
| 2   | C     | 166  | SER  | 2.1  |
| 1   | H     | 180  | VAL  | 2.1  |
| 2   | C     | 1163 | THR  | 2.0  |
| 2   | I     | 493  | ILE  | 2.0  |
| 2   | I     | 610  | GLU  | 2.0  |
| 3   | J     | 1151 | LYS  | 2.0  |
| 1   | H     | 31   | LEU  | 2.0  |
| 2   | I     | 521  | LEU  | 2.0  |
| 2   | I     | 1220 | GLN  | 2.0  |
| 3   | D     | 441  | LEU  | 2.0  |
| 3   | D     | 788  | LEU  | 2.0  |
| 1   | H     | 61   | ILE  | 2.0  |
| 1   | A     | 7    | GLU  | 2.0  |
| 3   | D     | 830  | ASP  | 2.0  |
| 3   | D     | 1334 | GLU  | 2.0  |
| 1   | A     | 260  | LEU  | 2.0  |
| 2   | C     | 1122 | LYS  | 2.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | C     | 605  | TYR  | 2.0  |
| 3   | D     | 135  | ILE  | 2.0  |
| 2   | C     | 554  | HIS  | 2.0  |
| 3   | D     | 1211 | SER  | 2.0  |

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. 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  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 6   | D4P  | N     | 4   | 11/12 | 0.75 | 0.11 | 133,140,153,159            | 0     |
| 6   | D4P  | M     | 4   | 11/12 | 0.84 | 0.09 | 102,118,135,137            | 0     |
| 6   | MEA  | M     | 5   | 12/13 | 0.87 | 0.09 | 79,91,106,106              | 0     |
| 6   | MEA  | N     | 5   | 12/13 | 0.87 | 0.12 | 109,123,128,130            | 0     |
| 6   | 2TL  | N     | 6   | 7/8   | 0.87 | 0.08 | 124,127,132,147            | 0     |
| 6   | 2TL  | M     | 6   | 7/8   | 0.89 | 0.12 | 91,110,113,123             | 0     |
| 6   | 28J  | N     | 3   | 8/9   | 0.93 | 0.11 | 106,127,131,132            | 0     |
| 6   | 28J  | M     | 3   | 8/9   | 0.95 | 0.11 | 97,105,111,114             | 0     |

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 7   | MG   | J     | 2000 | 1/1   | 0.32 | 0.23 | 98,98,98,98                | 0     |
| 7   | MG   | D     | 2000 | 1/1   | 0.45 | 0.19 | 258,258,258,258            | 0     |
| 8   | ZN   | J     | 2001 | 1/1   | 0.98 | 0.03 | 106,106,106,106            | 0     |
| 8   | ZN   | D     | 2001 | 1/1   | 0.99 | 0.03 | 87,87,87,87                | 0     |
| 8   | ZN   | J     | 2002 | 1/1   | 0.99 | 0.07 | 80,80,80,80                | 0     |
| 8   | ZN   | D     | 2002 | 1/1   | 1.00 | 0.07 | 64,64,64,64                | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.