



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2021 – 01:22 PM EDT

PDB ID : 2NV2  
Title : Structure of the PLP synthase complex Pdx1/2 (YaaD/E) from *Bacillus subtilis*  
Authors : Strohmeier, M.; Tews, I.; Sinning, I.  
Deposited on : 2006-11-10  
Resolution : 2.12 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

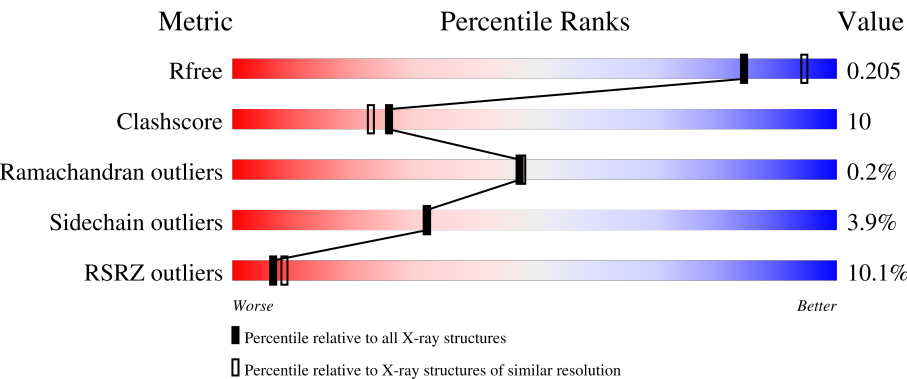
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

# 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 2.12 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 6241 (2.14-2.10)                                      |
| Clashscore            | 141614                      | 6778 (2.14-2.10)                                      |
| Ramachandran outliers | 138981                      | 6705 (2.14-2.10)                                      |
| Sidechain outliers    | 138945                      | 6706 (2.14-2.10)                                      |
| RSRZ outliers         | 127900                      | 6112 (2.14-2.10)                                      |

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     | 294    | <div><div>4%</div><div><div></div><div>78%</div><div>13%</div><div>•</div><div>9%</div></div></div> |
| 1   | C     | 294    | <div><div>4%</div><div><div></div><div>80%</div><div>11%</div><div>•</div><div>9%</div></div></div> |
| 1   | E     | 294    | <div><div>4%</div><div><div></div><div>76%</div><div>14%</div><div>•</div><div>9%</div></div></div> |
| 1   | G     | 294    | <div><div>4%</div><div><div></div><div>78%</div><div>13%</div><div>•</div><div>9%</div></div></div> |
| 1   | I     | 294    | <div><div>4%</div><div><div></div><div>77%</div><div>14%</div><div>•</div><div>8%</div></div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | K     | 294    |                  |
| 1   | M     | 294    |                  |
| 1   | O     | 294    |                  |
| 1   | Q     | 294    |                  |
| 1   | S     | 294    |                  |
| 1   | U     | 294    |                  |
| 1   | W     | 294    |                  |
| 2   | B     | 204    |                  |
| 2   | D     | 204    |                  |
| 2   | F     | 204    |                  |
| 2   | H     | 204    |                  |
| 2   | J     | 204    |                  |
| 2   | L     | 204    |                  |
| 2   | N     | 204    |                  |
| 2   | P     | 204    |                  |
| 2   | R     | 204    |                  |
| 2   | T     | 204    |                  |
| 2   | V     | 204    |                  |
| 2   | X     | 204    |                  |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 3   | CL   | A     | 6001 | -         | -        | X       | -                |
| 3   | CL   | C     | 6005 | -         | -        | X       | -                |
| 3   | CL   | E     | 6009 | -         | -        | X       | -                |
| 3   | CL   | I     | 6017 | -         | -        | X       | -                |
| 3   | CL   | Q     | 6033 | -         | -        | X       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 3   | CL   | S     | 6037 | -         | -        | X       | -                |
| 3   | CL   | U     | 6041 | -         | -        | X       | -                |
| 3   | CL   | W     | 6045 | -         | -        | X       | -                |
| 4   | EDO  | A     | 6031 | -         | -        | X       | -                |
| 4   | EDO  | E     | 6047 | -         | -        | X       | -                |
| 4   | EDO  | G     | 6043 | -         | -        | X       | -                |
| 4   | EDO  | I     | 6039 | -         | -        | X       | -                |
| 4   | EDO  | M     | 6007 | -         | -        | X       | -                |
| 4   | EDO  | Q     | 6035 | -         | -        | X       | -                |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 48293 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 Pyridoxal biosynthesis lyase pdxS.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 268      | Total | C    | N   | O   | S  | 0       | 6       | 0     |
|     |       |          | 2028  | 1270 | 354 | 388 | 16 |         |         |       |
| 1   | C     | 269      | Total | C    | N   | O   | S  | 0       | 5       | 0     |
|     |       |          | 2037  | 1273 | 355 | 393 | 16 |         |         |       |
| 1   | E     | 269      | Total | C    | N   | O   | S  | 0       | 5       | 0     |
|     |       |          | 2037  | 1273 | 356 | 392 | 16 |         |         |       |
| 1   | G     | 268      | Total | C    | N   | O   | S  | 0       | 3       | 0     |
|     |       |          | 2007  | 1255 | 348 | 388 | 16 |         |         |       |
| 1   | I     | 271      | Total | C    | N   | O   | S  | 0       | 4       | 0     |
|     |       |          | 2042  | 1276 | 357 | 393 | 16 |         |         |       |
| 1   | K     | 270      | Total | C    | N   | O   | S  | 0       | 4       | 0     |
|     |       |          | 2032  | 1272 | 356 | 388 | 16 |         |         |       |
| 1   | M     | 269      | Total | C    | N   | O   | S  | 0       | 5       | 0     |
|     |       |          | 2036  | 1273 | 356 | 391 | 16 |         |         |       |
| 1   | O     | 268      | Total | C    | N   | O   | S  | 0       | 4       | 0     |
|     |       |          | 2024  | 1265 | 357 | 386 | 16 |         |         |       |
| 1   | Q     | 270      | Total | C    | N   | O   | S  | 0       | 3       | 0     |
|     |       |          | 2028  | 1268 | 356 | 388 | 16 |         |         |       |
| 1   | S     | 270      | Total | C    | N   | O   | S  | 0       | 3       | 0     |
|     |       |          | 2028  | 1267 | 355 | 390 | 16 |         |         |       |
| 1   | U     | 271      | Total | C    | N   | O   | S  | 0       | 4       | 0     |
|     |       |          | 2034  | 1271 | 356 | 391 | 16 |         |         |       |
| 1   | W     | 270      | Total | C    | N   | O   | S  | 0       | 6       | 0     |
|     |       |          | 2044  | 1280 | 357 | 391 | 16 |         |         |       |

- Molecule 2 is a protein called Glutamine amidotransferase subunit pdxT.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 193      | Total | C   | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1500  | 948 | 264 | 280 | 8 |         |         |       |
| 2   | D     | 194      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1497  | 946 | 262 | 281 | 8 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | F     | 191      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1474  | 932 | 257 | 277 | 8 |         |         |       |
| 2   | H     | 193      | Total | C   | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1494  | 944 | 260 | 282 | 8 |         |         |       |
| 2   | J     | 196      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1512  | 957 | 264 | 283 | 8 |         |         |       |
| 2   | L     | 192      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1483  | 937 | 259 | 279 | 8 |         |         |       |
| 2   | N     | 193      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1488  | 940 | 260 | 280 | 8 |         |         |       |
| 2   | P     | 193      | Total | C   | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1496  | 947 | 261 | 280 | 8 |         |         |       |
| 2   | R     | 193      | Total | C   | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1500  | 948 | 264 | 280 | 8 |         |         |       |
| 2   | T     | 194      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1493  | 944 | 262 | 279 | 8 |         |         |       |
| 2   | V     | 194      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1497  | 946 | 262 | 281 | 8 |         |         |       |
| 2   | X     | 195      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1505  | 952 | 263 | 282 | 8 |         |         |       |

There are 108 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| B     | 170     | ASN      | HIS    | engineered mutation | UNP P37528 |
| B     | 197     | LEU      | -      | expression tag      | UNP P37528 |
| B     | 198     | GLU      | -      | expression tag      | UNP P37528 |
| B     | 199     | HIS      | -      | expression tag      | UNP P37528 |
| B     | 200     | HIS      | -      | expression tag      | UNP P37528 |
| B     | 201     | HIS      | -      | expression tag      | UNP P37528 |
| B     | 202     | HIS      | -      | expression tag      | UNP P37528 |
| B     | 203     | HIS      | -      | expression tag      | UNP P37528 |
| B     | 204     | HIS      | -      | expression tag      | UNP P37528 |
| D     | 170     | ASN      | HIS    | engineered mutation | UNP P37528 |
| D     | 197     | LEU      | -      | expression tag      | UNP P37528 |
| D     | 198     | GLU      | -      | expression tag      | UNP P37528 |
| D     | 199     | HIS      | -      | expression tag      | UNP P37528 |
| D     | 200     | HIS      | -      | expression tag      | UNP P37528 |
| D     | 201     | HIS      | -      | expression tag      | UNP P37528 |
| D     | 202     | HIS      | -      | expression tag      | UNP P37528 |
| D     | 203     | HIS      | -      | expression tag      | UNP P37528 |
| D     | 204     | HIS      | -      | expression tag      | UNP P37528 |
| F     | 170     | ASN      | HIS    | engineered mutation | UNP P37528 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| F     | 197     | LEU      | -      | expression tag      | UNP P37528 |
| F     | 198     | GLU      | -      | expression tag      | UNP P37528 |
| F     | 199     | HIS      | -      | expression tag      | UNP P37528 |
| F     | 200     | HIS      | -      | expression tag      | UNP P37528 |
| F     | 201     | HIS      | -      | expression tag      | UNP P37528 |
| F     | 202     | HIS      | -      | expression tag      | UNP P37528 |
| F     | 203     | HIS      | -      | expression tag      | UNP P37528 |
| F     | 204     | HIS      | -      | expression tag      | UNP P37528 |
| H     | 170     | ASN      | HIS    | engineered mutation | UNP P37528 |
| H     | 197     | LEU      | -      | expression tag      | UNP P37528 |
| H     | 198     | GLU      | -      | expression tag      | UNP P37528 |
| H     | 199     | HIS      | -      | expression tag      | UNP P37528 |
| H     | 200     | HIS      | -      | expression tag      | UNP P37528 |
| H     | 201     | HIS      | -      | expression tag      | UNP P37528 |
| H     | 202     | HIS      | -      | expression tag      | UNP P37528 |
| H     | 203     | HIS      | -      | expression tag      | UNP P37528 |
| H     | 204     | HIS      | -      | expression tag      | UNP P37528 |
| J     | 170     | ASN      | HIS    | engineered mutation | UNP P37528 |
| J     | 197     | LEU      | -      | expression tag      | UNP P37528 |
| J     | 198     | GLU      | -      | expression tag      | UNP P37528 |
| J     | 199     | HIS      | -      | expression tag      | UNP P37528 |
| J     | 200     | HIS      | -      | expression tag      | UNP P37528 |
| J     | 201     | HIS      | -      | expression tag      | UNP P37528 |
| J     | 202     | HIS      | -      | expression tag      | UNP P37528 |
| J     | 203     | HIS      | -      | expression tag      | UNP P37528 |
| J     | 204     | HIS      | -      | expression tag      | UNP P37528 |
| L     | 170     | ASN      | HIS    | engineered mutation | UNP P37528 |
| L     | 197     | LEU      | -      | expression tag      | UNP P37528 |
| L     | 198     | GLU      | -      | expression tag      | UNP P37528 |
| L     | 199     | HIS      | -      | expression tag      | UNP P37528 |
| L     | 200     | HIS      | -      | expression tag      | UNP P37528 |
| L     | 201     | HIS      | -      | expression tag      | UNP P37528 |
| L     | 202     | HIS      | -      | expression tag      | UNP P37528 |
| L     | 203     | HIS      | -      | expression tag      | UNP P37528 |
| L     | 204     | HIS      | -      | expression tag      | UNP P37528 |
| N     | 170     | ASN      | HIS    | engineered mutation | UNP P37528 |
| N     | 197     | LEU      | -      | expression tag      | UNP P37528 |
| N     | 198     | GLU      | -      | expression tag      | UNP P37528 |
| N     | 199     | HIS      | -      | expression tag      | UNP P37528 |
| N     | 200     | HIS      | -      | expression tag      | UNP P37528 |
| N     | 201     | HIS      | -      | expression tag      | UNP P37528 |
| N     | 202     | HIS      | -      | expression tag      | UNP P37528 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| N     | 203     | HIS      | -      | expression tag      | UNP P37528 |
| N     | 204     | HIS      | -      | expression tag      | UNP P37528 |
| P     | 170     | ASN      | HIS    | engineered mutation | UNP P37528 |
| P     | 197     | LEU      | -      | expression tag      | UNP P37528 |
| P     | 198     | GLU      | -      | expression tag      | UNP P37528 |
| P     | 199     | HIS      | -      | expression tag      | UNP P37528 |
| P     | 200     | HIS      | -      | expression tag      | UNP P37528 |
| P     | 201     | HIS      | -      | expression tag      | UNP P37528 |
| P     | 202     | HIS      | -      | expression tag      | UNP P37528 |
| P     | 203     | HIS      | -      | expression tag      | UNP P37528 |
| P     | 204     | HIS      | -      | expression tag      | UNP P37528 |
| R     | 170     | ASN      | HIS    | engineered mutation | UNP P37528 |
| R     | 197     | LEU      | -      | expression tag      | UNP P37528 |
| R     | 198     | GLU      | -      | expression tag      | UNP P37528 |
| R     | 199     | HIS      | -      | expression tag      | UNP P37528 |
| R     | 200     | HIS      | -      | expression tag      | UNP P37528 |
| R     | 201     | HIS      | -      | expression tag      | UNP P37528 |
| R     | 202     | HIS      | -      | expression tag      | UNP P37528 |
| R     | 203     | HIS      | -      | expression tag      | UNP P37528 |
| R     | 204     | HIS      | -      | expression tag      | UNP P37528 |
| T     | 170     | ASN      | HIS    | engineered mutation | UNP P37528 |
| T     | 197     | LEU      | -      | expression tag      | UNP P37528 |
| T     | 198     | GLU      | -      | expression tag      | UNP P37528 |
| T     | 199     | HIS      | -      | expression tag      | UNP P37528 |
| T     | 200     | HIS      | -      | expression tag      | UNP P37528 |
| T     | 201     | HIS      | -      | expression tag      | UNP P37528 |
| T     | 202     | HIS      | -      | expression tag      | UNP P37528 |
| T     | 203     | HIS      | -      | expression tag      | UNP P37528 |
| T     | 204     | HIS      | -      | expression tag      | UNP P37528 |
| V     | 170     | ASN      | HIS    | engineered mutation | UNP P37528 |
| V     | 197     | LEU      | -      | expression tag      | UNP P37528 |
| V     | 198     | GLU      | -      | expression tag      | UNP P37528 |
| V     | 199     | HIS      | -      | expression tag      | UNP P37528 |
| V     | 200     | HIS      | -      | expression tag      | UNP P37528 |
| V     | 201     | HIS      | -      | expression tag      | UNP P37528 |
| V     | 202     | HIS      | -      | expression tag      | UNP P37528 |
| V     | 203     | HIS      | -      | expression tag      | UNP P37528 |
| V     | 204     | HIS      | -      | expression tag      | UNP P37528 |
| X     | 170     | ASN      | HIS    | engineered mutation | UNP P37528 |
| X     | 197     | LEU      | -      | expression tag      | UNP P37528 |
| X     | 198     | GLU      | -      | expression tag      | UNP P37528 |
| X     | 199     | HIS      | -      | expression tag      | UNP P37528 |

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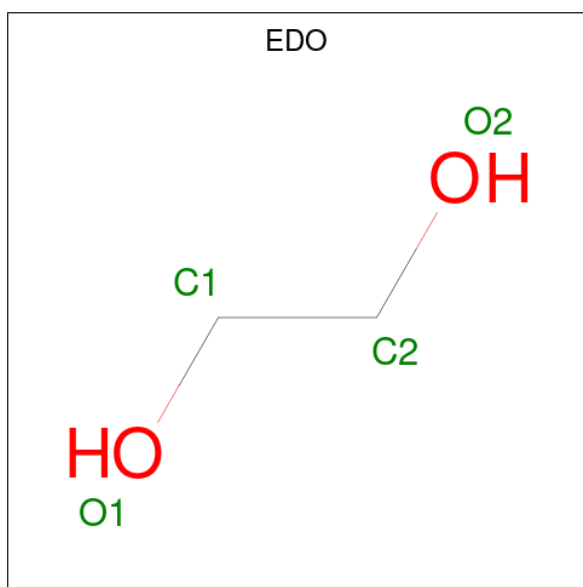
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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| X     | 200     | HIS      | -      | expression tag | UNP P37528 |
| X     | 201     | HIS      | -      | expression tag | UNP P37528 |
| X     | 202     | HIS      | -      | expression tag | UNP P37528 |
| X     | 203     | HIS      | -      | expression tag | UNP P37528 |
| X     | 204     | HIS      | -      | expression tag | UNP P37528 |

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3   | A     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 3   | C     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 3   | E     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 3   | G     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 3   | I     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 3   | K     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 3   | M     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 3   | O     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 3   | Q     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 3   | S     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 3   | U     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 3   | W     | 1        | Total Cl<br>1 1 | 0       | 0       |

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



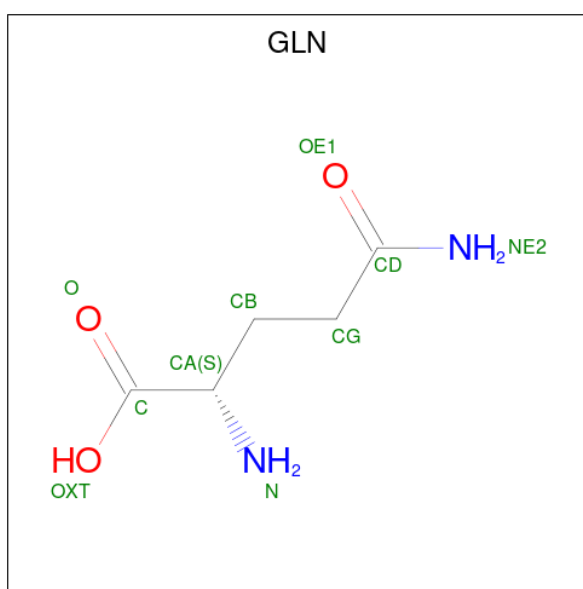
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | I     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | I     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | I     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | K     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | M     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | Q     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | Q     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | U     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | U     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 4   | W     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |

- Molecule 5 is GLUTAMINE (three-letter code: GLN) (formula:  $C_5H_{10}N_2O_3$ ).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 5   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 10    | 5 | 2 | 3 |         |         |
| 5   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 10    | 5 | 2 | 3 |         |         |
| 5   | F     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 10    | 5 | 2 | 3 |         |         |
| 5   | H     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 10    | 5 | 2 | 3 |         |         |
| 5   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 10    | 5 | 2 | 3 |         |         |
| 5   | L     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 10    | 5 | 2 | 3 |         |         |
| 5   | N     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 10    | 5 | 2 | 3 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 5   | P     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 10    | 5 | 2 | 3 |         |         |
| 5   | R     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 10    | 5 | 2 | 3 |         |         |
| 5   | T     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 10    | 5 | 2 | 3 |         |         |
| 5   | V     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 10    | 5 | 2 | 3 |         |         |
| 5   | X     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 9     | 5 | 2 | 2 |         |         |

- Molecule 6 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 6   | A     | 295      | Total | O   | 0       | 0       |
|     |       |          | 295   | 295 |         |         |
| 6   | B     | 120      | Total | O   | 0       | 0       |
|     |       |          | 120   | 120 |         |         |
| 6   | C     | 348      | Total | O   | 0       | 0       |
|     |       |          | 348   | 348 |         |         |
| 6   | D     | 142      | Total | O   | 0       | 0       |
|     |       |          | 142   | 142 |         |         |
| 6   | E     | 335      | Total | O   | 0       | 0       |
|     |       |          | 335   | 335 |         |         |
| 6   | F     | 115      | Total | O   | 0       | 0       |
|     |       |          | 115   | 115 |         |         |
| 6   | G     | 330      | Total | O   | 0       | 0       |
|     |       |          | 330   | 330 |         |         |
| 6   | H     | 164      | Total | O   | 0       | 0       |
|     |       |          | 164   | 164 |         |         |
| 6   | I     | 330      | Total | O   | 0       | 0       |
|     |       |          | 330   | 330 |         |         |
| 6   | J     | 204      | Total | O   | 0       | 0       |
|     |       |          | 204   | 204 |         |         |
| 6   | K     | 303      | Total | O   | 0       | 0       |
|     |       |          | 303   | 303 |         |         |
| 6   | L     | 153      | Total | O   | 0       | 0       |
|     |       |          | 153   | 153 |         |         |
| 6   | M     | 334      | Total | O   | 0       | 0       |
|     |       |          | 334   | 334 |         |         |
| 6   | N     | 198      | Total | O   | 0       | 0       |
|     |       |          | 198   | 198 |         |         |

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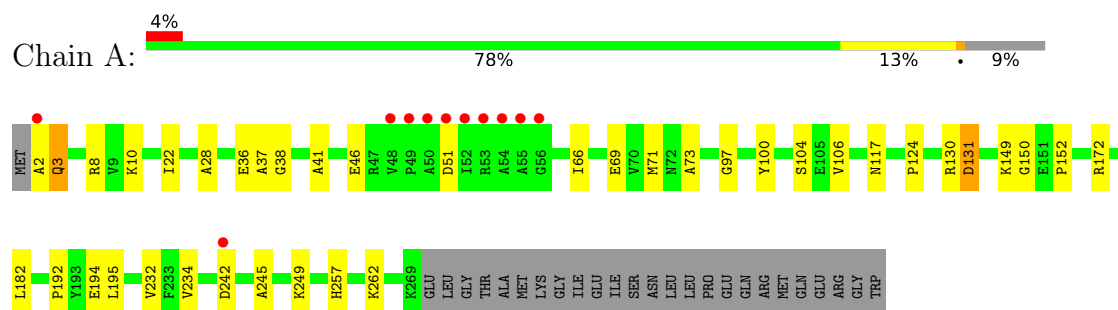
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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 6   | O     | 343      | Total<br>343 | O<br>343 | 0       | 0       |
| 6   | P     | 177      | Total<br>177 | O<br>177 | 0       | 0       |
| 6   | Q     | 323      | Total<br>323 | O<br>323 | 0       | 0       |
| 6   | R     | 173      | Total<br>173 | O<br>173 | 0       | 0       |
| 6   | S     | 311      | Total<br>311 | O<br>311 | 0       | 0       |
| 6   | T     | 134      | Total<br>134 | O<br>134 | 0       | 0       |
| 6   | U     | 285      | Total<br>285 | O<br>285 | 0       | 0       |
| 6   | V     | 104      | Total<br>104 | O<br>104 | 0       | 0       |
| 6   | W     | 334      | Total<br>334 | O<br>334 | 0       | 0       |
| 6   | X     | 219      | Total<br>219 | O<br>219 | 0       | 0       |

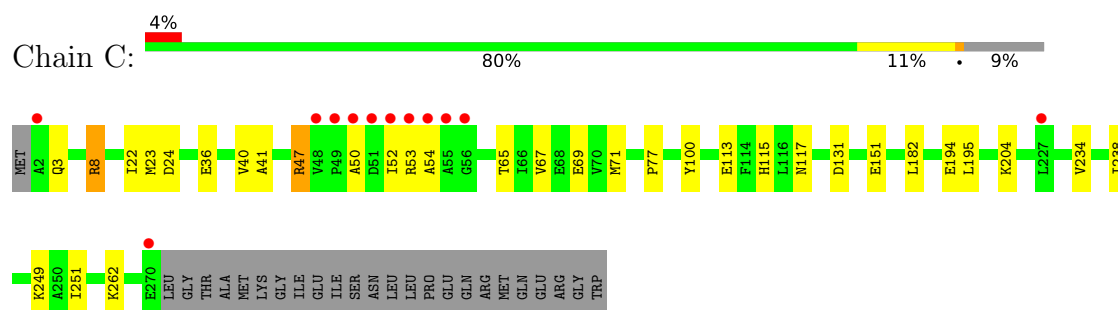
### 3 Residue-property plots [i](#)

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.

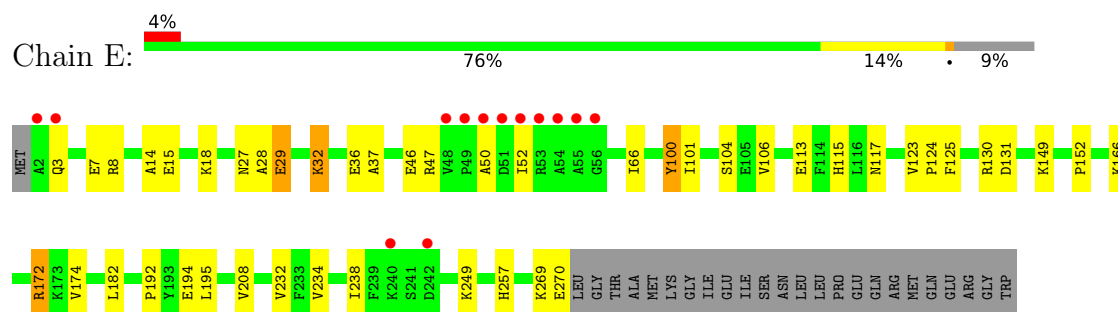
#### • Molecule 1: Pyridoxal biosynthesis lyase pdxS



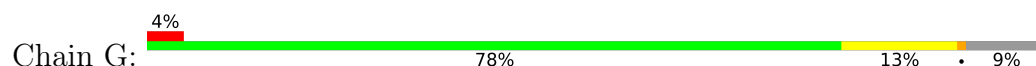
#### • Molecule 1: Pyridoxal biosynthesis lyase pdxS

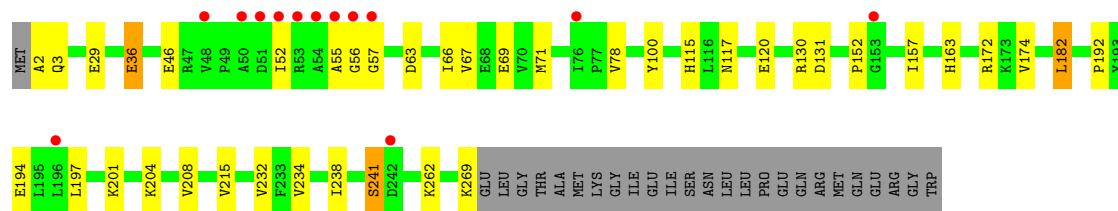


#### • Molecule 1: Pyridoxal biosynthesis lyase pdxS

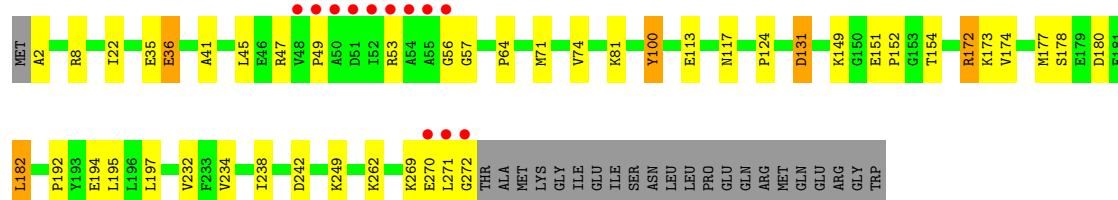
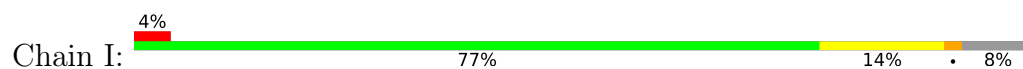


#### • Molecule 1: Pyridoxal biosynthesis lyase pdxS

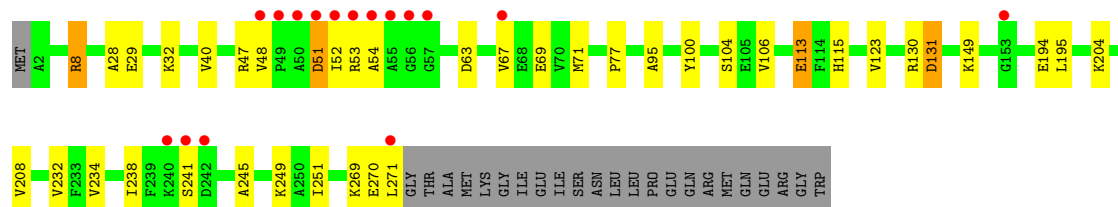
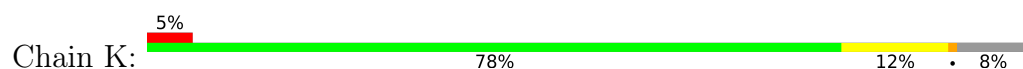




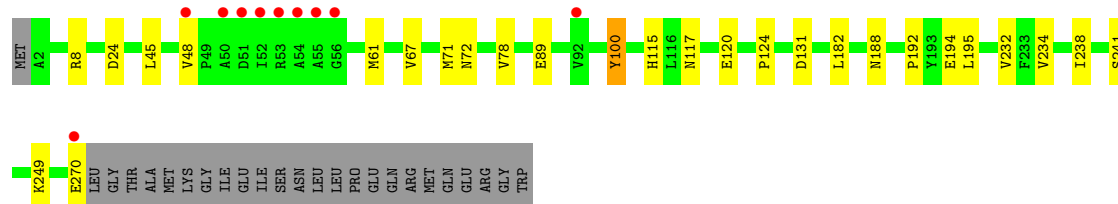
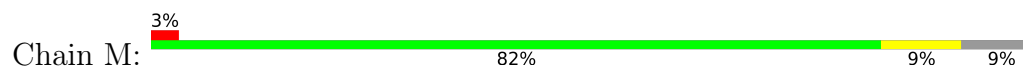
• Molecule 1: Pyridoxal biosynthesis lyase pdxS



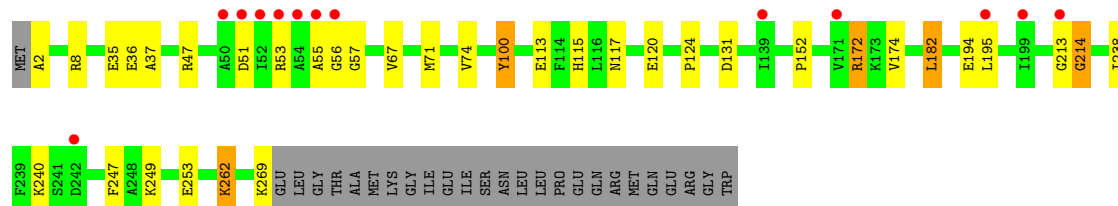
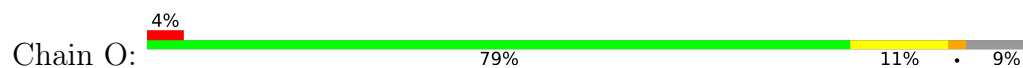
• Molecule 1: Pyridoxal biosynthesis lyase pdxS



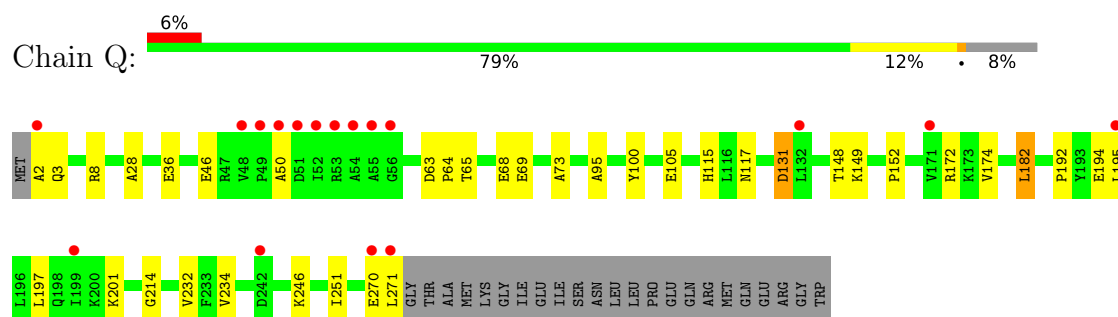
• Molecule 1: Pyridoxal biosynthesis lyase pdxS



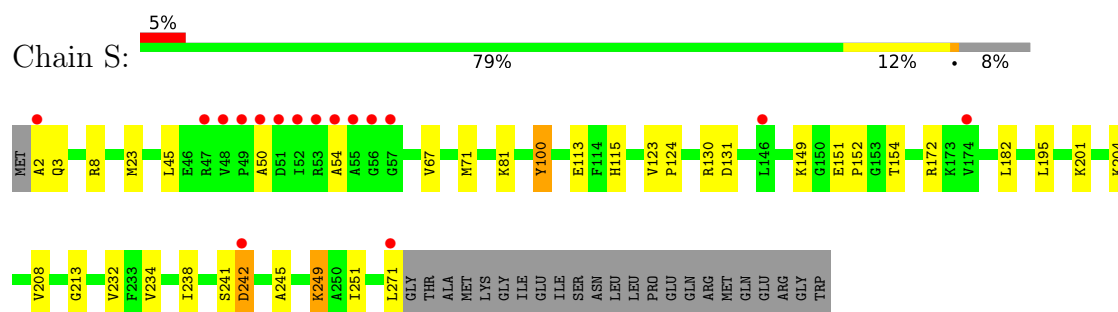
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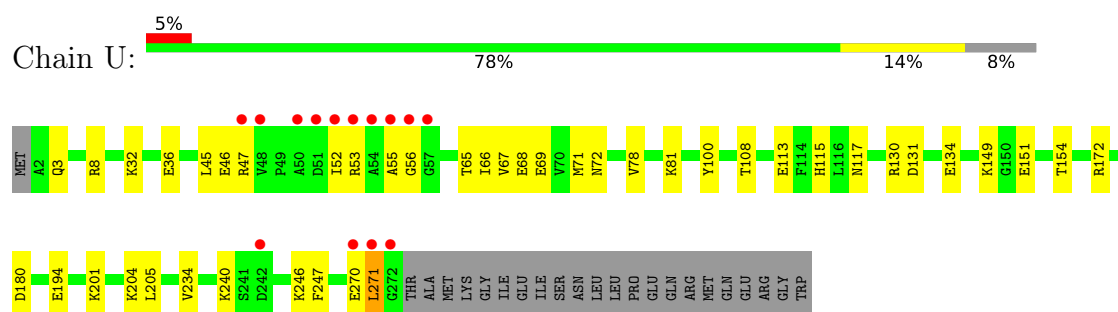
- Molecule 1: Pyridoxal biosynthesis lyase pdxS



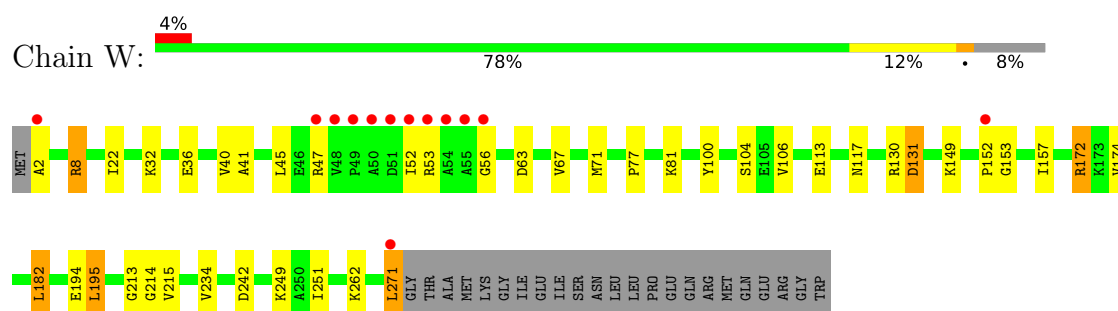
- Molecule 1: Pyridoxal biosynthesis lyase pdxS



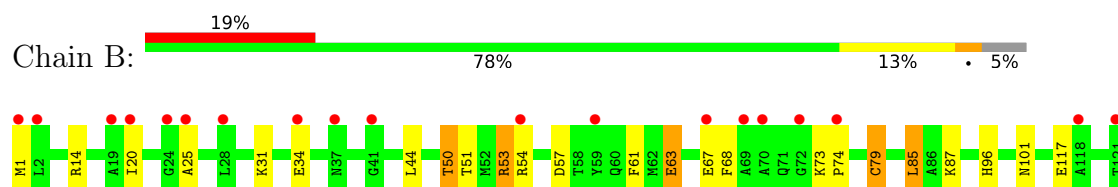
- Molecule 1: Pyridoxal biosynthesis lyase pdxS

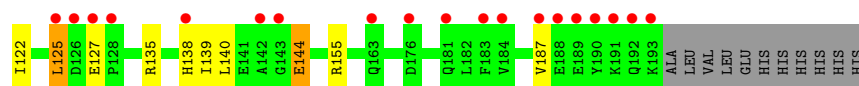


- Molecule 1: Pyridoxal biosynthesis lyase pdxS

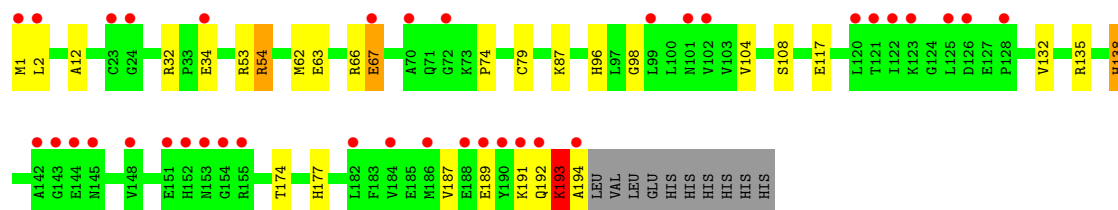
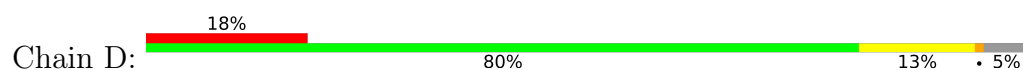


- Molecule 2: Glutamine amidotransferase subunit pdxT

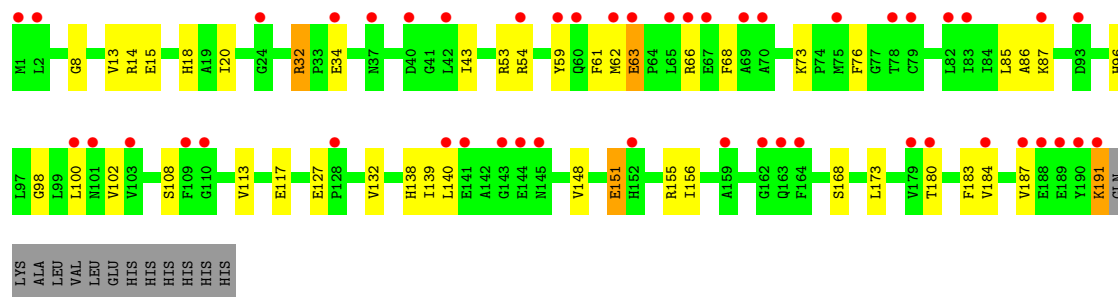
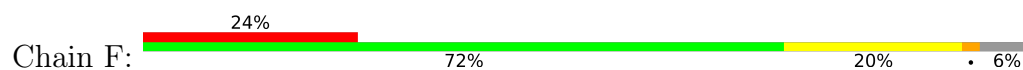




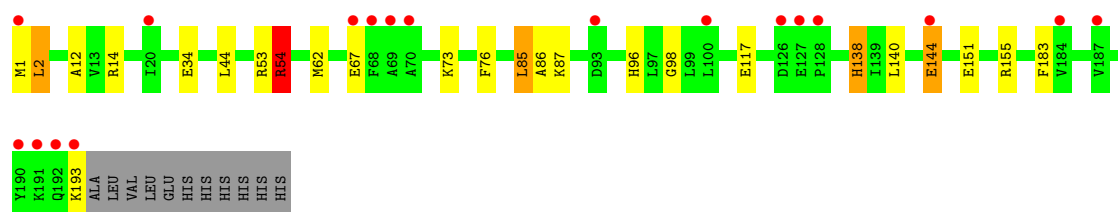
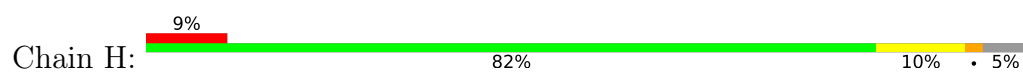
- Molecule 2: Glutamine amidotransferase subunit pdxT



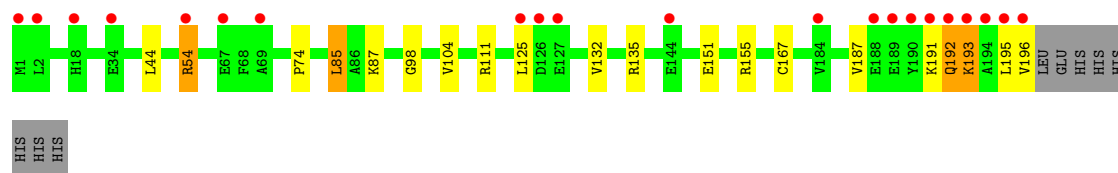
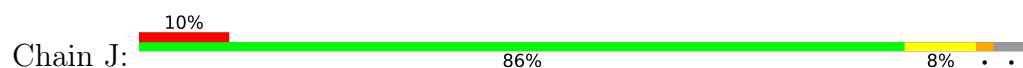
- Molecule 2: Glutamine amidotransferase subunit pdxT




- Molecule 2: Glutamine amidotransferase subunit pdxT

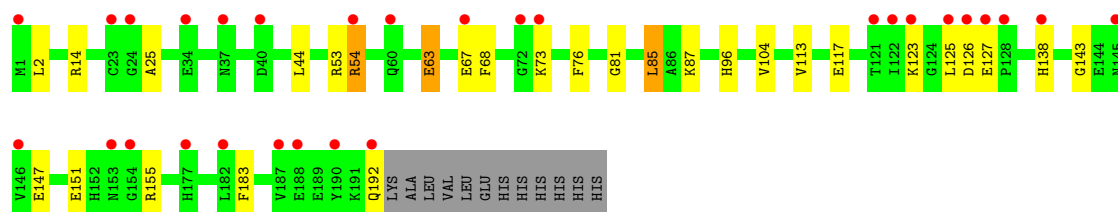


- Molecule 2: Glutamine amidotransferase subunit pdxT




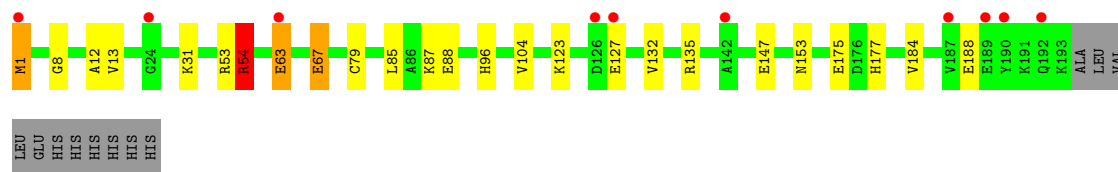
- Molecule 2: Glutamine amidotransferase subunit pdxT

Chain L: 




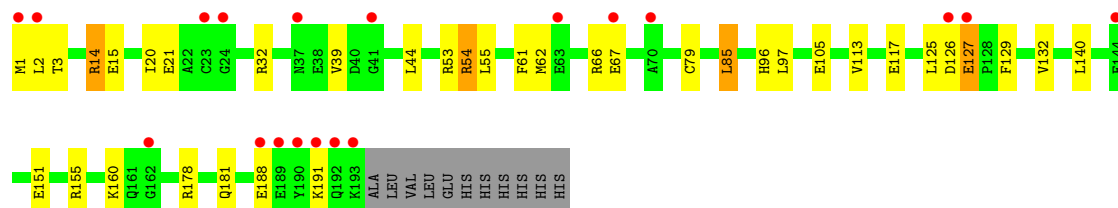
• Molecule 2: Glutamine amidotransferase subunit pdxT

Chain N: 




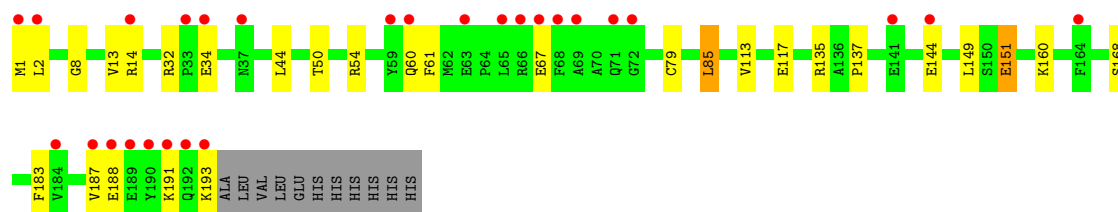
• Molecule 2: Glutamine amidotransferase subunit pdxT

Chain P: 




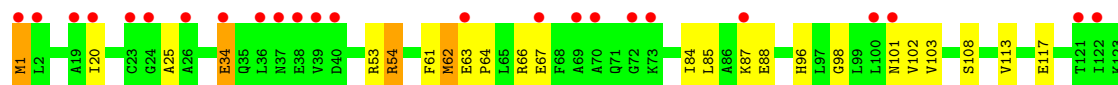
• Molecule 2: Glutamine amidotransferase subunit pdxT

Chain R: 



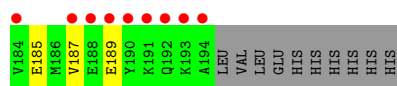
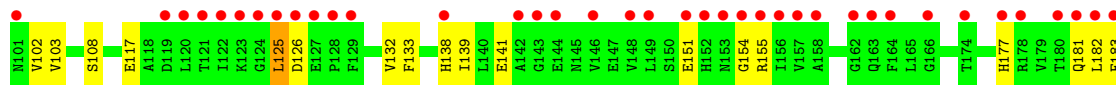
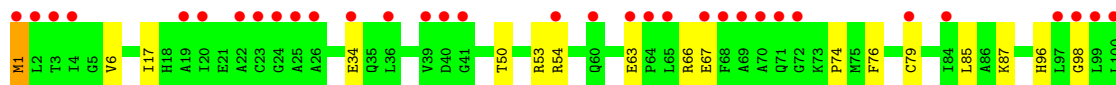
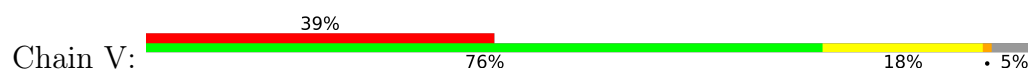
• Molecule 2: Glutamine amidotransferase subunit pdxT

Chain T: 

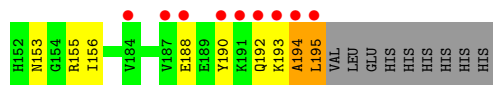
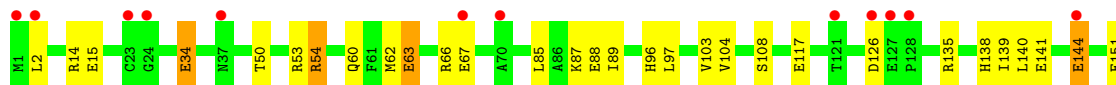
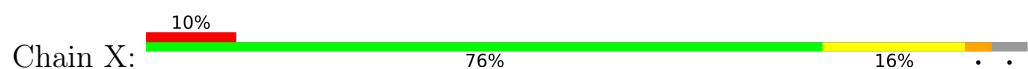




- Molecule 2: Glutamine amidotransferase subunit pdxT



- Molecule 2: Glutamine amidotransferase subunit pdxT



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 93.51Å 259.01Å 144.96Å<br>90.00° 92.13° 90.00°              | Depositor        |
| Resolution (Å)  | 50.00 – 2.12<br>49.62 – 2.12                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.2 (50.00-2.12)<br>98.2 (49.62-2.12)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | 0.08  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.89 (at 2.12Å)   | Xtriage          |
| Refinement program  | REFMAC 5.2.0019   | Depositor        |
| R, $R_{free}$   | 0.146 , 0.198<br>0.157 , 0.205                              | Depositor<br>DCC |
| $R_{free}$ test set   | 19065 reflections (5.01%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 28.3  | Xtriage          |
| Anisotropy  | 0.049   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 60.6   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction   | 0.016 for h,-k,-l   | Xtriage          |
| $F_o, F_c$ correlation  | 0.96  | EDS              |
| Total number of atoms   | 48293   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 45.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: EDO, CL

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     | 0.72         | 0/2070         | 0.77        | 5/2792 (0.2%)   |
| 1   | C     | 0.80         | 0/2076         | 0.80        | 2/2799 (0.1%)   |
| 1   | E     | 0.76         | 0/2076         | 0.79        | 4/2799 (0.1%)   |
| 1   | G     | 0.76         | 0/2040         | 0.81        | 3/2753 (0.1%)   |
| 1   | I     | 0.77         | 0/2078         | 0.85        | 4/2802 (0.1%)   |
| 1   | K     | 0.75         | 0/2068         | 0.78        | 3/2790 (0.1%)   |
| 1   | M     | 0.78         | 0/2075         | 0.81        | 1/2797 (0.0%)   |
| 1   | O     | 0.77         | 0/2060         | 0.85        | 4/2777 (0.1%)   |
| 1   | Q     | 0.75         | 0/2061         | 0.80        | 5/2780 (0.2%)   |
| 1   | S     | 0.73         | 0/2061         | 0.79        | 4/2781 (0.1%)   |
| 1   | U     | 0.73         | 0/2070         | 0.77        | 4/2793 (0.1%)   |
| 1   | W     | 0.83         | 0/2086         | 0.80        | 4/2814 (0.1%)   |
| 2   | B     | 0.56         | 0/1531         | 0.71        | 2/2066 (0.1%)   |
| 2   | D     | 0.54         | 0/1525         | 0.71        | 2/2059 (0.1%)   |
| 2   | F     | 0.53         | 0/1502         | 0.63        | 0/2029          |
| 2   | H     | 0.57         | 0/1525         | 0.72        | 1/2060 (0.0%)   |
| 2   | J     | 0.62         | 1/1540 (0.1%)  | 0.75        | 1/2080 (0.0%)   |
| 2   | L     | 0.54         | 0/1511         | 0.66        | 0/2041          |
| 2   | N     | 0.66         | 0/1516         | 0.76        | 4/2048 (0.2%)   |
| 2   | P     | 0.60         | 0/1527         | 0.70        | 0/2062          |
| 2   | R     | 0.57         | 0/1531         | 0.69        | 2/2066 (0.1%)   |
| 2   | T     | 0.53         | 0/1521         | 0.69        | 1/2054 (0.0%)   |
| 2   | V     | 0.48         | 0/1525         | 0.69        | 0/2059          |
| 2   | X     | 0.62         | 0/1533         | 0.73        | 2/2070 (0.1%)   |
| All | All   | 0.69         | 1/43108 (0.0%) | 0.76        | 58/58171 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | G     | 0                   | 1                   |
| 1   | I     | 0                   | 1                   |
| 2   | D     | 0                   | 1                   |
| 2   | P     | 1                   | 0                   |
| 2   | X     | 0                   | 1                   |
| All | All   | 1                   | 4                   |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | J     | 167 | CYS  | CB-SG | -5.57 | 1.72        | 1.81     |

All (58) bond angle outliers are listed below:

| Mol | Chain | Res    | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1   | W     | 8      | ARG  | NE-CZ-NH2 | -7.29 | 116.65      | 120.30   |
| 1   | O     | 172[A] | ARG  | NE-CZ-NH1 | 6.74  | 123.67      | 120.30   |
| 1   | O     | 172[B] | ARG  | NE-CZ-NH1 | 6.74  | 123.67      | 120.30   |
| 1   | Q     | 63     | ASP  | CB-CG-OD2 | 6.62  | 124.26      | 118.30   |
| 1   | K     | 63     | ASP  | CB-CG-OD1 | -6.62 | 112.35      | 118.30   |
| 1   | I     | 172[A] | ARG  | NE-CZ-NH1 | 6.53  | 123.56      | 120.30   |
| 1   | I     | 172[B] | ARG  | NE-CZ-NH1 | 6.53  | 123.56      | 120.30   |
| 1   | O     | 172[A] | ARG  | NE-CZ-NH2 | -6.52 | 117.04      | 120.30   |
| 1   | O     | 172[B] | ARG  | NE-CZ-NH2 | -6.52 | 117.04      | 120.30   |
| 1   | K     | 63     | ASP  | CB-CG-OD2 | 6.34  | 124.00      | 118.30   |
| 2   | B     | 135    | ARG  | NE-CZ-NH2 | -6.22 | 117.19      | 120.30   |
| 2   | H     | 54     | ARG  | NE-CZ-NH1 | 6.13  | 123.37      | 120.30   |
| 2   | N     | 135    | ARG  | NE-CZ-NH2 | -6.10 | 117.25      | 120.30   |
| 1   | G     | 172    | ARG  | NE-CZ-NH1 | 6.09  | 123.34      | 120.30   |
| 1   | C     | 8      | ARG  | NE-CZ-NH2 | -6.04 | 117.28      | 120.30   |
| 1   | G     | 63     | ASP  | CB-CG-OD1 | -5.91 | 112.98      | 118.30   |
| 2   | R     | 135    | ARG  | NE-CZ-NH2 | -5.90 | 117.35      | 120.30   |
| 1   | U     | 180    | ASP  | CB-CG-OD1 | 5.79  | 123.51      | 118.30   |
| 1   | E     | 172[A] | ARG  | NE-CZ-NH2 | -5.78 | 117.41      | 120.30   |
| 1   | E     | 172[B] | ARG  | NE-CZ-NH2 | -5.78 | 117.41      | 120.30   |
| 2   | X     | 135    | ARG  | NE-CZ-NH1 | 5.74  | 123.17      | 120.30   |
| 2   | R     | 135    | ARG  | NE-CZ-NH1 | 5.68  | 123.14      | 120.30   |
| 1   | G     | 63     | ASP  | CB-CG-OD2 | 5.61  | 123.35      | 118.30   |
| 1   | U     | 172[A] | ARG  | NE-CZ-NH1 | 5.59  | 123.09      | 120.30   |
| 1   | U     | 172[B] | ARG  | NE-CZ-NH1 | 5.59  | 123.09      | 120.30   |
| 2   | D     | 135    | ARG  | NE-CZ-NH2 | -5.58 | 117.51      | 120.30   |
| 1   | A     | 182    | LEU  | CB-CG-CD2 | -5.56 | 101.55      | 111.00   |
| 2   | T     | 135    | ARG  | NE-CZ-NH2 | -5.55 | 117.53      | 120.30   |

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| Mol | Chain | Res    | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1   | C     | 24     | ASP  | CB-CG-OD2 | -5.53 | 113.32      | 118.30   |
| 1   | I     | 172[A] | ARG  | NE-CZ-NH2 | -5.47 | 117.57      | 120.30   |
| 1   | I     | 172[B] | ARG  | NE-CZ-NH2 | -5.47 | 117.57      | 120.30   |
| 2   | J     | 135    | ARG  | NE-CZ-NH2 | -5.45 | 117.57      | 120.30   |
| 1   | S     | 172[A] | ARG  | NE-CZ-NH2 | -5.45 | 117.58      | 120.30   |
| 1   | S     | 172[B] | ARG  | NE-CZ-NH2 | -5.45 | 117.58      | 120.30   |
| 1   | A     | 172[A] | ARG  | NE-CZ-NH2 | -5.36 | 117.62      | 120.30   |
| 1   | A     | 172[B] | ARG  | NE-CZ-NH2 | -5.36 | 117.62      | 120.30   |
| 2   | N     | 135    | ARG  | NE-CZ-NH1 | 5.31  | 122.95      | 120.30   |
| 2   | B     | 53     | ARG  | NE-CZ-NH1 | 5.30  | 122.95      | 120.30   |
| 1   | E     | 172[A] | ARG  | NE-CZ-NH1 | 5.29  | 122.95      | 120.30   |
| 1   | E     | 172[B] | ARG  | NE-CZ-NH1 | 5.29  | 122.95      | 120.30   |
| 2   | D     | 135    | ARG  | NE-CZ-NH1 | 5.28  | 122.94      | 120.30   |
| 2   | X     | 135    | ARG  | NE-CZ-NH2 | -5.24 | 117.68      | 120.30   |
| 1   | Q     | 63     | ASP  | CB-CG-OD1 | -5.22 | 113.60      | 118.30   |
| 1   | W     | 63     | ASP  | CB-CG-OD2 | 5.21  | 122.99      | 118.30   |
| 1   | K     | 8      | ARG  | NE-CZ-NH2 | -5.20 | 117.70      | 120.30   |
| 1   | W     | 172[A] | ARG  | NE-CZ-NH2 | -5.16 | 117.72      | 120.30   |
| 1   | W     | 172[B] | ARG  | NE-CZ-NH2 | -5.16 | 117.72      | 120.30   |
| 1   | Q     | 172[A] | ARG  | NE-CZ-NH1 | 5.14  | 122.87      | 120.30   |
| 1   | Q     | 172[B] | ARG  | NE-CZ-NH1 | 5.14  | 122.87      | 120.30   |
| 1   | U     | 205    | LEU  | CB-CG-CD1 | -5.06 | 102.41      | 111.00   |
| 1   | S     | 172[A] | ARG  | NE-CZ-NH1 | 5.04  | 122.82      | 120.30   |
| 1   | S     | 172[B] | ARG  | NE-CZ-NH1 | 5.04  | 122.82      | 120.30   |
| 1   | A     | 172[A] | ARG  | NE-CZ-NH1 | 5.03  | 122.81      | 120.30   |
| 1   | A     | 172[B] | ARG  | NE-CZ-NH1 | 5.03  | 122.81      | 120.30   |
| 2   | N     | 54[A]  | ARG  | NE-CZ-NH1 | 5.03  | 122.81      | 120.30   |
| 2   | N     | 54[B]  | ARG  | NE-CZ-NH1 | 5.03  | 122.81      | 120.30   |
| 1   | M     | 24     | ASP  | CB-CG-OD2 | -5.02 | 113.78      | 118.30   |
| 1   | Q     | 8      | ARG  | NE-CZ-NH2 | -5.01 | 117.80      | 120.30   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res   | Type | Atom |
|-----|-------|-------|------|------|
| 2   | P     | 54[B] | ARG  | CA   |

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | D     | 193 | LYS  | Peptide |
| 1   | G     | 56  | GLY  | Peptide |
| 1   | I     | 56  | GLY  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | X     | 194 | ALA  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2028  | 0        | 2078     | 33      | 0            |
| 1   | C     | 2037  | 0        | 2079     | 39      | 0            |
| 1   | E     | 2037  | 0        | 2081     | 73      | 0            |
| 1   | G     | 2007  | 0        | 2041     | 40      | 0            |
| 1   | I     | 2042  | 0        | 2085     | 54      | 0            |
| 1   | K     | 2032  | 0        | 2081     | 35      | 0            |
| 1   | M     | 2036  | 0        | 2084     | 29      | 0            |
| 1   | O     | 2024  | 0        | 2074     | 46      | 0            |
| 1   | Q     | 2028  | 0        | 2072     | 37      | 0            |
| 1   | S     | 2028  | 0        | 2065     | 34      | 0            |
| 1   | U     | 2034  | 0        | 2070     | 43      | 0            |
| 1   | W     | 2044  | 0        | 2095     | 51      | 0            |
| 2   | B     | 1500  | 0        | 1512     | 35      | 0            |
| 2   | D     | 1497  | 0        | 1504     | 33      | 0            |
| 2   | F     | 1474  | 0        | 1478     | 36      | 0            |
| 2   | H     | 1494  | 0        | 1494     | 21      | 0            |
| 2   | J     | 1512  | 0        | 1524     | 10      | 0            |
| 2   | L     | 1483  | 0        | 1486     | 28      | 1            |
| 2   | N     | 1488  | 0        | 1488     | 28      | 0            |
| 2   | P     | 1496  | 0        | 1508     | 48      | 0            |
| 2   | R     | 1500  | 0        | 1512     | 28      | 0            |
| 2   | T     | 1493  | 0        | 1500     | 57      | 0            |
| 2   | V     | 1497  | 0        | 1504     | 39      | 0            |
| 2   | X     | 1505  | 0        | 1515     | 43      | 1            |
| 3   | A     | 1     | 0        | 0        | 2       | 0            |
| 3   | C     | 1     | 0        | 0        | 2       | 0            |
| 3   | E     | 1     | 0        | 0        | 2       | 0            |
| 3   | G     | 1     | 0        | 0        | 1       | 0            |
| 3   | I     | 1     | 0        | 0        | 2       | 0            |
| 3   | K     | 1     | 0        | 0        | 1       | 0            |
| 3   | M     | 1     | 0        | 0        | 0       | 0            |
| 3   | O     | 1     | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | Q     | 1     | 0        | 0        | 2       | 0            |
| 3   | S     | 1     | 0        | 0        | 2       | 0            |
| 3   | U     | 1     | 0        | 0        | 2       | 0            |
| 3   | W     | 1     | 0        | 0        | 2       | 0            |
| 4   | A     | 12    | 0        | 18       | 8       | 0            |
| 4   | C     | 8     | 0        | 12       | 0       | 0            |
| 4   | E     | 8     | 0        | 11       | 9       | 0            |
| 4   | G     | 4     | 0        | 6        | 9       | 0            |
| 4   | I     | 12    | 0        | 17       | 9       | 0            |
| 4   | K     | 4     | 0        | 6        | 0       | 0            |
| 4   | M     | 4     | 0        | 5        | 5       | 0            |
| 4   | Q     | 8     | 0        | 11       | 11      | 0            |
| 4   | U     | 8     | 0        | 12       | 0       | 0            |
| 4   | W     | 4     | 0        | 6        | 0       | 0            |
| 5   | B     | 10    | 0        | 7        | 1       | 0            |
| 5   | D     | 10    | 0        | 7        | 1       | 0            |
| 5   | F     | 10    | 0        | 7        | 0       | 0            |
| 5   | H     | 10    | 0        | 7        | 0       | 0            |
| 5   | J     | 10    | 0        | 7        | 0       | 0            |
| 5   | L     | 10    | 0        | 7        | 0       | 0            |
| 5   | N     | 10    | 0        | 7        | 0       | 0            |
| 5   | P     | 10    | 0        | 7        | 2       | 0            |
| 5   | R     | 10    | 0        | 7        | 0       | 0            |
| 5   | T     | 10    | 0        | 7        | 0       | 0            |
| 5   | V     | 10    | 0        | 7        | 0       | 0            |
| 5   | X     | 9     | 0        | 7        | 0       | 0            |
| 6   | A     | 295   | 0        | 0        | 13      | 0            |
| 6   | B     | 120   | 0        | 0        | 19      | 0            |
| 6   | C     | 348   | 0        | 0        | 14      | 0            |
| 6   | D     | 142   | 0        | 0        | 14      | 0            |
| 6   | E     | 335   | 0        | 0        | 48      | 0            |
| 6   | F     | 115   | 0        | 0        | 10      | 0            |
| 6   | G     | 330   | 0        | 0        | 22      | 0            |
| 6   | H     | 164   | 0        | 0        | 6       | 0            |
| 6   | I     | 330   | 0        | 0        | 33      | 0            |
| 6   | J     | 204   | 0        | 0        | 1       | 0            |
| 6   | K     | 303   | 0        | 0        | 20      | 0            |
| 6   | L     | 153   | 0        | 0        | 15      | 0            |
| 6   | M     | 334   | 0        | 0        | 17      | 0            |
| 6   | N     | 198   | 0        | 0        | 19      | 0            |
| 6   | O     | 343   | 0        | 0        | 28      | 0            |
| 6   | P     | 177   | 0        | 0        | 21      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6   | Q     | 323   | 0        | 0        | 21      | 0            |
| 6   | R     | 173   | 0        | 0        | 14      | 1            |
| 6   | S     | 311   | 0        | 0        | 25      | 0            |
| 6   | T     | 134   | 0        | 0        | 32      | 0            |
| 6   | U     | 285   | 0        | 0        | 22      | 0            |
| 6   | V     | 104   | 0        | 0        | 16      | 0            |
| 6   | W     | 334   | 0        | 0        | 35      | 1            |
| 6   | X     | 219   | 0        | 0        | 24      | 0            |
| All | All   | 48293 | 0        | 43118    | 897     | 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 (897) 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) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:R:54[B]:ARG:NH1  | 6:R:3257:HOH:O    | 1.57                     | 1.31              |
| 1:S:234:VAL:HB     | 6:S:6294:HOH:O    | 1.32                     | 1.28              |
| 1:E:172[B]:ARG:NH1 | 6:E:6234:HOH:O    | 1.67                     | 1.28              |
| 1:C:36[B]:GLU:HG3  | 2:D:54[B]:ARG:NH2 | 1.48                     | 1.27              |
| 6:A:6321:HOH:O     | 2:B:31:LYS:HB3    | 1.27                     | 1.27              |
| 2:N:54[B]:ARG:NH2  | 6:N:6095:HOH:O    | 1.64                     | 1.26              |
| 2:T:34:GLU:HG3     | 6:T:4725:HOH:O    | 1.20                     | 1.26              |
| 1:G:120:GLU:HG2    | 6:G:6327:HOH:O    | 1.25                     | 1.26              |
| 1:E:113:GLU:HG3    | 6:E:6324:HOH:O    | 1.12                     | 1.25              |
| 1:E:36[B]:GLU:HG3  | 6:E:6377:HOH:O    | 1.26                     | 1.25              |
| 1:M:120:GLU:HG2    | 6:M:6354:HOH:O    | 1.34                     | 1.23              |
| 2:V:151:GLU:HB3    | 6:V:5669:HOH:O    | 1.38                     | 1.23              |
| 1:Q:152:PRO:HD2    | 6:Q:6356:HOH:O    | 1.11                     | 1.23              |
| 2:T:155:ARG:HD3    | 6:T:5384:HOH:O    | 1.38                     | 1.23              |
| 1:I:172[B]:ARG:NH1 | 6:I:6173:HOH:O    | 1.66                     | 1.21              |
| 2:B:155[B]:ARG:NH1 | 6:B:5061:HOH:O    | 1.73                     | 1.19              |
| 1:C:234:VAL:HB     | 6:C:6342:HOH:O    | 1.39                     | 1.18              |
| 1:U:234:VAL:HB     | 6:U:6316:HOH:O    | 1.03                     | 1.18              |
| 1:U:201:LYS:HE3    | 6:U:6288:HOH:O    | 1.43                     | 1.17              |
| 2:B:138:HIS:CD2    | 6:B:5449:HOH:O    | 1.96                     | 1.16              |
| 1:E:36[B]:GLU:CG   | 6:E:6377:HOH:O    | 1.80                     | 1.15              |
| 2:P:20:ILE:HG22    | 6:P:6201:HOH:O    | 1.45                     | 1.14              |
| 2:T:54[A]:ARG:CD   | 6:T:4784:HOH:O    | 1.96                     | 1.14              |
| 1:O:172[B]:ARG:NH1 | 6:O:6309:HOH:O    | 1.81                     | 1.13              |
| 2:L:54[B]:ARG:NH2  | 6:L:6170:HOH:O    | 1.74                     | 1.12              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 6:K:6320:HOH:O     | 3:Q:6033:CL:CL   | 2.05                     | 1.12              |
| 2:D:54[B]:ARG:NH2  | 6:D:6075:HOH:O   | 1.84                     | 1.10              |
| 1:E:29[B]:GLU:OE2  | 6:E:6338:HOH:O   | 1.69                     | 1.10              |
| 3:E:6009:CL:CL     | 6:W:6353:HOH:O   | 2.07                     | 1.09              |
| 1:Q:201:LYS:HE3    | 6:Q:6332:HOH:O   | 1.51                     | 1.09              |
| 1:I:131[B]:ASP:OD1 | 6:I:6172:HOH:O   | 1.72                     | 1.07              |
| 1:O:67:VAL:HG12    | 1:O:71:MET:HE2   | 1.30                     | 1.07              |
| 2:T:138:HIS:HB2    | 6:T:5332:HOH:O   | 1.55                     | 1.06              |
| 1:W:172[B]:ARG:NH1 | 6:W:6289:HOH:O   | 1.87                     | 1.06              |
| 2:N:147:GLU:HG2    | 6:N:6225:HOH:O   | 1.53                     | 1.06              |
| 2:N:54[B]:ARG:CZ   | 6:N:6095:HOH:O   | 1.90                     | 1.05              |
| 2:T:1:MET:HG2      | 6:T:5143:HOH:O   | 1.56                     | 1.04              |
| 2:X:104:VAL:HB     | 6:X:6200:HOH:O   | 1.58                     | 1.03              |
| 1:C:194:GLU:HG2    | 4:M:6007:EDO:H12 | 1.36                     | 1.03              |
| 1:E:234:VAL:HB     | 6:E:6336:HOH:O   | 1.57                     | 1.03              |
| 1:W:113[B]:GLU:OE2 | 6:W:6305:HOH:O   | 1.73                     | 1.03              |
| 1:I:234:VAL:HB     | 6:I:6296:HOH:O   | 1.56                     | 1.03              |
| 1:U:72:ASN:HB3     | 6:U:6313:HOH:O   | 1.55                     | 1.03              |
| 2:D:54[B]:ARG:CZ   | 6:D:6075:HOH:O   | 2.01                     | 1.02              |
| 1:G:194:GLU:HB2    | 4:G:6043:EDO:H11 | 1.37                     | 1.02              |
| 2:T:54[A]:ARG:CG   | 6:T:4784:HOH:O   | 2.07                     | 1.02              |
| 1:E:36[B]:GLU:OE2  | 6:E:6278:HOH:O   | 1.76                     | 1.01              |
| 1:I:113[B]:GLU:OE2 | 6:I:6244:HOH:O   | 1.78                     | 1.01              |
| 1:Q:234:VAL:HB     | 6:Q:6324:HOH:O   | 0.84                     | 1.00              |
| 1:G:262:LYS:HE2    | 6:I:6350:HOH:O   | 1.61                     | 1.00              |
| 1:Q:50:ALA:HB2     | 6:Q:6349:HOH:O   | 1.59                     | 1.00              |
| 1:M:131[A]:ASP:OD2 | 6:M:6198:HOH:O   | 1.77                     | 1.00              |
| 1:C:113[B]:GLU:OE2 | 6:C:6292:HOH:O   | 1.79                     | 1.00              |
| 1:E:194:GLU:HB2    | 4:E:6047:EDO:H11 | 1.43                     | 0.99              |
| 1:Q:197:LEU:HD12   | 6:Q:6339:HOH:O   | 1.62                     | 0.99              |
| 2:T:155:ARG:HG3    | 6:T:5723:HOH:O   | 1.60                     | 0.99              |
| 1:A:36[B]:GLU:OE1  | 6:A:6188:HOH:O   | 1.80                     | 0.99              |
| 2:V:6:VAL:HG23     | 6:V:5626:HOH:O   | 1.62                     | 0.98              |
| 1:A:131[B]:ASP:OD2 | 6:A:6181:HOH:O   | 1.81                     | 0.97              |
| 2:B:138:HIS:HD2    | 6:B:5449:HOH:O   | 1.36                     | 0.97              |
| 1:Q:148:THR:HG22   | 6:Q:6318:HOH:O   | 1.64                     | 0.97              |
| 2:X:192:GLN:HG3    | 6:X:6265:HOH:O   | 1.64                     | 0.97              |
| 6:Q:6353:HOH:O     | 1:S:113:GLU:HG2  | 1.62                     | 0.96              |
| 1:G:192:PRO:HB3    | 4:G:6043:EDO:H22 | 1.44                     | 0.96              |
| 3:I:6017:CL:CL     | 6:S:6347:HOH:O   | 2.18                     | 0.96              |
| 1:E:29[A]:GLU:HG2  | 6:E:6381:HOH:O   | 1.64                     | 0.95              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:M:67:VAL:HG12    | 1:M:71:MET:HE3     | 1.46                     | 0.95              |
| 2:X:54[B]:ARG:NH2  | 6:X:6143:HOH:O     | 1.99                     | 0.95              |
| 2:B:87:LYS:HG3     | 2:B:101:ASN:HA     | 1.47                     | 0.95              |
| 1:W:131[B]:ASP:OD1 | 6:W:6210:HOH:O     | 1.85                     | 0.95              |
| 2:T:139:ILE:HG22   | 6:T:5578:HOH:O     | 1.67                     | 0.95              |
| 2:L:87:LYS:HE3     | 6:L:6176:HOH:O     | 1.67                     | 0.94              |
| 2:B:144:GLU:H      | 2:B:144:GLU:CD     | 1.70                     | 0.94              |
| 1:G:234:VAL:HB     | 6:G:6331:HOH:O     | 1.68                     | 0.94              |
| 1:O:249:LYS:NZ     | 2:P:54[A]:ARG:HH21 | 1.65                     | 0.94              |
| 6:S:6328:HOH:O     | 2:T:113:VAL:HB     | 1.68                     | 0.94              |
| 1:K:131[B]:ASP:OD2 | 6:K:6189:HOH:O     | 1.83                     | 0.94              |
| 1:O:67:VAL:HG12    | 1:O:71:MET:CE      | 1.98                     | 0.94              |
| 1:A:194:GLU:HB2    | 4:A:6031:EDO:H12   | 1.50                     | 0.93              |
| 6:E:6262:HOH:O     | 2:F:113:VAL:HB     | 1.66                     | 0.93              |
| 1:K:32:LYS:HE2     | 6:K:6296:HOH:O     | 1.69                     | 0.93              |
| 1:O:249:LYS:HZ2    | 2:P:54[A]:ARG:HH21 | 1.15                     | 0.92              |
| 1:M:45:LEU:HD13    | 6:M:6331:HOH:O     | 1.67                     | 0.92              |
| 1:I:47:ARG:HG3     | 6:I:6354:HOH:O     | 1.68                     | 0.92              |
| 1:I:194:GLU:HB2    | 4:I:6039:EDO:H11   | 1.50                     | 0.92              |
| 1:G:197:LEU:HD12   | 6:G:6333:HOH:O     | 1.68                     | 0.92              |
| 2:H:144:GLU:CD     | 2:H:144:GLU:H      | 1.73                     | 0.91              |
| 1:S:152:PRO:HA     | 6:S:6346:HOH:O     | 1.70                     | 0.91              |
| 1:G:36[B]:GLU:OE1  | 6:G:6276:HOH:O     | 1.87                     | 0.90              |
| 1:E:36[B]:GLU:OE1  | 6:E:6220:HOH:O     | 1.88                     | 0.90              |
| 2:T:1:MET:CG       | 6:T:5143:HOH:O     | 2.14                     | 0.90              |
| 2:X:195:LEU:HG     | 6:X:6267:HOH:O     | 1.71                     | 0.90              |
| 2:F:191:LYS:C      | 6:F:5703:HOH:O     | 2.08                     | 0.89              |
| 1:K:245:ALA:O      | 1:K:249:LYS:HD3    | 1.73                     | 0.89              |
| 2:B:139:ILE:CD1    | 6:B:5510:HOH:O     | 2.20                     | 0.89              |
| 1:M:67:VAL:HG12    | 1:M:71:MET:CE      | 2.03                     | 0.89              |
| 3:W:6045:CL:CL     | 6:W:6141:HOH:O     | 2.27                     | 0.88              |
| 2:R:60:GLN:HG3     | 6:R:5326:HOH:O     | 1.74                     | 0.88              |
| 3:A:6001:CL:CL     | 6:O:6244:HOH:O     | 2.26                     | 0.88              |
| 1:S:152:PRO:HD2    | 6:S:6344:HOH:O     | 1.71                     | 0.88              |
| 2:T:1:MET:CB       | 6:T:5143:HOH:O     | 2.21                     | 0.88              |
| 1:G:194:GLU:HB2    | 4:G:6043:EDO:C1    | 2.04                     | 0.87              |
| 1:Q:115:HIS:HD2    | 6:Q:6346:HOH:O     | 1.57                     | 0.87              |
| 2:V:17:ILE:CD1     | 6:V:5626:HOH:O     | 2.21                     | 0.87              |
| 1:W:152:PRO:CG     | 6:W:6343:HOH:O     | 2.22                     | 0.87              |
| 1:E:194:GLU:HB2    | 4:E:6047:EDO:C1    | 2.04                     | 0.87              |
| 2:D:194:ALA:HA     | 6:D:6133:HOH:O     | 1.74                     | 0.87              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:E:270:GLU:C      | 6:E:6353:HOH:O     | 2.13                     | 0.86              |
| 6:K:6292:HOH:O     | 2:L:113:VAL:HB     | 1.74                     | 0.86              |
| 2:X:54[A]:ARG:NH1  | 6:X:6147:HOH:O     | 1.64                     | 0.86              |
| 1:C:36[B]:GLU:HG3  | 2:D:54[B]:ARG:HH21 | 1.33                     | 0.86              |
| 1:W:47:ARG:HD2     | 6:W:6352:HOH:O     | 1.74                     | 0.86              |
| 1:C:67:VAL:HG12    | 1:C:71:MET:CE      | 2.05                     | 0.86              |
| 1:S:50:ALA:HB2     | 6:S:6286:HOH:O     | 1.76                     | 0.86              |
| 6:K:6188:HOH:O     | 3:Q:6033:CL:CL     | 2.33                     | 0.84              |
| 1:S:213:GLY:HA2    | 6:S:6346:HOH:O     | 1.77                     | 0.84              |
| 1:I:194:GLU:HB2    | 4:I:6039:EDO:C1    | 2.08                     | 0.83              |
| 1:W:152:PRO:HB2    | 6:W:6343:HOH:O     | 1.78                     | 0.83              |
| 1:E:29[B]:GLU:CD   | 6:E:6338:HOH:O     | 2.11                     | 0.83              |
| 1:E:29[B]:GLU:HG3  | 6:E:6381:HOH:O     | 1.78                     | 0.83              |
| 2:R:54[A]:ARG:CZ   | 6:R:3513:HOH:O     | 2.25                     | 0.83              |
| 1:E:27:ASN:OD1     | 1:E:29[B]:GLU:HG2  | 1.78                     | 0.83              |
| 1:W:113[A]:GLU:OE2 | 6:W:6357:HOH:O     | 1.97                     | 0.83              |
| 2:B:139:ILE:HD12   | 6:B:5510:HOH:O     | 1.78                     | 0.83              |
| 2:T:54[A]:ARG:HG2  | 6:T:4784:HOH:O     | 1.71                     | 0.83              |
| 2:T:139:ILE:CG2    | 6:T:5578:HOH:O     | 2.21                     | 0.83              |
| 1:G:46:GLU:HG3     | 1:G:66:ILE:HD12    | 1.62                     | 0.82              |
| 2:X:54[B]:ARG:NH1  | 6:X:6193:HOH:O     | 2.10                     | 0.82              |
| 1:S:67:VAL:HG12    | 1:S:71:MET:CE      | 2.10                     | 0.82              |
| 3:W:6045:CL:CL     | 6:W:6307:HOH:O     | 2.33                     | 0.82              |
| 1:U:72:ASN:CB      | 6:U:6313:HOH:O     | 2.20                     | 0.81              |
| 2:T:54[B]:ARG:HG3  | 6:T:4784:HOH:O     | 1.79                     | 0.81              |
| 1:C:36[B]:GLU:HG3  | 2:D:54[B]:ARG:HH22 | 1.44                     | 0.81              |
| 1:W:152:PRO:CB     | 6:W:6343:HOH:O     | 2.29                     | 0.81              |
| 2:L:125:LEU:HA     | 6:L:6171:HOH:O     | 1.81                     | 0.80              |
| 3:C:6005:CL:CL     | 6:C:6144:HOH:O     | 2.36                     | 0.80              |
| 2:X:144:GLU:H      | 2:X:144:GLU:CD     | 1.85                     | 0.80              |
| 3:A:6001:CL:CL     | 6:O:6194:HOH:O     | 2.37                     | 0.80              |
| 1:E:130:ARG:HH12   | 1:E:149:LYS:NZ     | 1.80                     | 0.80              |
| 6:S:6328:HOH:O     | 2:T:113:VAL:CB     | 2.27                     | 0.80              |
| 2:X:34:GLU:CG      | 6:X:6094:HOH:O     | 2.29                     | 0.80              |
| 2:X:34:GLU:HG2     | 6:X:6094:HOH:O     | 1.81                     | 0.80              |
| 1:G:29:GLU:HG2     | 6:G:6309:HOH:O     | 1.81                     | 0.79              |
| 1:Q:115:HIS:CD2    | 6:Q:6346:HOH:O     | 2.34                     | 0.79              |
| 1:W:32:LYS:HE2     | 6:W:6252:HOH:O     | 1.81                     | 0.79              |
| 1:M:270:GLU:HG2    | 6:O:6362:HOH:O     | 1.81                     | 0.79              |
| 2:V:17:ILE:HD13    | 6:V:5626:HOH:O     | 1.82                     | 0.79              |
| 2:X:138:HIS:CE1    | 6:X:6214:HOH:O     | 2.35                     | 0.79              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:C:36[B]:GLU:CG   | 2:D:54[B]:ARG:NH2 | 2.39                     | 0.79              |
| 1:C:262:LYS:HE3    | 6:E:6351:HOH:O    | 1.82                     | 0.79              |
| 1:Q:152:PRO:CD     | 6:Q:6356:HOH:O    | 1.87                     | 0.79              |
| 1:O:120[A]:GLU:OE2 | 6:O:6153:HOH:O    | 2.01                     | 0.79              |
| 2:V:1:MET:HB2      | 6:V:4934:HOH:O    | 1.83                     | 0.79              |
| 2:N:147:GLU:CG     | 6:N:6225:HOH:O    | 2.17                     | 0.78              |
| 2:F:102:VAL:HG22   | 6:F:4875:HOH:O    | 1.81                     | 0.78              |
| 1:U:240:LYS:CB     | 6:U:6314:HOH:O    | 2.30                     | 0.78              |
| 1:G:192:PRO:CB     | 4:G:6043:EDO:H22  | 2.13                     | 0.78              |
| 2:X:195:LEU:HA     | 6:X:6225:HOH:O    | 1.83                     | 0.78              |
| 1:G:194:GLU:CB     | 4:G:6043:EDO:H11  | 2.13                     | 0.78              |
| 2:P:129:PHE:HB2    | 6:P:6192:HOH:O    | 1.84                     | 0.78              |
| 1:O:113:GLU:HG2    | 6:O:6344:HOH:O    | 1.84                     | 0.77              |
| 2:R:44:LEU:CD1     | 2:R:85:LEU:HD13   | 2.13                     | 0.77              |
| 1:U:246:LYS:HD3    | 6:U:6323:HOH:O    | 1.84                     | 0.77              |
| 1:U:113[B]:GLU:OE1 | 6:U:6203:HOH:O    | 2.02                     | 0.77              |
| 1:G:197:LEU:CD1    | 6:G:6333:HOH:O    | 2.28                     | 0.76              |
| 1:U:69:GLU:HG3     | 6:U:6318:HOH:O    | 1.85                     | 0.76              |
| 2:N:53:ARG:HH11    | 2:N:96:HIS:HD2    | 1.33                     | 0.76              |
| 1:G:152:PRO:HD2    | 6:G:6302:HOH:O    | 1.83                     | 0.76              |
| 1:E:270:GLU:CB     | 6:E:6343:HOH:O    | 2.33                     | 0.76              |
| 1:M:194:GLU:HB2    | 4:M:6007:EDO:H11  | 1.67                     | 0.76              |
| 1:W:214:GLY:CA     | 6:W:6367:HOH:O    | 2.33                     | 0.76              |
| 1:W:271:LEU:HD23   | 6:W:6356:HOH:O    | 1.86                     | 0.76              |
| 2:X:153:ASN:ND2    | 6:X:6259:HOH:O    | 2.16                     | 0.75              |
| 1:E:130:ARG:NH1    | 1:E:149:LYS:NZ    | 2.33                     | 0.75              |
| 6:S:6328:HOH:O     | 2:T:113:VAL:CG2   | 2.33                     | 0.75              |
| 2:R:191:LYS:HE2    | 6:R:4894:HOH:O    | 1.85                     | 0.75              |
| 3:O:6029:CL:CL     | 6:O:6307:HOH:O    | 2.41                     | 0.75              |
| 4:A:6031:EDO:H21   | 1:O:194:GLU:HG2   | 1.68                     | 0.75              |
| 1:Q:131[B]:ASP:OD1 | 6:Q:6211:HOH:O    | 2.04                     | 0.75              |
| 2:F:100:LEU:HB3    | 6:F:4875:HOH:O    | 1.86                     | 0.75              |
| 2:B:57:ASP:OD2     | 6:B:5438:HOH:O    | 2.04                     | 0.75              |
| 1:K:269:LYS:O      | 1:K:271:LEU:HD13  | 1.85                     | 0.74              |
| 1:S:67:VAL:HG12    | 1:S:71:MET:HE1    | 1.69                     | 0.74              |
| 2:L:25:ALA:HA      | 6:L:6172:HOH:O    | 1.86                     | 0.74              |
| 2:B:139:ILE:HG13   | 6:B:5510:HOH:O    | 1.87                     | 0.74              |
| 1:C:67:VAL:HG12    | 1:C:71:MET:HE3    | 1.70                     | 0.74              |
| 1:O:214:GLY:CA     | 6:O:6333:HOH:O    | 2.34                     | 0.74              |
| 2:X:2:LEU:HD21     | 2:X:188:GLU:HG3   | 1.70                     | 0.74              |
| 1:I:49:PRO:HG3     | 6:I:6366:HOH:O    | 1.86                     | 0.74              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:Q:246:LYS:HE2    | 6:Q:6354:HOH:O    | 1.86                     | 0.74              |
| 2:X:138:HIS:HB2    | 6:X:6135:HOH:O    | 1.87                     | 0.73              |
| 1:E:270:GLU:HB3    | 6:E:6343:HOH:O    | 1.87                     | 0.73              |
| 2:H:53:ARG:HH11    | 2:H:96:HIS:HD2    | 1.36                     | 0.73              |
| 1:I:197:LEU:HD12   | 6:I:6364:HOH:O    | 1.87                     | 0.73              |
| 2:P:125:LEU:CD1    | 6:P:6192:HOH:O    | 2.35                     | 0.73              |
| 1:W:214:GLY:HA3    | 6:W:6367:HOH:O    | 1.88                     | 0.73              |
| 1:K:245:ALA:O      | 1:K:249:LYS:CD    | 2.36                     | 0.73              |
| 2:X:138:HIS:ND1    | 6:X:6214:HOH:O    | 2.21                     | 0.73              |
| 1:O:214:GLY:HA3    | 6:O:6333:HOH:O    | 1.89                     | 0.73              |
| 1:C:262:LYS:CE     | 6:E:6351:HOH:O    | 2.37                     | 0.72              |
| 2:X:60:GLN:HG2     | 6:X:6213:HOH:O    | 1.87                     | 0.72              |
| 1:U:55:ALA:HB3     | 1:U:56:GLY:HA2    | 1.70                     | 0.72              |
| 2:V:54[B]:ARG:HH11 | 2:V:54[B]:ARG:CG  | 2.02                     | 0.72              |
| 1:K:29:GLU:CD      | 6:K:6296:HOH:O    | 2.27                     | 0.72              |
| 1:A:257:HIS:CE1    | 6:A:6321:HOH:O    | 2.42                     | 0.72              |
| 2:V:54[B]:ARG:HH11 | 2:V:54[B]:ARG:HG2 | 1.54                     | 0.72              |
| 1:E:50:ALA:HB2     | 6:E:6364:HOH:O    | 1.90                     | 0.71              |
| 1:A:3:GLN:HA       | 6:A:6303:HOH:O    | 1.90                     | 0.71              |
| 2:H:144:GLU:CD     | 2:H:144:GLU:N     | 2.42                     | 0.71              |
| 1:E:130:ARG:HH12   | 1:E:149:LYS:HZ1   | 1.36                     | 0.71              |
| 1:Q:36:GLU:O       | 2:R:54[B]:ARG:HD3 | 1.91                     | 0.71              |
| 1:C:67:VAL:HG12    | 1:C:71:MET:HE2    | 1.71                     | 0.71              |
| 1:O:36:GLU:O       | 2:P:54[B]:ARG:HD2 | 1.89                     | 0.71              |
| 1:O:47[B]:ARG:HA   | 6:O:6357:HOH:O    | 1.90                     | 0.71              |
| 2:R:160:LYS:HE2    | 6:R:5551:HOH:O    | 1.89                     | 0.71              |
| 3:E:6009:CL:CL     | 6:E:6345:HOH:O    | 2.45                     | 0.71              |
| 1:O:47[B]:ARG:HG3  | 6:O:6357:HOH:O    | 1.91                     | 0.71              |
| 2:P:188:GLU:HG2    | 6:P:6209:HOH:O    | 1.90                     | 0.71              |
| 1:E:36[B]:GLU:HG2  | 6:E:6377:HOH:O    | 1.65                     | 0.71              |
| 2:T:54[A]:ARG:HD2  | 6:T:4784:HOH:O    | 1.72                     | 0.71              |
| 1:C:194:GLU:CG     | 4:M:6007:EDO:H12  | 2.18                     | 0.70              |
| 1:O:47[A]:ARG:HA   | 6:O:6357:HOH:O    | 1.90                     | 0.70              |
| 2:V:17:ILE:HD11    | 6:V:5626:HOH:O    | 1.83                     | 0.70              |
| 2:N:63:GLU:HG3     | 6:N:6220:HOH:O    | 1.88                     | 0.70              |
| 2:R:54[B]:ARG:NE   | 6:R:3929:HOH:O    | 2.24                     | 0.70              |
| 2:F:66:ARG:HD2     | 6:F:5427:HOH:O    | 1.90                     | 0.70              |
| 2:B:139:ILE:CG1    | 6:B:5510:HOH:O    | 2.36                     | 0.70              |
| 6:S:6328:HOH:O     | 2:T:113:VAL:HG23  | 1.91                     | 0.70              |
| 1:U:69:GLU:CG      | 6:U:6318:HOH:O    | 2.39                     | 0.70              |
| 1:W:152:PRO:CD     | 6:W:6343:HOH:O    | 2.39                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:Q:192:PRO:HB3   | 4:Q:6035:EDO:H11  | 1.72                     | 0.70              |
| 3:S:6037:CL:CL    | 6:S:6243:HOH:O    | 2.46                     | 0.70              |
| 1:W:152:PRO:HD2   | 6:W:6343:HOH:O    | 1.91                     | 0.70              |
| 1:G:3:GLN:HB3     | 6:G:6362:HOH:O    | 1.91                     | 0.70              |
| 2:N:67:GLU:CG     | 6:N:6216:HOH:O    | 2.40                     | 0.70              |
| 2:D:194:ALA:C     | 6:D:6131:HOH:O    | 2.30                     | 0.69              |
| 1:M:115:HIS:HD2   | 6:M:6112:HOH:O    | 1.75                     | 0.69              |
| 2:F:62:MET:C      | 6:F:5427:HOH:O    | 2.31                     | 0.69              |
| 1:E:192:PRO:HB3   | 4:E:6047:EDO:H22  | 1.75                     | 0.69              |
| 2:B:144:GLU:CD    | 2:B:144:GLU:N     | 2.45                     | 0.69              |
| 2:V:177:HIS:HD2   | 6:V:5109:HOH:O    | 1.75                     | 0.69              |
| 1:C:3:GLN:HB3     | 6:C:6328:HOH:O    | 1.91                     | 0.69              |
| 1:E:194:GLU:CB    | 4:E:6047:EDO:H11  | 2.21                     | 0.69              |
| 2:T:87:LYS:HG3    | 2:T:101:ASN:HA    | 1.72                     | 0.69              |
| 1:O:214:GLY:N     | 6:O:6333:HOH:O    | 2.26                     | 0.69              |
| 1:U:47:ARG:HB2    | 1:U:52:ILE:HD11   | 1.74                     | 0.68              |
| 1:W:213:GLY:O     | 6:W:6367:HOH:O    | 2.10                     | 0.68              |
| 6:M:6287:HOH:O    | 1:W:262:LYS:CE    | 2.41                     | 0.68              |
| 3:U:6041:CL:CL    | 6:U:6242:HOH:O    | 2.48                     | 0.68              |
| 2:J:44:LEU:HD12   | 2:J:85:LEU:HD13   | 1.76                     | 0.67              |
| 1:O:36:GLU:CD     | 6:O:6348:HOH:O    | 2.31                     | 0.67              |
| 2:B:53:ARG:HH11   | 2:B:96:HIS:HD2    | 1.42                     | 0.67              |
| 2:D:34:GLU:HG2    | 6:D:6046:HOH:O    | 1.95                     | 0.67              |
| 1:E:113:GLU:CG    | 6:E:6324:HOH:O    | 1.89                     | 0.67              |
| 2:N:88:GLU:OE1    | 6:N:6199:HOH:O    | 2.12                     | 0.67              |
| 1:W:271:LEU:CD2   | 6:W:6356:HOH:O    | 2.41                     | 0.67              |
| 2:F:18:HIS:CD2    | 6:F:5556:HOH:O    | 2.47                     | 0.67              |
| 1:I:194:GLU:CB    | 4:I:6039:EDO:H11  | 2.23                     | 0.67              |
| 2:J:44:LEU:CD1    | 2:J:85:LEU:HD13   | 2.25                     | 0.67              |
| 2:D:194:ALA:CA    | 6:D:6133:HOH:O    | 2.37                     | 0.67              |
| 1:I:232:VAL:HG12  | 1:I:234:VAL:HG23  | 1.76                     | 0.67              |
| 1:Q:194:GLU:N     | 4:Q:6035:EDO:H21  | 2.10                     | 0.66              |
| 1:S:67:VAL:HG12   | 1:S:71:MET:HE2    | 1.76                     | 0.66              |
| 2:V:50:THR:O      | 2:V:54[A]:ARG:HG2 | 1.94                     | 0.66              |
| 1:E:36[A]:GLU:OE2 | 6:E:6301:HOH:O    | 2.13                     | 0.66              |
| 1:G:46:GLU:HG3    | 1:G:66:ILE:CD1    | 2.26                     | 0.66              |
| 2:F:86:ALA:HA     | 6:F:4875:HOH:O    | 1.94                     | 0.66              |
| 2:P:129:PHE:HD1   | 6:P:6192:HOH:O    | 1.78                     | 0.66              |
| 1:A:242:ASP:OD1   | 6:A:6322:HOH:O    | 2.13                     | 0.66              |
| 2:P:53:ARG:HH11   | 2:P:96:HIS:HD2    | 1.42                     | 0.66              |
| 2:V:34:GLU:HG2    | 6:V:3608:HOH:O    | 1.94                     | 0.66              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:E:192:PRO:CB    | 4:E:6047:EDO:H22 | 2.26                     | 0.66              |
| 2:L:138:HIS:HB2   | 6:L:6083:HOH:O   | 1.94                     | 0.66              |
| 1:I:192:PRO:CB    | 4:I:6039:EDO:H22 | 2.26                     | 0.65              |
| 2:L:54[A]:ARG:CZ  | 6:L:6107:HOH:O   | 2.44                     | 0.65              |
| 1:Q:201:LYS:CE    | 6:Q:6332:HOH:O   | 2.24                     | 0.65              |
| 2:B:54[B]:ARG:HD2 | 6:B:3460:HOH:O   | 1.95                     | 0.65              |
| 2:X:138:HIS:CD2   | 6:X:6227:HOH:O   | 2.49                     | 0.65              |
| 1:I:197:LEU:CD1   | 6:I:6364:HOH:O   | 2.43                     | 0.65              |
| 1:A:245:ALA:O     | 1:A:249:LYS:HG3  | 1.97                     | 0.64              |
| 1:S:152:PRO:O     | 6:S:6344:HOH:O   | 2.15                     | 0.64              |
| 2:X:53:ARG:HH11   | 2:X:96:HIS:HD2   | 1.45                     | 0.64              |
| 2:V:66:ARG:HG2    | 2:V:66:ARG:HH11  | 1.62                     | 0.64              |
| 1:Q:246:LYS:CE    | 6:Q:6354:HOH:O   | 2.44                     | 0.64              |
| 1:M:48:VAL:HG22   | 6:M:6331:HOH:O   | 1.98                     | 0.64              |
| 1:G:2:ALA:HA      | 2:H:117:GLU:O    | 1.98                     | 0.64              |
| 1:I:36:GLU:HG2    | 6:I:6092:HOH:O   | 1.97                     | 0.64              |
| 1:I:45:LEU:HD21   | 1:I:81:LYS:HE2   | 1.79                     | 0.64              |
| 1:M:232:VAL:HG12  | 1:M:234:VAL:HG23 | 1.78                     | 0.64              |
| 1:W:67:VAL:HG12   | 1:W:71:MET:CE    | 2.27                     | 0.64              |
| 1:G:232:VAL:HG12  | 1:G:234:VAL:HG23 | 1.79                     | 0.64              |
| 1:K:29:GLU:OE2    | 6:K:6296:HOH:O   | 2.15                     | 0.64              |
| 2:P:125:LEU:HD13  | 6:P:6192:HOH:O   | 1.96                     | 0.64              |
| 1:Q:105:GLU:HB3   | 6:Q:6310:HOH:O   | 1.98                     | 0.64              |
| 2:X:62:MET:SD     | 2:X:97:LEU:HD23  | 2.38                     | 0.63              |
| 2:L:44:LEU:HD12   | 2:L:85:LEU:HD13  | 1.80                     | 0.63              |
| 1:U:204:LYS:HD3   | 6:U:6280:HOH:O   | 1.99                     | 0.63              |
| 1:M:270:GLU:C     | 6:M:6281:HOH:O   | 2.36                     | 0.63              |
| 1:Q:194:GLU:H     | 4:Q:6035:EDO:H21 | 1.64                     | 0.63              |
| 2:F:108:SER:OG    | 2:F:138:HIS:HD2  | 1.82                     | 0.63              |
| 1:I:53:ARG:HD3    | 6:I:6284:HOH:O   | 1.98                     | 0.63              |
| 2:H:53:ARG:HH11   | 2:H:96:HIS:CD2   | 2.17                     | 0.62              |
| 2:F:34:GLU:H      | 2:F:34:GLU:CD    | 2.03                     | 0.62              |
| 2:F:62:MET:HG3    | 6:F:5427:HOH:O   | 1.99                     | 0.62              |
| 2:N:53:ARG:HH11   | 2:N:96:HIS:CD2   | 2.16                     | 0.62              |
| 1:W:67:VAL:HG12   | 1:W:71:MET:HE2   | 1.82                     | 0.62              |
| 2:B:63:GLU:HG3    | 6:B:4744:HOH:O   | 2.00                     | 0.62              |
| 2:D:138:HIS:HB3   | 6:D:6113:HOH:O   | 1.99                     | 0.62              |
| 1:O:55:ALA:N      | 1:O:56:GLY:HA2   | 2.15                     | 0.62              |
| 2:X:144:GLU:CD    | 2:X:144:GLU:N    | 2.53                     | 0.62              |
| 1:E:270:GLU:C     | 6:E:6371:HOH:O   | 2.38                     | 0.61              |
| 1:E:8:ARG:HD3     | 6:E:6359:HOH:O   | 1.99                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:L:44:LEU:CD1     | 2:L:85:LEU:HD13    | 2.30                     | 0.61              |
| 2:N:123:LYS:NZ     | 6:N:6225:HOH:O     | 2.33                     | 0.61              |
| 1:O:213:GLY:C      | 6:O:6333:HOH:O     | 2.37                     | 0.61              |
| 2:T:54[B]:ARG:HD2  | 6:T:2551:HOH:O     | 1.99                     | 0.61              |
| 1:M:45:LEU:CD1     | 6:M:6331:HOH:O     | 2.36                     | 0.61              |
| 1:A:192:PRO:HB3    | 4:A:6031:EDO:H22   | 1.82                     | 0.61              |
| 2:R:60:GLN:CD      | 6:R:5326:HOH:O     | 2.39                     | 0.61              |
| 2:X:34:GLU:HG3     | 6:X:6094:HOH:O     | 1.97                     | 0.61              |
| 2:R:60:GLN:CG      | 6:R:5326:HOH:O     | 2.36                     | 0.61              |
| 1:E:192:PRO:HB3    | 4:E:6047:EDO:C2    | 2.30                     | 0.61              |
| 2:P:181:GLN:HG2    | 6:P:6196:HOH:O     | 2.01                     | 0.61              |
| 3:U:6041:CL:CL     | 6:U:6205:HOH:O     | 2.53                     | 0.61              |
| 1:C:65:THR:O       | 1:C:69[A]:GLU:HG3  | 2.01                     | 0.61              |
| 1:W:242:ASP:O      | 6:W:6181:HOH:O     | 2.17                     | 0.61              |
| 1:I:192:PRO:HB3    | 4:I:6039:EDO:H22   | 1.82                     | 0.60              |
| 1:C:36[B]:GLU:CG   | 2:D:54[B]:ARG:HH21 | 2.11                     | 0.60              |
| 1:K:8:ARG:HD2      | 2:L:117:GLU:OE2    | 2.00                     | 0.60              |
| 4:A:6031:EDO:H21   | 1:O:194:GLU:H      | 1.66                     | 0.60              |
| 1:M:249[A]:LYS:HG2 | 2:N:54[A]:ARG:HH21 | 1.67                     | 0.60              |
| 2:N:31:LYS:HG3     | 6:N:6191:HOH:O     | 2.01                     | 0.60              |
| 2:P:125:LEU:HD12   | 6:P:6192:HOH:O     | 2.00                     | 0.60              |
| 1:E:130:ARG:NH1    | 1:E:149:LYS:HZ2    | 1.99                     | 0.60              |
| 1:O:37:ALA:O       | 2:P:54[A]:ARG:HD2  | 2.01                     | 0.60              |
| 2:X:14:ARG:NH1     | 2:X:15:GLU:OE2     | 2.35                     | 0.60              |
| 2:F:53:ARG:HH11    | 2:F:96:HIS:HD2     | 1.49                     | 0.60              |
| 1:K:47:ARG:HG3     | 1:K:48:VAL:N       | 2.16                     | 0.60              |
| 1:Q:197:LEU:CD1    | 6:Q:6339:HOH:O     | 2.34                     | 0.60              |
| 2:R:44:LEU:HD12    | 2:R:85:LEU:HD13    | 1.82                     | 0.60              |
| 1:S:45:LEU:HD21    | 1:S:81:LYS:HE2     | 1.83                     | 0.60              |
| 1:C:23:MET:HG2     | 6:C:6342:HOH:O     | 2.01                     | 0.60              |
| 2:H:138:HIS:CE1    | 2:H:140:LEU:HD23   | 2.37                     | 0.60              |
| 1:Q:194:GLU:HB2    | 4:Q:6035:EDO:H21   | 1.83                     | 0.60              |
| 2:D:67:GLU:OE2     | 6:D:6125:HOH:O     | 2.16                     | 0.60              |
| 1:E:232:VAL:HG12   | 1:E:234:VAL:HG23   | 1.83                     | 0.60              |
| 1:K:8:ARG:NH1      | 6:K:6321:HOH:O     | 2.34                     | 0.60              |
| 1:M:8:ARG:HD3      | 2:N:132:VAL:HG21   | 1.84                     | 0.59              |
| 2:N:67:GLU:CB      | 6:N:6216:HOH:O     | 2.50                     | 0.59              |
| 1:S:232:VAL:HG12   | 1:S:234:VAL:HG23   | 1.84                     | 0.59              |
| 2:T:87:LYS:HB3     | 6:T:4753:HOH:O     | 2.02                     | 0.59              |
| 2:T:139:ILE:CB     | 6:T:5578:HOH:O     | 2.50                     | 0.59              |
| 1:I:173:LYS:HE2    | 1:I:177:MET:HE1    | 1.85                     | 0.59              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:K:194:GLU:H      | 4:Q:6035:EDO:H12  | 1.68                     | 0.59              |
| 2:R:54[B]:ARG:CD   | 6:R:3929:HOH:O    | 2.51                     | 0.59              |
| 1:C:151:GLU:HB3    | 6:C:6366:HOH:O    | 2.03                     | 0.59              |
| 1:I:64:PRO:HG3     | 6:I:6358:HOH:O    | 2.02                     | 0.59              |
| 2:V:87:LYS:HA      | 2:V:98:GLY:HA2    | 1.85                     | 0.59              |
| 1:W:130:ARG:NE     | 6:W:6359:HOH:O    | 2.23                     | 0.59              |
| 2:T:156:ILE:HB     | 6:T:5578:HOH:O    | 2.02                     | 0.58              |
| 1:W:113[B]:GLU:OE1 | 6:W:6103:HOH:O    | 2.17                     | 0.58              |
| 1:K:123:VAL:HB     | 6:K:6292:HOH:O    | 2.04                     | 0.58              |
| 1:W:149:LYS:NZ     | 6:W:6355:HOH:O    | 2.36                     | 0.58              |
| 2:P:126:ASP:HB2    | 6:P:6155:HOH:O    | 2.02                     | 0.58              |
| 2:D:174:THR:HG21   | 6:D:6073:HOH:O    | 2.04                     | 0.58              |
| 1:O:253:GLU:OE2    | 2:P:54[A]:ARG:NH2 | 2.36                     | 0.58              |
| 2:V:54[B]:ARG:CZ   | 6:V:4748:HOH:O    | 2.50                     | 0.58              |
| 2:P:125:LEU:HD22   | 6:P:6151:HOH:O    | 2.04                     | 0.58              |
| 2:D:189:GLU:HG2    | 6:D:6110:HOH:O    | 2.03                     | 0.58              |
| 1:W:152:PRO:HG2    | 6:W:6343:HOH:O    | 1.94                     | 0.57              |
| 1:K:51:ASP:CG      | 6:K:6233:HOH:O    | 2.43                     | 0.57              |
| 2:D:53:ARG:HH11    | 2:D:96:HIS:HD2    | 1.52                     | 0.57              |
| 2:D:177:HIS:HE1    | 6:D:6144:HOH:O    | 1.85                     | 0.57              |
| 2:H:73:LYS:NZ      | 6:H:6157:HOH:O    | 2.16                     | 0.57              |
| 3:S:6037:CL:CL     | 6:S:6321:HOH:O    | 2.54                     | 0.57              |
| 1:M:188[A]:ASN:ND2 | 6:M:6157:HOH:O    | 2.37                     | 0.57              |
| 2:T:1:MET:HB2      | 6:T:5143:HOH:O    | 1.93                     | 0.57              |
| 1:A:257:HIS:ND1    | 6:A:6321:HOH:O    | 2.32                     | 0.57              |
| 1:G:67:VAL:HG12    | 1:G:71:MET:CE     | 2.34                     | 0.57              |
| 2:T:54[A]:ARG:NE   | 6:T:4784:HOH:O    | 2.25                     | 0.57              |
| 2:T:87:LYS:HD2     | 6:T:4753:HOH:O    | 2.05                     | 0.57              |
| 2:T:155:ARG:CG     | 6:T:5723:HOH:O    | 2.33                     | 0.57              |
| 2:V:53:ARG:HH11    | 2:V:96:HIS:HD2    | 1.51                     | 0.57              |
| 2:V:108:SER:OG     | 2:V:138:HIS:CD2   | 2.58                     | 0.57              |
| 2:X:63:GLU:HG3     | 6:X:6229:HOH:O    | 2.03                     | 0.57              |
| 1:E:130:ARG:HH11   | 1:E:149:LYS:HD2   | 1.68                     | 0.57              |
| 1:G:69:GLU:HG3     | 6:G:6336:HOH:O    | 2.05                     | 0.57              |
| 2:F:148:VAL:HG13   | 2:F:156:ILE:HG23  | 1.87                     | 0.57              |
| 2:V:138:HIS:CD2    | 2:V:155:ARG:NH1   | 2.73                     | 0.57              |
| 1:M:249[A]:LYS:HG2 | 2:N:54[A]:ARG:NH2 | 2.20                     | 0.56              |
| 1:O:37:ALA:C       | 2:P:54[A]:ARG:HD2 | 2.25                     | 0.56              |
| 1:O:269:LYS:C      | 6:O:6335:HOH:O    | 2.43                     | 0.56              |
| 1:S:238:ILE:O      | 1:S:241:SER:HB3   | 2.05                     | 0.56              |
| 2:V:54[A]:ARG:NH2  | 6:V:2884:HOH:O    | 2.36                     | 0.56              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 2:B:122:ILE:HB      | 2:B:125:LEU:HG    | 1.87                     | 0.56              |
| 1:E:28:ALA:O        | 1:E:32:LYS:HG2    | 2.05                     | 0.56              |
| 1:E:46:GLU:HA       | 1:E:66:ILE:HD13   | 1.86                     | 0.56              |
| 1:I:234:VAL:CB      | 6:I:6296:HOH:O    | 2.32                     | 0.56              |
| 2:L:123:LYS:NZ      | 2:L:147:GLU:OE2   | 2.28                     | 0.56              |
| 1:M:270:GLU:CD      | 6:M:6337:HOH:O    | 2.42                     | 0.56              |
| 1:S:23:MET:HG2      | 6:S:6294:HOH:O    | 2.04                     | 0.56              |
| 2:T:63:GLU:HB3      | 2:T:64:PRO:HD3    | 1.87                     | 0.56              |
| 1:K:270:GLU:O       | 1:K:271:LEU:HD12  | 2.05                     | 0.56              |
| 1:W:234[A]:VAL:HG21 | 1:W:251:ILE:HG21  | 1.87                     | 0.56              |
| 1:M:100:TYR:CZ      | 1:M:124:PRO:HB2   | 2.41                     | 0.56              |
| 2:X:138:HIS:CB      | 6:X:6135:HOH:O    | 2.50                     | 0.56              |
| 1:O:249:LYS:HZ2     | 2:P:54[A]:ARG:NH2 | 1.96                     | 0.56              |
| 2:T:139:ILE:HB      | 6:T:5578:HOH:O    | 2.06                     | 0.56              |
| 1:E:270:GLU:HB2     | 6:E:6343:HOH:O    | 2.01                     | 0.56              |
| 2:F:32:ARG:HB3      | 2:F:34:GLU:OE1    | 2.05                     | 0.56              |
| 2:R:34:GLU:H        | 2:R:34:GLU:CD     | 2.10                     | 0.56              |
| 2:R:54[B]:ARG:HD3   | 6:R:3929:HOH:O    | 2.06                     | 0.56              |
| 1:K:51:ASP:HA       | 1:K:54:ALA:HB3    | 1.88                     | 0.56              |
| 2:N:12:ALA:HB3      | 6:N:6065:HOH:O    | 2.05                     | 0.56              |
| 2:P:2:LEU:HD21      | 6:P:6209:HOH:O    | 2.06                     | 0.56              |
| 1:Q:192:PRO:HB2     | 4:Q:6035:EDO:H22  | 1.87                     | 0.56              |
| 2:B:53:ARG:HH11     | 2:B:96:HIS:CD2    | 2.23                     | 0.55              |
| 1:C:151:GLU:CB      | 6:C:6366:HOH:O    | 2.53                     | 0.55              |
| 6:K:6292:HOH:O      | 2:L:113:VAL:CB    | 2.45                     | 0.55              |
| 2:R:2:LEU:CD2       | 2:R:188:GLU:HG2   | 2.36                     | 0.55              |
| 1:U:204:LYS:HE2     | 6:U:6211:HOH:O    | 2.05                     | 0.55              |
| 1:I:271:LEU:HD12    | 6:I:6304:HOH:O    | 2.06                     | 0.55              |
| 1:S:245:ALA:O       | 1:S:249:LYS:HD3   | 2.06                     | 0.55              |
| 2:X:2:LEU:CD2       | 2:X:188:GLU:HG3   | 2.36                     | 0.55              |
| 2:L:53:ARG:HH11     | 2:L:96:HIS:HD2    | 1.54                     | 0.55              |
| 2:R:149:LEU:HD11    | 2:R:160:LYS:HB2   | 1.89                     | 0.55              |
| 2:X:53:ARG:HH11     | 2:X:96:HIS:CD2    | 2.23                     | 0.55              |
| 3:K:6021:CL:CL      | 6:K:6236:HOH:O    | 2.55                     | 0.55              |
| 2:V:108:SER:HB2     | 2:V:138:HIS:NE2   | 2.22                     | 0.55              |
| 2:X:144:GLU:HB3     | 6:X:6191:HOH:O    | 2.05                     | 0.55              |
| 1:U:270:GLU:N       | 6:U:6312:HOH:O    | 2.39                     | 0.55              |
| 1:I:22:ILE:HG12     | 1:I:41:ALA:HB3    | 1.89                     | 0.54              |
| 2:L:138:HIS:CG      | 6:L:6132:HOH:O    | 2.60                     | 0.54              |
| 2:P:44:LEU:CD1      | 2:P:85:LEU:HD13   | 2.36                     | 0.54              |
| 2:P:178:ARG:CZ      | 6:P:6192:HOH:O    | 2.55                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:O:152:PRO:HD2   | 6:O:6323:HOH:O    | 2.07                     | 0.54              |
| 1:C:23:MET:CE     | 1:C:238:ILE:HD12  | 2.37                     | 0.54              |
| 2:P:53:ARG:HH11   | 2:P:96:HIS:CD2    | 2.24                     | 0.54              |
| 1:G:29:GLU:HB2    | 6:G:6361:HOH:O    | 2.06                     | 0.54              |
| 1:G:67:VAL:HG12   | 1:G:71:MET:HE2    | 1.90                     | 0.54              |
| 2:H:12:ALA:HB3    | 6:H:6040:HOH:O    | 2.07                     | 0.54              |
| 1:M:249[B]:LYS:NZ | 6:M:6318:HOH:O    | 2.36                     | 0.54              |
| 1:O:36:GLU:HB3    | 6:O:6348:HOH:O    | 2.05                     | 0.54              |
| 2:T:138:HIS:CD2   | 2:T:155:ARG:HD2   | 2.42                     | 0.54              |
| 1:U:53:ARG:O      | 1:U:56:GLY:HA3    | 2.08                     | 0.54              |
| 1:S:123:VAL:HB    | 6:S:6328:HOH:O    | 2.07                     | 0.54              |
| 2:T:62:MET:O      | 2:T:66:ARG:HG3    | 2.08                     | 0.54              |
| 2:T:138:HIS:HD2   | 6:T:5384:HOH:O    | 1.91                     | 0.54              |
| 1:K:47:ARG:HG2    | 1:K:52:ILE:CG1    | 2.38                     | 0.54              |
| 2:P:21:GLU:N      | 6:P:6201:HOH:O    | 2.39                     | 0.54              |
| 1:I:272:GLY:N     | 6:I:6360:HOH:O    | 2.41                     | 0.54              |
| 1:Q:232:VAL:HG12  | 1:Q:234:VAL:HG23  | 1.90                     | 0.53              |
| 2:X:66:ARG:HG2    | 2:X:66:ARG:HH11   | 1.73                     | 0.53              |
| 1:E:194:GLU:HB2   | 4:E:6047:EDO:H12  | 1.89                     | 0.53              |
| 1:E:257:HIS:HE1   | 2:F:59:TYR:CE1    | 2.27                     | 0.53              |
| 1:Q:192:PRO:CB    | 4:Q:6035:EDO:H22  | 2.39                     | 0.53              |
| 1:S:152:PRO:CD    | 6:S:6344:HOH:O    | 2.40                     | 0.53              |
| 2:T:156:ILE:HD12  | 6:T:5578:HOH:O    | 2.07                     | 0.53              |
| 2:F:66:ARG:HH11   | 2:F:66:ARG:HG2    | 1.74                     | 0.53              |
| 2:F:183:PHE:O     | 2:F:187:VAL:HG23  | 2.07                     | 0.53              |
| 1:A:3:GLN:HB3     | 6:A:6279:HOH:O    | 2.08                     | 0.53              |
| 2:N:123:LYS:HD3   | 6:N:6225:HOH:O    | 2.08                     | 0.53              |
| 1:U:130:ARG:NH1   | 1:U:149:LYS:NZ    | 2.57                     | 0.53              |
| 2:V:133:PHE:HE2   | 6:V:5124:HOH:O    | 1.92                     | 0.53              |
| 1:W:8:ARG:HD2     | 2:X:117:GLU:OE2   | 2.09                     | 0.53              |
| 2:X:50:THR:O      | 2:X:54[B]:ARG:HG2 | 2.09                     | 0.53              |
| 1:G:192:PRO:HB3   | 4:G:6043:EDO:C2   | 2.29                     | 0.53              |
| 1:E:8:ARG:HD3     | 2:F:132:VAL:HG21  | 1.91                     | 0.52              |
| 2:V:125:LEU:CD2   | 2:V:182:LEU:HD11  | 2.39                     | 0.52              |
| 1:A:150:GLY:O     | 6:A:6294:HOH:O    | 2.19                     | 0.52              |
| 1:K:8:ARG:CZ      | 6:K:6321:HOH:O    | 2.56                     | 0.52              |
| 2:V:154:GLY:C     | 6:V:5669:HOH:O    | 2.47                     | 0.52              |
| 1:W:53:ARG:O      | 1:W:56:GLY:N      | 2.32                     | 0.52              |
| 1:A:262:LYS:HE3   | 6:C:6286:HOH:O    | 2.08                     | 0.52              |
| 3:I:6017:CL:CL    | 6:S:6181:HOH:O    | 2.56                     | 0.52              |
| 4:I:6039:EDO:O1   | 6:I:6162:HOH:O    | 2.19                     | 0.52              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:L:155:ARG:HG2     | 2:L:155:ARG:HH11    | 1.73                     | 0.52              |
| 1:S:130:ARG:NH1     | 1:S:149:LYS:HZ2     | 2.07                     | 0.52              |
| 2:T:155:ARG:CD      | 6:T:5723:HOH:O      | 2.56                     | 0.52              |
| 2:D:62:MET:O        | 2:D:66:ARG:HG3      | 2.09                     | 0.52              |
| 2:D:194:ALA:C       | 6:D:6133:HOH:O      | 2.47                     | 0.52              |
| 2:P:44:LEU:HD12     | 2:P:85:LEU:HD13     | 1.91                     | 0.52              |
| 1:U:270:GLU:CA      | 6:U:6312:HOH:O      | 2.57                     | 0.52              |
| 1:A:194:GLU:CB      | 4:A:6031:EDO:H12    | 2.33                     | 0.52              |
| 1:C:23:MET:HE3      | 1:C:238:ILE:CD1     | 2.39                     | 0.52              |
| 6:G:6105:HOH:O      | 2:H:54:ARG:HD2      | 2.09                     | 0.52              |
| 2:V:138:HIS:HB2     | 6:V:5292:HOH:O      | 2.10                     | 0.52              |
| 1:O:2:ALA:HA        | 2:P:117:GLU:O       | 2.09                     | 0.52              |
| 2:X:89:ILE:HG12     | 6:X:6200:HOH:O      | 2.09                     | 0.52              |
| 1:A:46:GLU:HG3      | 1:A:66:ILE:HD12     | 1.92                     | 0.52              |
| 1:C:50:ALA:O        | 1:C:54:ALA:CB       | 2.58                     | 0.52              |
| 2:P:127:GLU:CD      | 2:P:127:GLU:H       | 2.13                     | 0.52              |
| 1:G:269:LYS:C       | 6:G:6314:HOH:O      | 2.47                     | 0.51              |
| 1:O:117:ASN:ND2     | 1:O:120[A]:GLU:OE2  | 2.43                     | 0.51              |
| 1:W:174:VAL:HG13    | 1:W:182:LEU:HD11    | 1.92                     | 0.51              |
| 2:J:193:LYS:HE2     | 6:J:6222:HOH:O      | 2.09                     | 0.51              |
| 2:L:138:HIS:CD2     | 6:L:6132:HOH:O      | 2.62                     | 0.51              |
| 1:O:172[B]:ARG:CZ   | 6:O:6309:HOH:O      | 2.37                     | 0.51              |
| 2:P:129:PHE:CD1     | 6:P:6192:HOH:O      | 2.54                     | 0.51              |
| 1:A:38:GLY:O        | 2:B:51:THR:HG23     | 2.10                     | 0.51              |
| 2:B:50:THR:OG1      | 6:B:2702:HOH:O      | 2.19                     | 0.51              |
| 2:L:2:LEU:O         | 6:L:6172:HOH:O      | 2.18                     | 0.51              |
| 2:T:155:ARG:CD      | 6:T:5384:HOH:O      | 2.19                     | 0.51              |
| 1:W:153:GLY:C       | 6:W:6298:HOH:O      | 2.49                     | 0.51              |
| 1:G:152:PRO:CD      | 6:G:6302:HOH:O      | 2.51                     | 0.51              |
| 4:M:6007:EDO:O2     | 6:M:6107:HOH:O      | 2.19                     | 0.51              |
| 2:R:2:LEU:HD22      | 2:R:188:GLU:HG2     | 1.93                     | 0.51              |
| 1:E:104:SER:OG      | 1:E:106:VAL:HG22    | 2.11                     | 0.51              |
| 1:I:249:LYS:HG3     | 2:J:54[A]:ARG:NH1   | 2.25                     | 0.51              |
| 1:O:8:ARG:HD3       | 2:P:132:VAL:HG21    | 1.91                     | 0.51              |
| 1:W:213:GLY:C       | 6:W:6367:HOH:O      | 2.47                     | 0.51              |
| 1:A:28:ALA:HB1      | 1:A:73:ALA:HB2      | 1.92                     | 0.51              |
| 2:F:14:ARG:NH1      | 2:F:15:GLU:OE2      | 2.44                     | 0.51              |
| 2:P:151:GLU:HA      | 2:P:155:ARG:O       | 2.11                     | 0.51              |
| 1:K:232:VAL:HG12    | 1:K:234[A]:VAL:HG23 | 1.93                     | 0.51              |
| 1:K:234[A]:VAL:HG21 | 1:K:251:ILE:HG21    | 1.93                     | 0.51              |
| 1:C:67:VAL:CG1      | 1:C:71:MET:HE2      | 2.39                     | 0.51              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 6:E:6359:HOH:O    | 2:F:132:VAL:HG21    | 2.09                     | 0.51              |
| 2:F:180:THR:O     | 2:F:184:VAL:HG23    | 2.11                     | 0.51              |
| 2:N:1:MET:HE2     | 6:N:6223:HOH:O      | 2.10                     | 0.51              |
| 2:H:2:LEU:H       | 2:H:2:LEU:HD22      | 1.75                     | 0.51              |
| 1:I:49:PRO:HD3    | 6:I:6366:HOH:O      | 2.11                     | 0.51              |
| 2:B:74:PRO:HG2    | 2:B:187:VAL:HA      | 1.92                     | 0.50              |
| 2:D:192:GLN:O     | 2:D:193:LYS:HB2     | 2.10                     | 0.50              |
| 1:O:53:ARG:O      | 1:O:56:GLY:HA2      | 2.11                     | 0.50              |
| 1:U:246:LYS:NZ    | 6:U:6323:HOH:O      | 2.44                     | 0.50              |
| 1:W:36:GLU:HG3    | 6:W:6304:HOH:O      | 2.11                     | 0.50              |
| 1:A:8:ARG:HD2     | 2:B:117:GLU:OE2     | 2.11                     | 0.50              |
| 2:F:63:GLU:N      | 6:F:5427:HOH:O      | 2.43                     | 0.50              |
| 1:W:45:LEU:HD21   | 1:W:81:LYS:HE2      | 1.93                     | 0.50              |
| 1:I:271:LEU:HD11  | 6:I:6252:HOH:O      | 2.11                     | 0.50              |
| 2:L:68:PHE:CE1    | 2:L:73:LYS:HD3      | 2.46                     | 0.50              |
| 2:P:3:THR:HG22    | 2:P:39:VAL:HG12     | 1.93                     | 0.50              |
| 1:I:272:GLY:C     | 6:I:6368:HOH:O      | 2.50                     | 0.50              |
| 6:K:6292:HOH:O    | 2:L:113:VAL:CG2     | 2.59                     | 0.50              |
| 6:O:6271:HOH:O    | 2:P:113[B]:VAL:HG11 | 2.10                     | 0.50              |
| 2:V:54[B]:ARG:HG2 | 2:V:54[B]:ARG:NH1   | 2.20                     | 0.50              |
| 2:X:108:SER:HG    | 2:X:138:HIS:CE1     | 2.30                     | 0.50              |
| 1:C:115:HIS:HD2   | 6:C:6240:HOH:O      | 1.95                     | 0.50              |
| 1:A:37:ALA:O      | 2:B:54[B]:ARG:HD3   | 2.11                     | 0.50              |
| 1:A:46:GLU:HG3    | 1:A:66:ILE:CD1      | 2.41                     | 0.50              |
| 2:D:192:GLN:O     | 2:D:193:LYS:CB      | 2.59                     | 0.50              |
| 1:I:269:LYS:O     | 1:I:271:LEU:HD13    | 2.11                     | 0.50              |
| 1:O:115:HIS:HE1   | 6:O:6094:HOH:O      | 1.95                     | 0.50              |
| 1:E:269:LYS:O     | 1:E:270:GLU:HB2     | 2.12                     | 0.50              |
| 1:I:238:ILE:HD11  | 6:I:6296:HOH:O      | 2.12                     | 0.50              |
| 2:N:67:GLU:HG2    | 6:N:6216:HOH:O      | 2.10                     | 0.50              |
| 1:K:47:ARG:HG2    | 1:K:52:ILE:HG13     | 1.93                     | 0.50              |
| 1:O:2:ALA:N       | 6:O:6173:HOH:O      | 2.44                     | 0.50              |
| 1:A:36[B]:GLU:HB2 | 6:B:5598:HOH:O      | 2.12                     | 0.50              |
| 1:I:234:VAL:CG1   | 6:I:6296:HOH:O      | 2.57                     | 0.50              |
| 1:W:2:ALA:N       | 6:W:6320:HOH:O      | 2.45                     | 0.50              |
| 1:E:8:ARG:HG2     | 6:E:6359:HOH:O      | 2.11                     | 0.49              |
| 1:Q:149:LYS:HE2   | 6:Q:6310:HOH:O      | 2.11                     | 0.49              |
| 1:U:36:GLU:HG3    | 6:V:5545:HOH:O      | 2.12                     | 0.49              |
| 1:E:47:ARG:HB2    | 1:E:52:ILE:HD11     | 1.92                     | 0.49              |
| 1:W:47:ARG:HG3    | 1:W:52:ILE:HD11     | 1.94                     | 0.49              |
| 2:B:44:LEU:CD1    | 2:B:85:LEU:HD13     | 2.42                     | 0.49              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 2:F:138:HIS:CE1    | 2:F:140:LEU:HD23 | 2.47                     | 0.49              |
| 1:G:130:ARG:NE     | 6:G:6332:HOH:O   | 2.44                     | 0.49              |
| 2:H:54:ARG:HG2     | 6:H:6135:HOH:O   | 2.12                     | 0.49              |
| 2:B:20:ILE:HG23    | 2:B:25:ALA:HB3   | 1.92                     | 0.49              |
| 3:C:6005:CL:CL     | 6:C:6284:HOH:O   | 2.57                     | 0.49              |
| 1:I:232:VAL:CG1    | 1:I:234:VAL:HG23 | 2.42                     | 0.49              |
| 2:V:53:ARG:HH11    | 2:V:96:HIS:CD2   | 2.28                     | 0.49              |
| 2:D:53:ARG:HH11    | 2:D:96:HIS:CD2   | 2.29                     | 0.49              |
| 1:E:50:ALA:CB      | 6:E:6364:HOH:O   | 2.52                     | 0.49              |
| 2:P:2:LEU:HD21     | 2:P:188:GLU:HG2  | 1.95                     | 0.49              |
| 2:H:86:ALA:O       | 2:H:98:GLY:HA2   | 2.13                     | 0.49              |
| 2:H:193:LYS:C      | 6:H:6179:HOH:O   | 2.50                     | 0.49              |
| 1:I:197:LEU:HG     | 6:I:6364:HOH:O   | 2.12                     | 0.49              |
| 2:P:105:GLU:HB2    | 2:P:140:LEU:HD11 | 1.95                     | 0.49              |
| 1:A:130[A]:ARG:NH1 | 1:A:149:LYS:NZ   | 2.61                     | 0.49              |
| 2:D:32:ARG:HE      | 2:D:34:GLU:CD    | 2.16                     | 0.49              |
| 1:G:130:ARG:HG2    | 1:G:163:HIS:CE1  | 2.48                     | 0.49              |
| 1:A:22:ILE:HG12    | 1:A:41:ALA:HB3   | 1.94                     | 0.49              |
| 1:C:3:GLN:NE2      | 6:C:6234:HOH:O   | 2.45                     | 0.49              |
| 1:I:173:LYS:HE3    | 6:Q:6066:HOH:O   | 2.12                     | 0.49              |
| 1:I:262:LYS:NZ     | 1:K:95:ALA:O     | 2.45                     | 0.49              |
| 2:P:178:ARG:NH2    | 6:P:6192:HOH:O   | 2.45                     | 0.49              |
| 1:E:152:PRO:HG2    | 6:E:6363:HOH:O   | 2.13                     | 0.49              |
| 1:M:72:ASN:HB3     | 6:M:6328:HOH:O   | 2.12                     | 0.49              |
| 2:P:66:ARG:HH11    | 2:P:66:ARG:HG2   | 1.78                     | 0.49              |
| 1:Q:194:GLU:CB     | 4:Q:6035:EDO:H21 | 2.43                     | 0.48              |
| 1:U:65:THR:HB      | 6:U:6303:HOH:O   | 2.12                     | 0.48              |
| 2:X:88:GLU:HG2     | 2:X:103:VAL:HG13 | 1.95                     | 0.48              |
| 1:K:53:ARG:HD3     | 6:K:6272:HOH:O   | 2.14                     | 0.48              |
| 1:I:192:PRO:HB3    | 4:I:6039:EDO:C2  | 2.42                     | 0.48              |
| 2:X:151:GLU:HG3    | 6:X:6236:HOH:O   | 2.13                     | 0.48              |
| 1:G:234:VAL:CB     | 6:G:6331:HOH:O   | 2.43                     | 0.48              |
| 2:N:127:GLU:HG2    | 6:N:6204:HOH:O   | 2.13                     | 0.48              |
| 2:D:96:HIS:HE1     | 6:D:6028:HOH:O   | 1.95                     | 0.48              |
| 1:E:8:ARG:CG       | 6:E:6359:HOH:O   | 2.62                     | 0.48              |
| 2:P:14:ARG:NH1     | 2:P:15:GLU:OE2   | 2.46                     | 0.48              |
| 1:U:8:ARG:HD3      | 2:V:132:VAL:HG21 | 1.95                     | 0.48              |
| 1:C:234:VAL:HG21   | 1:C:251:ILE:HG21 | 1.95                     | 0.48              |
| 2:P:127:GLU:HG3    | 6:P:6198:HOH:O   | 2.13                     | 0.48              |
| 1:Q:271:LEU:C      | 6:Q:6289:HOH:O   | 2.52                     | 0.48              |
| 1:S:2:ALA:HA       | 2:T:117:GLU:O    | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:T:53:ARG:HH11  | 2:T:96:HIS:HD2   | 1.60                     | 0.48              |
| 1:W:271:LEU:C    | 6:W:6338:HOH:O   | 2.51                     | 0.48              |
| 2:B:138:HIS:NE2  | 2:B:140:LEU:HD23 | 2.29                     | 0.48              |
| 1:I:174:VAL:HG13 | 1:I:182:LEU:HD11 | 1.96                     | 0.48              |
| 1:I:8:ARG:HD3    | 2:J:132:VAL:HG21 | 1.96                     | 0.48              |
| 1:K:269:LYS:O    | 1:K:271:LEU:CD1  | 2.61                     | 0.48              |
| 1:M:48:VAL:HA    | 6:M:6331:HOH:O   | 2.14                     | 0.48              |
| 1:O:238:ILE:HD13 | 1:O:247:PHE:HD2  | 1.79                     | 0.48              |
| 1:U:201:LYS:CE   | 6:U:6288:HOH:O   | 2.25                     | 0.48              |
| 1:U:67:VAL:HG12  | 1:U:71:MET:HE2   | 1.96                     | 0.48              |
| 1:M:67:VAL:HG12  | 1:M:71:MET:HE2   | 1.92                     | 0.48              |
| 1:U:45:LEU:HD21  | 1:U:81:LYS:HE2   | 1.96                     | 0.48              |
| 1:O:152:PRO:HB2  | 6:O:6323:HOH:O   | 2.14                     | 0.47              |
| 4:A:6031:EDO:H21 | 1:O:194:GLU:CG   | 2.40                     | 0.47              |
| 1:E:123:VAL:HB   | 6:E:6262:HOH:O   | 2.14                     | 0.47              |
| 1:I:100:TYR:CZ   | 1:I:124:PRO:HB2  | 2.50                     | 0.47              |
| 2:T:20:ILE:HG23  | 2:T:25:ALA:HB3   | 1.96                     | 0.47              |
| 1:K:249:LYS:HE3  | 6:K:6123:HOH:O   | 2.12                     | 0.47              |
| 1:C:53:ARG:HB2   | 6:C:6344:HOH:O   | 2.13                     | 0.47              |
| 1:K:130:ARG:NH1  | 1:K:149:LYS:NZ   | 2.63                     | 0.47              |
| 1:U:46:GLU:HA    | 1:U:66:ILE:HD13  | 1.95                     | 0.47              |
| 1:E:152:PRO:HB3  | 6:E:6327:HOH:O   | 2.15                     | 0.47              |
| 2:F:87:LYS:HA    | 2:F:98:GLY:HA2   | 1.95                     | 0.47              |
| 1:I:197:LEU:CG   | 6:I:6364:HOH:O   | 2.61                     | 0.47              |
| 1:S:242:ASP:OD1  | 6:S:6334:HOH:O   | 2.20                     | 0.47              |
| 1:U:68:GLU:CG    | 6:U:6293:HOH:O   | 2.63                     | 0.47              |
| 1:U:151:GLU:OE2  | 1:U:154:THR:HG21 | 2.14                     | 0.47              |
| 2:V:125:LEU:HD21 | 2:V:182:LEU:HD11 | 1.96                     | 0.47              |
| 1:C:22:ILE:HG12  | 1:C:41:ALA:HB3   | 1.97                     | 0.47              |
| 1:E:15:GLU:OE1   | 1:E:18:LYS:NZ    | 2.47                     | 0.47              |
| 2:P:32:ARG:NH2   | 6:P:6178:HOH:O   | 2.47                     | 0.47              |
| 2:R:2:LEU:HD11   | 2:R:187:VAL:HG12 | 1.95                     | 0.47              |
| 2:R:32:ARG:HB3   | 2:R:34:GLU:OE1   | 2.15                     | 0.47              |
| 2:R:183:PHE:O    | 2:R:187:VAL:HG23 | 2.14                     | 0.47              |
| 2:T:87:LYS:HD3   | 2:T:98:GLY:O     | 2.15                     | 0.47              |
| 2:F:20:ILE:HD11  | 2:F:43:ILE:HD12  | 1.96                     | 0.47              |
| 1:G:204:LYS:HE2  | 6:G:6310:HOH:O   | 2.13                     | 0.47              |
| 1:Q:65:THR:O     | 1:Q:69:GLU:HG3   | 2.14                     | 0.47              |
| 1:C:50:ALA:O     | 1:C:54:ALA:HB3   | 2.15                     | 0.47              |
| 1:E:174:VAL:HG13 | 1:E:182:LEU:HD11 | 1.96                     | 0.47              |
| 1:E:238:ILE:HD11 | 6:E:6336:HOH:O   | 2.14                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:I:152:PRO:HB3   | 6:I:6330:HOH:O   | 2.15                     | 0.47              |
| 1:O:35:GLU:OE2    | 1:O:74:VAL:HB    | 2.15                     | 0.47              |
| 1:O:36:GLU:CB     | 6:O:6348:HOH:O   | 2.61                     | 0.47              |
| 1:O:240:LYS:NZ    | 6:O:6316:HOH:O   | 2.43                     | 0.47              |
| 1:O:262:LYS:HE3   | 1:Q:95:ALA:HB1   | 1.97                     | 0.47              |
| 1:G:152:PRO:HB2   | 6:G:6302:HOH:O   | 2.14                     | 0.47              |
| 2:P:191:LYS:HE2   | 6:P:6186:HOH:O   | 2.15                     | 0.47              |
| 1:I:71:MET:HE2    | 2:J:111:ARG:CZ   | 2.44                     | 0.46              |
| 2:X:54[B]:ARG:CZ  | 6:X:6143:HOH:O   | 2.48                     | 0.46              |
| 4:E:6047:EDO:H12  | 1:W:194:GLU:HG2  | 1.96                     | 0.46              |
| 2:V:74:PRO:HG2    | 2:V:187:VAL:HA   | 1.96                     | 0.46              |
| 1:I:194:GLU:HB2   | 4:I:6039:EDO:H12 | 1.91                     | 0.46              |
| 1:U:67:VAL:HG12   | 1:U:71:MET:CE    | 2.46                     | 0.46              |
| 1:W:172[B]:ARG:CZ | 6:W:6289:HOH:O   | 2.47                     | 0.46              |
| 1:E:8:ARG:HD2     | 2:F:117:GLU:OE2  | 2.15                     | 0.46              |
| 1:S:204:LYS:HE2   | 6:S:6305:HOH:O   | 2.14                     | 0.46              |
| 1:G:201:LYS:HG3   | 6:G:6333:HOH:O   | 2.16                     | 0.46              |
| 1:S:201:LYS:NZ    | 6:S:6260:HOH:O   | 2.47                     | 0.46              |
| 2:F:68:PHE:CE1    | 2:F:73:LYS:HD2   | 2.50                     | 0.46              |
| 1:K:28:ALA:HB2    | 1:K:69:GLU:HG2   | 1.97                     | 0.46              |
| 1:S:151:GLU:HB3   | 6:S:6248:HOH:O   | 2.15                     | 0.46              |
| 1:U:134:GLU:OE2   | 1:U:149:LYS:HE3  | 2.16                     | 0.46              |
| 1:U:115:HIS:HE1   | 6:U:6106:HOH:O   | 1.98                     | 0.46              |
| 1:W:104:SER:OG    | 1:W:106:VAL:HG22 | 2.16                     | 0.46              |
| 2:X:54[A]:ARG:NH2 | 6:X:6147:HOH:O   | 2.46                     | 0.46              |
| 4:A:6031:EDO:C2   | 1:O:194:GLU:H    | 2.29                     | 0.46              |
| 2:D:74:PRO:HG2    | 2:D:187:VAL:HA   | 1.97                     | 0.46              |
| 1:E:14:ALA:HB1    | 1:E:208:VAL:HG22 | 1.96                     | 0.46              |
| 6:E:6359:HOH:O    | 2:F:173:LEU:HB3  | 2.15                     | 0.46              |
| 1:G:29:GLU:OE1    | 6:G:6205:HOH:O   | 2.21                     | 0.46              |
| 1:A:104:SER:OG    | 1:A:106:VAL:HG22 | 2.15                     | 0.46              |
| 1:E:7:GLU:CD      | 6:E:6372:HOH:O   | 2.54                     | 0.46              |
| 6:E:6359:HOH:O    | 2:F:132:VAL:HG11 | 2.15                     | 0.46              |
| 1:Q:28:ALA:HB1    | 1:Q:73:ALA:HB2   | 1.97                     | 0.46              |
| 1:A:2:ALA:HA      | 2:B:117:GLU:O    | 2.16                     | 0.46              |
| 1:C:23:MET:HE2    | 1:C:238:ILE:HD12 | 1.98                     | 0.46              |
| 2:P:160:LYS:HE2   | 6:P:6176:HOH:O   | 2.15                     | 0.46              |
| 1:E:257:HIS:CE1   | 2:F:59:TYR:CE1   | 3.04                     | 0.45              |
| 1:M:8:ARG:HD3     | 2:N:132:VAL:CG2  | 2.45                     | 0.45              |
| 1:Q:192:PRO:HB3   | 4:Q:6035:EDO:C1  | 2.42                     | 0.45              |
| 2:B:67:GLU:HG3    | 6:B:4729:HOH:O   | 2.15                     | 0.45              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:I:194:GLU:CA    | 4:I:6039:EDO:H11    | 2.46                     | 0.45              |
| 2:N:87:LYS:NZ     | 6:N:6132:HOH:O      | 2.48                     | 0.45              |
| 1:O:249:LYS:HZ3   | 2:P:54[A]:ARG:HH21  | 1.57                     | 0.45              |
| 2:R:191:LYS:C     | 6:R:4702:HOH:O      | 2.54                     | 0.45              |
| 1:I:2:ALA:N       | 6:I:6303:HOH:O      | 2.49                     | 0.45              |
| 1:M:192:PRO:HB3   | 4:M:6007:EDO:H21    | 1.97                     | 0.45              |
| 1:Q:2:ALA:HA      | 2:R:117:GLU:O       | 2.16                     | 0.45              |
| 1:A:106:VAL:HG12  | 1:A:152:PRO:HG2     | 1.99                     | 0.45              |
| 1:E:101:ILE:CD1   | 1:E:123:VAL:HG11    | 2.46                     | 0.45              |
| 2:F:66:ARG:CD     | 6:F:5427:HOH:O      | 2.58                     | 0.45              |
| 2:R:50:THR:HB     | 2:R:54[B]:ARG:NH1   | 2.31                     | 0.45              |
| 2:T:156:ILE:CD1   | 6:T:5578:HOH:O      | 2.64                     | 0.45              |
| 2:D:66:ARG:HG2    | 2:D:66:ARG:HH11     | 1.81                     | 0.45              |
| 1:G:194:GLU:CA    | 4:G:6043:EDO:H11    | 2.46                     | 0.45              |
| 2:V:1:MET:HE2     | 2:V:1:MET:O         | 2.17                     | 0.45              |
| 1:I:238:ILE:CD1   | 6:I:6296:HOH:O      | 2.64                     | 0.45              |
| 2:T:88:GLU:HG3    | 2:T:103:VAL:HG13    | 1.98                     | 0.45              |
| 1:I:271:LEU:CD1   | 6:I:6304:HOH:O      | 2.62                     | 0.45              |
| 2:J:151:GLU:HB2   | 2:J:155:ARG:O       | 2.17                     | 0.45              |
| 1:C:204:LYS:HE2   | 6:C:6202:HOH:O      | 2.15                     | 0.45              |
| 2:L:151:GLU:CD    | 6:L:6162:HOH:O      | 2.55                     | 0.45              |
| 2:L:151:GLU:HA    | 2:L:155:ARG:O       | 2.17                     | 0.45              |
| 6:M:6287:HOH:O    | 1:W:262:LYS:HE2     | 2.13                     | 0.45              |
| 1:S:234:VAL:HG21  | 1:S:251:ILE:HG21    | 1.99                     | 0.45              |
| 1:U:151:GLU:HG2   | 1:U:154:THR:CG2     | 2.47                     | 0.45              |
| 2:B:54[A]:ARG:NH2 | 6:B:3835:HOH:O      | 2.51                     | 0.44              |
| 6:O:6271:HOH:O    | 2:P:113[A]:VAL:HG21 | 2.16                     | 0.44              |
| 1:U:71:MET:HA     | 1:U:78:VAL:HG21     | 1.99                     | 0.44              |
| 1:W:157:ILE:HD13  | 1:W:215:VAL:HA      | 1.98                     | 0.44              |
| 3:G:6013:CL:CL    | 6:G:6293:HOH:O      | 2.59                     | 0.44              |
| 2:N:177:HIS:HD2   | 6:N:6066:HOH:O      | 2.00                     | 0.44              |
| 2:R:32:ARG:NH2    | 6:R:5656:HOH:O      | 2.50                     | 0.44              |
| 2:V:1:MET:O       | 2:V:1:MET:CE        | 2.65                     | 0.44              |
| 1:W:40:VAL:O      | 1:W:77:PRO:HD2      | 2.17                     | 0.44              |
| 1:I:270:GLU:HB2   | 6:I:6367:HOH:O      | 2.17                     | 0.44              |
| 1:M:115:HIS:CD2   | 6:M:6112:HOH:O      | 2.60                     | 0.44              |
| 2:T:88:GLU:HG2    | 2:T:103:VAL:HG22    | 2.00                     | 0.44              |
| 1:W:67:VAL:HG12   | 1:W:71:MET:HE1      | 1.97                     | 0.44              |
| 1:E:238:ILE:CD1   | 6:E:6336:HOH:O      | 2.65                     | 0.44              |
| 1:G:115:HIS:HE1   | 6:G:6087:HOH:O      | 2.00                     | 0.44              |
| 1:G:174:VAL:HG13  | 1:G:182:LEU:HD11    | 2.00                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:H:76:PHE:HB2     | 2:H:183:PHE:CD1   | 2.52                     | 0.44              |
| 1:K:104:SER:OG     | 1:K:106:VAL:HG22  | 2.17                     | 0.44              |
| 2:L:53:ARG:HH11    | 2:L:96:HIS:CD2    | 2.34                     | 0.44              |
| 2:P:62:MET:SD      | 2:P:97:LEU:HD23   | 2.58                     | 0.44              |
| 1:A:36[B]:GLU:CD   | 6:A:6188:HOH:O    | 2.43                     | 0.44              |
| 4:A:6031:EDO:O1    | 6:A:6169:HOH:O    | 2.21                     | 0.44              |
| 2:F:53:ARG:HH11    | 2:F:96:HIS:CD2    | 2.32                     | 0.44              |
| 1:W:153:GLY:CA     | 6:W:6298:HOH:O    | 2.65                     | 0.44              |
| 1:C:47:ARG:HG3     | 1:C:52:ILE:HD11   | 1.99                     | 0.44              |
| 2:F:102:VAL:HB     | 2:F:139:ILE:HG23  | 2.00                     | 0.44              |
| 1:G:238:ILE:O      | 1:G:241:SER:HB3   | 2.17                     | 0.44              |
| 2:N:31:LYS:HB2     | 6:N:6191:HOH:O    | 2.17                     | 0.43              |
| 1:O:100:TYR:CZ     | 1:O:124:PRO:HB2   | 2.53                     | 0.43              |
| 1:S:50:ALA:O       | 1:S:54:ALA:HB3    | 2.18                     | 0.43              |
| 2:B:68:PHE:CE1     | 2:B:73:LYS:HD3    | 2.53                     | 0.43              |
| 2:B:155[A]:ARG:HD3 | 6:B:5018:HOH:O    | 2.17                     | 0.43              |
| 1:I:149:LYS:NZ     | 6:I:6292:HOH:O    | 2.49                     | 0.43              |
| 1:C:36[A]:GLU:HG3  | 6:C:6281:HOH:O    | 2.18                     | 0.43              |
| 1:E:194:GLU:CA     | 4:E:6047:EDO:H11  | 2.49                     | 0.43              |
| 1:K:115:HIS:HD2    | 6:K:6212:HOH:O    | 2.00                     | 0.43              |
| 1:U:247:PHE:CE1    | 1:U:271:LEU:HG    | 2.54                     | 0.43              |
| 1:U:8:ARG:HD2      | 2:V:117:GLU:OE2   | 2.18                     | 0.43              |
| 2:V:125:LEU:HA     | 6:V:5630:HOH:O    | 2.19                     | 0.43              |
| 2:H:151:GLU:HA     | 2:H:155:ARG:O     | 2.19                     | 0.43              |
| 1:S:8:ARG:HD2      | 2:T:117:GLU:OE2   | 2.19                     | 0.43              |
| 1:S:8:ARG:HD3      | 2:T:132:VAL:HG21  | 2.01                     | 0.43              |
| 2:V:54[B]:ARG:CG   | 2:V:54[B]:ARG:NH1 | 2.69                     | 0.43              |
| 1:C:262:LYS:HE2    | 6:E:6351:HOH:O    | 2.12                     | 0.43              |
| 1:G:262:LYS:CE     | 6:I:6350:HOH:O    | 2.38                     | 0.43              |
| 1:I:35:GLU:OE2     | 1:I:74:VAL:HB     | 2.18                     | 0.43              |
| 1:I:151:GLU:OE2    | 1:I:154:THR:OG1   | 2.32                     | 0.43              |
| 2:P:54[A]:ARG:HG2  | 6:P:6109:HOH:O    | 2.18                     | 0.43              |
| 2:R:54[B]:ARG:NH2  | 6:R:3386:HOH:O    | 2.52                     | 0.43              |
| 2:D:108:SER:HB2    | 2:D:138:HIS:CE1   | 2.54                     | 0.43              |
| 1:E:115:HIS:HD2    | 6:E:6237:HOH:O    | 2.01                     | 0.43              |
| 2:H:44:LEU:CD1     | 2:H:85:LEU:HD13   | 2.49                     | 0.43              |
| 1:A:10:LYS:HB3     | 1:A:124:PRO:HB3   | 2.01                     | 0.43              |
| 1:C:23:MET:HE3     | 1:C:238:ILE:HD12  | 1.99                     | 0.43              |
| 2:D:87:LYS:HA      | 2:D:98:GLY:HA2    | 2.01                     | 0.43              |
| 2:H:2:LEU:HD23     | 6:H:6138:HOH:O    | 2.19                     | 0.43              |
| 2:T:138:HIS:CE1    | 6:T:4026:HOH:O    | 2.72                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:71:MET:HE1    | 1:A:97:GLY:C     | 2.39                     | 0.43              |
| 2:B:54[B]:ARG:CD  | 6:B:3460:HOH:O   | 2.62                     | 0.43              |
| 1:K:40:VAL:O      | 1:K:77:PRO:HD2   | 2.19                     | 0.43              |
| 2:P:54[A]:ARG:NH1 | 2:P:55:LEU:HD23  | 2.34                     | 0.43              |
| 2:T:87:LYS:HA     | 2:T:98:GLY:HA2   | 2.01                     | 0.43              |
| 2:L:76:PHE:HB2    | 2:L:183:PHE:CE1  | 2.54                     | 0.42              |
| 2:N:8:GLY:HA2     | 2:N:13:VAL:HG21  | 2.00                     | 0.42              |
| 1:Q:64:PRO:O      | 1:Q:68:GLU:HG3   | 2.19                     | 0.42              |
| 1:Q:105:GLU:CG    | 6:Q:6310:HOH:O   | 2.66                     | 0.42              |
| 1:Q:174:VAL:HG13  | 1:Q:182:LEU:HD11 | 2.01                     | 0.42              |
| 4:G:6043:EDO:H21  | 1:U:194:GLU:H    | 1.84                     | 0.42              |
| 2:L:143:GLY:HA2   | 6:L:6169:HOH:O   | 2.18                     | 0.42              |
| 2:X:192:GLN:O     | 2:X:194:ALA:N    | 2.52                     | 0.42              |
| 1:E:100:TYR:CZ    | 1:E:124:PRO:HB2  | 2.53                     | 0.42              |
| 2:P:96:HIS:HE1    | 6:P:6052:HOH:O   | 2.01                     | 0.42              |
| 2:T:88:GLU:CG     | 2:T:103:VAL:HG13 | 2.49                     | 0.42              |
| 2:V:181:GLN:HE21  | 2:V:185:GLU:HG3  | 1.84                     | 0.42              |
| 2:B:79:CYS:SG     | 5:B:6004:GLN:NE2 | 2.92                     | 0.42              |
| 1:G:71:MET:HA     | 1:G:78:VAL:HG21  | 2.01                     | 0.42              |
| 1:Q:46:GLU:O      | 6:Q:6315:HOH:O   | 2.22                     | 0.42              |
| 1:W:157:ILE:HD12  | 6:W:6367:HOH:O   | 2.20                     | 0.42              |
| 1:C:8:ARG:HD3     | 2:D:132:VAL:HG21 | 2.02                     | 0.42              |
| 2:P:79:CYS:SG     | 5:P:6032:GLN:CD  | 2.98                     | 0.42              |
| 1:U:247:PHE:HE1   | 1:U:271:LEU:HG   | 1.84                     | 0.42              |
| 2:V:125:LEU:CD2   | 2:V:125:LEU:N    | 2.82                     | 0.42              |
| 2:X:138:HIS:CD2   | 2:X:140:LEU:HD23 | 2.55                     | 0.42              |
| 1:E:8:ARG:CD      | 6:E:6359:HOH:O   | 2.61                     | 0.42              |
| 1:S:130:ARG:HD3   | 6:S:6211:HOH:O   | 2.19                     | 0.42              |
| 1:W:195:LEU:HD12  | 1:W:195:LEU:HA   | 1.96                     | 0.42              |
| 1:E:3[B]:GLN:NE2  | 6:E:6256:HOH:O   | 2.53                     | 0.42              |
| 2:T:87:LYS:CB     | 6:T:4753:HOH:O   | 2.64                     | 0.42              |
| 1:E:172[B]:ARG:CZ | 6:E:6234:HOH:O   | 2.40                     | 0.42              |
| 2:F:151:GLU:HA    | 2:F:155:ARG:O    | 2.20                     | 0.42              |
| 2:J:192:GLN:O     | 2:J:193:LYS:C    | 2.57                     | 0.42              |
| 2:L:192:GLN:C     | 6:L:6177:HOH:O   | 2.58                     | 0.42              |
| 1:O:115:HIS:HD2   | 6:O:6176:HOH:O   | 2.03                     | 0.42              |
| 2:T:108:SER:CB    | 2:T:138:HIS:HD1  | 2.33                     | 0.42              |
| 2:V:66:ARG:HH11   | 2:V:66:ARG:CG    | 2.31                     | 0.42              |
| 1:A:36[A]:GLU:HG2 | 6:B:5598:HOH:O   | 2.20                     | 0.42              |
| 1:E:152:PRO:CD    | 6:E:6363:HOH:O   | 2.68                     | 0.42              |
| 2:J:74:PRO:HG2    | 2:J:187:VAL:HA   | 2.02                     | 0.42              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:K:238:ILE:O      | 1:K:241:SER:HB3     | 2.20                     | 0.42              |
| 1:M:232:VAL:CG1    | 1:M:234:VAL:HG23    | 2.49                     | 0.42              |
| 2:N:175:GLU:OE2    | 2:N:175:GLU:HA      | 2.20                     | 0.42              |
| 2:T:149:LEU:HD11   | 2:T:160:LYS:HB2     | 2.00                     | 0.42              |
| 2:V:103:VAL:HG23   | 2:V:141:GLU:HG3     | 2.02                     | 0.42              |
| 2:B:14:ARG:HD3     | 6:B:3011:HOH:O      | 2.20                     | 0.41              |
| 1:C:8:ARG:HD2      | 2:D:117:GLU:OE2     | 2.20                     | 0.41              |
| 1:C:40:VAL:O       | 1:C:77:PRO:HD2      | 2.20                     | 0.41              |
| 1:E:36[A]:GLU:HG3  | 6:E:6282:HOH:O      | 2.19                     | 0.41              |
| 1:I:49:PRO:CD      | 6:I:6366:HOH:O      | 2.68                     | 0.41              |
| 1:I:81:LYS:NZ      | 6:I:6163:HOH:O      | 2.52                     | 0.41              |
| 1:Q:194:GLU:CA     | 4:Q:6035:EDO:H21    | 2.50                     | 0.41              |
| 1:S:115:HIS:HE1    | 6:S:6073:HOH:O      | 2.03                     | 0.41              |
| 1:S:130:ARG:NH1    | 1:S:149:LYS:NZ      | 2.68                     | 0.41              |
| 2:X:139:ILE:HB     | 2:X:156:ILE:HB      | 2.02                     | 0.41              |
| 4:G:6043:EDO:H12   | 1:U:194:GLU:HG2     | 2.01                     | 0.41              |
| 1:I:178:SER:OG     | 1:I:180:ASP:OD1     | 2.34                     | 0.41              |
| 2:T:181:GLN:HG2    | 6:T:5402:HOH:O      | 2.19                     | 0.41              |
| 2:X:151:GLU:HA     | 2:X:155:ARG:O       | 2.20                     | 0.41              |
| 1:G:157:ILE:HD13   | 1:G:215:VAL:HA      | 2.02                     | 0.41              |
| 1:W:22:ILE:HG12    | 1:W:41:ALA:HB3      | 2.03                     | 0.41              |
| 1:A:232:VAL:HG12   | 1:A:234[B]:VAL:HG23 | 2.03                     | 0.41              |
| 2:D:12:ALA:HB3     | 6:D:6037:HOH:O      | 2.21                     | 0.41              |
| 1:E:270:GLU:O      | 6:E:6343:HOH:O      | 2.22                     | 0.41              |
| 1:W:152:PRO:HG3    | 6:W:6373:HOH:O      | 2.19                     | 0.41              |
| 1:W:153:GLY:HA2    | 6:W:6298:HOH:O      | 2.20                     | 0.41              |
| 1:A:3:GLN:CA       | 6:A:6303:HOH:O      | 2.61                     | 0.41              |
| 2:B:155[A]:ARG:HG2 | 6:B:5449:HOH:O      | 2.21                     | 0.41              |
| 1:C:23:MET:HE3     | 1:C:238:ILE:HD13    | 2.01                     | 0.41              |
| 2:H:87:LYS:HA      | 2:H:98:GLY:HA2      | 2.02                     | 0.41              |
| 2:L:126:ASP:N      | 6:L:6171:HOH:O      | 2.32                     | 0.41              |
| 6:M:6287:HOH:O     | 1:W:262:LYS:HE3     | 2.17                     | 0.41              |
| 1:S:151:GLU:HG2    | 1:S:154:THR:CG2     | 2.50                     | 0.41              |
| 2:T:102:VAL:HB     | 2:T:139:ILE:HG23    | 2.03                     | 0.41              |
| 2:X:66:ARG:NH1     | 2:X:97:LEU:O        | 2.47                     | 0.41              |
| 2:D:191:LYS:O      | 2:D:194:ALA:HB3     | 2.21                     | 0.41              |
| 1:E:101:ILE:HD12   | 1:E:123:VAL:HG11    | 2.02                     | 0.41              |
| 1:E:166:LYS:HG2    | 6:G:6348:HOH:O      | 2.21                     | 0.41              |
| 1:I:262:LYS:NZ     | 6:I:6319:HOH:O      | 2.53                     | 0.41              |
| 1:S:271:LEU:HD12   | 6:S:6267:HOH:O      | 2.20                     | 0.41              |
| 2:T:138:HIS:NE2    | 2:T:140:LEU:HD23    | 2.36                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:U:3:GLN:HB3     | 6:U:6292:HOH:O   | 2.19                     | 0.41              |
| 2:X:54[A]:ARG:CZ  | 6:X:6147:HOH:O   | 2.34                     | 0.41              |
| 2:F:76:PHE:HB2    | 2:F:183:PHE:CD1  | 2.56                     | 0.41              |
| 1:M:61:MET:HB2    | 1:M:89:GLU:CD    | 2.41                     | 0.41              |
| 2:X:53:ARG:HD3    | 2:X:96:HIS:HD2   | 1.85                     | 0.41              |
| 1:E:36[A]:GLU:CD  | 6:E:6301:HOH:O   | 2.56                     | 0.41              |
| 1:E:37:ALA:HA     | 1:E:249:LYS:HE2  | 2.02                     | 0.41              |
| 1:G:52:ILE:O      | 1:G:55:ALA:HB3   | 2.21                     | 0.41              |
| 2:J:87:LYS:HA     | 2:J:98:GLY:HA2   | 2.01                     | 0.41              |
| 1:O:174:VAL:HG13  | 1:O:182:LEU:HD11 | 2.03                     | 0.41              |
| 2:R:137:PRO:O     | 2:R:168:SER:HB2  | 2.21                     | 0.41              |
| 1:E:101:ILE:O     | 1:E:125:PHE:HA   | 2.21                     | 0.41              |
| 2:F:8:GLY:HA2     | 2:F:13:VAL:HG21  | 2.03                     | 0.41              |
| 2:L:81:GLY:HA2    | 6:L:6111:HOH:O   | 2.21                     | 0.41              |
| 1:S:100:TYR:CZ    | 1:S:124:PRO:HB2  | 2.56                     | 0.41              |
| 2:T:53:ARG:HH11   | 2:T:96:HIS:CD2   | 2.38                     | 0.41              |
| 2:T:183:PHE:O     | 2:T:187:VAL:HG23 | 2.20                     | 0.41              |
| 2:V:76:PHE:HB2    | 2:V:183:PHE:CD1  | 2.55                     | 0.41              |
| 2:V:102:VAL:HB    | 2:V:139:ILE:HG23 | 2.02                     | 0.41              |
| 1:W:47:ARG:HE     | 1:W:47:ARG:HB3   | 1.63                     | 0.41              |
| 2:H:76:PHE:HB2    | 2:H:183:PHE:CE1  | 2.56                     | 0.41              |
| 1:K:194:GLU:HG2   | 4:Q:6035:EDO:H12 | 2.02                     | 0.41              |
| 1:M:71:MET:HA     | 1:M:78:VAL:HG21  | 2.03                     | 0.41              |
| 2:R:151:GLU:CD    | 6:R:3363:HOH:O   | 2.59                     | 0.41              |
| 2:T:63:GLU:HB2    | 6:T:4130:HOH:O   | 2.19                     | 0.41              |
| 2:D:79:CYS:SG     | 5:D:6008:GLN:CD  | 2.99                     | 0.40              |
| 1:K:204:LYS:HE2   | 6:K:6249:HOH:O   | 2.21                     | 0.40              |
| 1:O:249:LYS:HG3   | 6:O:6272:HOH:O   | 2.21                     | 0.40              |
| 1:Q:234:VAL:HG21  | 1:Q:251:ILE:HG21 | 2.04                     | 0.40              |
| 1:U:53:ARG:HD3    | 1:U:108:THR:OG1  | 2.21                     | 0.40              |
| 1:U:130:ARG:NE    | 6:U:6223:HOH:O   | 2.53                     | 0.40              |
| 1:W:262:LYS:HG3   | 6:W:6378:HOH:O   | 2.21                     | 0.40              |
| 1:E:50:ALA:CA     | 6:E:6364:HOH:O   | 2.69                     | 0.40              |
| 2:P:79:CYS:SG     | 5:P:6032:GLN:NE2 | 2.94                     | 0.40              |
| 2:T:84:ILE:O      | 2:T:96:HIS:HB2   | 2.22                     | 0.40              |
| 1:K:115:HIS:HE1   | 6:K:6040:HOH:O   | 2.04                     | 0.40              |
| 2:N:54[B]:ARG:NH1 | 6:N:6095:HOH:O   | 2.31                     | 0.40              |
| 2:N:184:VAL:O     | 2:N:188:GLU:HG3  | 2.21                     | 0.40              |
| 2:R:8:GLY:HA2     | 2:R:13:VAL:HG21  | 2.03                     | 0.40              |
| 1:U:3:GLN:NE2     | 6:V:2913:HOH:O   | 2.50                     | 0.40              |
| 1:U:130:ARG:NH1   | 1:U:149:LYS:HZ1  | 2.19                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:38:GLY:HA3    | 2:B:54[B]:ARG:HG2 | 2.04                     | 0.40              |
| 1:A:69:GLU:HG3    | 6:A:6232:HOH:O    | 2.21                     | 0.40              |
| 1:E:249:LYS:NZ    | 6:E:6278:HOH:O    | 2.53                     | 0.40              |
| 2:H:14[A]:ARG:NH2 | 6:H:6176:HOH:O    | 2.54                     | 0.40              |
| 1:M:238:ILE:O     | 1:M:241:SER:HB3   | 2.20                     | 0.40              |
| 1:S:152:PRO:N     | 6:S:6344:HOH:O    | 2.53                     | 0.40              |
| 1:K:67:VAL:HG12   | 1:K:71:MET:HE2    | 2.02                     | 0.40              |
| 1:K:113:GLU:HB3   | 6:K:6210:HOH:O    | 2.20                     | 0.40              |
| 2:L:63:GLU:HB2    | 6:L:6152:HOH:O    | 2.20                     | 0.40              |
| 1:U:130:ARG:HH12  | 1:U:149:LYS:NZ    | 2.20                     | 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) |
|----------------|------------------------|--------------------------|-------------------|
| 2:L:87:LYS:NZ  | 2:X:141:GLU:OE1[1_656] | 1.83                     | 0.37              |
| 6:R:1160:HOH:O | 6:W:6293:HOH:O[1_556]  | 2.16                     | 0.04              |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 272/294 (92%) | 269 (99%) | 3 (1%)  | 0        | 100         | 100 |
| 1   | C     | 272/294 (92%) | 266 (98%) | 6 (2%)  | 0        | 100         | 100 |
| 1   | E     | 272/294 (92%) | 266 (98%) | 6 (2%)  | 0        | 100         | 100 |
| 1   | G     | 269/294 (92%) | 264 (98%) | 4 (2%)  | 1 (0%)   | 34          | 32  |
| 1   | I     | 273/294 (93%) | 265 (97%) | 7 (3%)  | 1 (0%)   | 34          | 32  |
| 1   | K     | 272/294 (92%) | 265 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 1   | M     | 272/294 (92%) | 270 (99%) | 2 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | O     | 270/294 (92%)   | 266 (98%)  | 2 (1%)   | 2 (1%)   | 22          | 17  |
| 1   | Q     | 271/294 (92%)   | 266 (98%)  | 3 (1%)   | 2 (1%)   | 22          | 17  |
| 1   | S     | 271/294 (92%)   | 265 (98%)  | 6 (2%)   | 0        | 100         | 100 |
| 1   | U     | 273/294 (93%)   | 269 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 1   | W     | 274/294 (93%)   | 269 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 2   | B     | 193/204 (95%)   | 186 (96%)  | 6 (3%)   | 1 (0%)   | 29          | 25  |
| 2   | D     | 193/204 (95%)   | 187 (97%)  | 5 (3%)   | 1 (0%)   | 29          | 25  |
| 2   | F     | 190/204 (93%)   | 183 (96%)  | 7 (4%)   | 0        | 100         | 100 |
| 2   | H     | 193/204 (95%)   | 187 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 2   | J     | 195/204 (96%)   | 187 (96%)  | 7 (4%)   | 1 (0%)   | 29          | 25  |
| 2   | L     | 191/204 (94%)   | 183 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 2   | N     | 192/204 (94%)   | 185 (96%)  | 6 (3%)   | 1 (0%)   | 29          | 25  |
| 2   | P     | 193/204 (95%)   | 188 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 2   | R     | 193/204 (95%)   | 189 (98%)  | 3 (2%)   | 1 (0%)   | 29          | 25  |
| 2   | T     | 193/204 (95%)   | 188 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 2   | V     | 193/204 (95%)   | 183 (95%)  | 9 (5%)   | 1 (0%)   | 29          | 25  |
| 2   | X     | 194/204 (95%)   | 186 (96%)  | 7 (4%)   | 1 (0%)   | 29          | 25  |
| All | All   | 5574/5976 (93%) | 5432 (98%) | 129 (2%) | 13 (0%)  | 47          | 48  |

All (13) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 193 | LYS  |
| 1   | G     | 57  | GLY  |
| 1   | I     | 57  | GLY  |
| 1   | O     | 57  | GLY  |
| 2   | J     | 192 | GLN  |
| 1   | Q     | 270 | GLU  |
| 2   | X     | 193 | LYS  |
| 2   | B     | 79  | CYS  |
| 2   | V     | 79  | CYS  |
| 2   | N     | 79  | CYS  |
| 2   | R     | 79  | CYS  |
| 1   | O     | 214 | GLY  |
| 1   | Q     | 214 | GLY  |

### 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     | 210/227 (92%)   | 203 (97%)  | 7 (3%)   | 38          | 39 |
| 1   | C     | 211/227 (93%)   | 204 (97%)  | 7 (3%)   | 38          | 39 |
| 1   | E     | 211/227 (93%)   | 204 (97%)  | 7 (3%)   | 38          | 39 |
| 1   | G     | 207/227 (91%)   | 198 (96%)  | 9 (4%)   | 29          | 28 |
| 1   | I     | 211/227 (93%)   | 203 (96%)  | 8 (4%)   | 33          | 33 |
| 1   | K     | 210/227 (92%)   | 203 (97%)  | 7 (3%)   | 38          | 39 |
| 1   | M     | 211/227 (93%)   | 207 (98%)  | 4 (2%)   | 57          | 61 |
| 1   | O     | 209/227 (92%)   | 203 (97%)  | 6 (3%)   | 42          | 44 |
| 1   | Q     | 209/227 (92%)   | 202 (97%)  | 7 (3%)   | 38          | 39 |
| 1   | S     | 209/227 (92%)   | 200 (96%)  | 9 (4%)   | 29          | 28 |
| 1   | U     | 209/227 (92%)   | 203 (97%)  | 6 (3%)   | 42          | 44 |
| 1   | W     | 212/227 (93%)   | 204 (96%)  | 8 (4%)   | 33          | 33 |
| 2   | B     | 160/168 (95%)   | 151 (94%)  | 9 (6%)   | 21          | 18 |
| 2   | D     | 159/168 (95%)   | 151 (95%)  | 8 (5%)   | 24          | 22 |
| 2   | F     | 157/168 (94%)   | 147 (94%)  | 10 (6%)  | 17          | 14 |
| 2   | H     | 159/168 (95%)   | 149 (94%)  | 10 (6%)  | 18          | 14 |
| 2   | J     | 161/168 (96%)   | 152 (94%)  | 9 (6%)   | 21          | 18 |
| 2   | L     | 158/168 (94%)   | 150 (95%)  | 8 (5%)   | 24          | 21 |
| 2   | N     | 158/168 (94%)   | 150 (95%)  | 8 (5%)   | 24          | 21 |
| 2   | P     | 160/168 (95%)   | 152 (95%)  | 8 (5%)   | 24          | 22 |
| 2   | R     | 160/168 (95%)   | 150 (94%)  | 10 (6%)  | 18          | 14 |
| 2   | T     | 158/168 (94%)   | 149 (94%)  | 9 (6%)   | 20          | 17 |
| 2   | V     | 159/168 (95%)   | 152 (96%)  | 7 (4%)   | 28          | 27 |
| 2   | X     | 160/168 (95%)   | 149 (93%)  | 11 (7%)  | 15          | 12 |
| All | All   | 4428/4740 (93%) | 4236 (96%) | 192 (4%) | 32          | 28 |

All (192) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 3      | GLN  |
| 1   | A     | 51     | ASP  |
| 1   | A     | 100    | TYR  |
| 1   | A     | 117    | ASN  |
| 1   | A     | 131[A] | ASP  |
| 1   | A     | 131[B] | ASP  |
| 1   | A     | 195    | LEU  |
| 2   | B     | 1      | MET  |
| 2   | B     | 34     | GLU  |
| 2   | B     | 50     | THR  |
| 2   | B     | 61     | PHE  |
| 2   | B     | 63     | GLU  |
| 2   | B     | 85     | LEU  |
| 2   | B     | 125    | LEU  |
| 2   | B     | 127    | GLU  |
| 2   | B     | 144    | GLU  |
| 1   | C     | 47     | ARG  |
| 1   | C     | 100    | TYR  |
| 1   | C     | 117    | ASN  |
| 1   | C     | 131    | ASP  |
| 1   | C     | 182    | LEU  |
| 1   | C     | 195    | LEU  |
| 1   | C     | 249    | LYS  |
| 2   | D     | 1      | MET  |
| 2   | D     | 2      | LEU  |
| 2   | D     | 54[A]  | ARG  |
| 2   | D     | 54[B]  | ARG  |
| 2   | D     | 63     | GLU  |
| 2   | D     | 67     | GLU  |
| 2   | D     | 104    | VAL  |
| 2   | D     | 138    | HIS  |
| 1   | E     | 29[A]  | GLU  |
| 1   | E     | 29[B]  | GLU  |
| 1   | E     | 32     | LYS  |
| 1   | E     | 100    | TYR  |
| 1   | E     | 117    | ASN  |
| 1   | E     | 131    | ASP  |
| 1   | E     | 195    | LEU  |
| 2   | F     | 32     | ARG  |
| 2   | F     | 54[A]  | ARG  |
| 2   | F     | 54[B]  | ARG  |
| 2   | F     | 61     | PHE  |
| 2   | F     | 63     | GLU  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 2   | F     | 85     | LEU  |
| 2   | F     | 127    | GLU  |
| 2   | F     | 151    | GLU  |
| 2   | F     | 168    | SER  |
| 2   | F     | 191    | LYS  |
| 1   | G     | 36[A]  | GLU  |
| 1   | G     | 36[B]  | GLU  |
| 1   | G     | 100    | TYR  |
| 1   | G     | 117    | ASN  |
| 1   | G     | 131[A] | ASP  |
| 1   | G     | 131[B] | ASP  |
| 1   | G     | 182    | LEU  |
| 1   | G     | 208    | VAL  |
| 1   | G     | 241    | SER  |
| 2   | H     | 1      | MET  |
| 2   | H     | 2      | LEU  |
| 2   | H     | 34[A]  | GLU  |
| 2   | H     | 34[B]  | GLU  |
| 2   | H     | 54     | ARG  |
| 2   | H     | 62     | MET  |
| 2   | H     | 67     | GLU  |
| 2   | H     | 85     | LEU  |
| 2   | H     | 138    | HIS  |
| 2   | H     | 144    | GLU  |
| 1   | I     | 36     | GLU  |
| 1   | I     | 100    | TYR  |
| 1   | I     | 117    | ASN  |
| 1   | I     | 131[A] | ASP  |
| 1   | I     | 131[B] | ASP  |
| 1   | I     | 182    | LEU  |
| 1   | I     | 195    | LEU  |
| 1   | I     | 242    | ASP  |
| 2   | J     | 54[A]  | ARG  |
| 2   | J     | 54[B]  | ARG  |
| 2   | J     | 85     | LEU  |
| 2   | J     | 104    | VAL  |
| 2   | J     | 125    | LEU  |
| 2   | J     | 191    | LYS  |
| 2   | J     | 193    | LYS  |
| 2   | J     | 195    | LEU  |
| 2   | J     | 196    | VAL  |
| 1   | K     | 51     | ASP  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | K     | 100    | TYR  |
| 1   | K     | 113    | GLU  |
| 1   | K     | 131[A] | ASP  |
| 1   | K     | 131[B] | ASP  |
| 1   | K     | 195    | LEU  |
| 1   | K     | 208    | VAL  |
| 2   | L     | 14     | ARG  |
| 2   | L     | 54[A]  | ARG  |
| 2   | L     | 54[B]  | ARG  |
| 2   | L     | 63     | GLU  |
| 2   | L     | 67     | GLU  |
| 2   | L     | 85     | LEU  |
| 2   | L     | 104    | VAL  |
| 2   | L     | 127    | GLU  |
| 1   | M     | 100    | TYR  |
| 1   | M     | 117    | ASN  |
| 1   | M     | 182    | LEU  |
| 1   | M     | 195    | LEU  |
| 2   | N     | 1      | MET  |
| 2   | N     | 54[A]  | ARG  |
| 2   | N     | 54[B]  | ARG  |
| 2   | N     | 63     | GLU  |
| 2   | N     | 67     | GLU  |
| 2   | N     | 85     | LEU  |
| 2   | N     | 104    | VAL  |
| 2   | N     | 153    | ASN  |
| 1   | O     | 51     | ASP  |
| 1   | O     | 100    | TYR  |
| 1   | O     | 131    | ASP  |
| 1   | O     | 182    | LEU  |
| 1   | O     | 195    | LEU  |
| 1   | O     | 262    | LYS  |
| 2   | P     | 1      | MET  |
| 2   | P     | 14     | ARG  |
| 2   | P     | 54[A]  | ARG  |
| 2   | P     | 54[B]  | ARG  |
| 2   | P     | 61     | PHE  |
| 2   | P     | 67     | GLU  |
| 2   | P     | 85     | LEU  |
| 2   | P     | 127    | GLU  |
| 1   | Q     | 3      | GLN  |
| 1   | Q     | 100    | TYR  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | Q     | 117    | ASN  |
| 1   | Q     | 131[A] | ASP  |
| 1   | Q     | 131[B] | ASP  |
| 1   | Q     | 182    | LEU  |
| 1   | Q     | 195    | LEU  |
| 2   | R     | 1      | MET  |
| 2   | R     | 14[A]  | ARG  |
| 2   | R     | 14[B]  | ARG  |
| 2   | R     | 61     | PHE  |
| 2   | R     | 67     | GLU  |
| 2   | R     | 85     | LEU  |
| 2   | R     | 113    | VAL  |
| 2   | R     | 144    | GLU  |
| 2   | R     | 151    | GLU  |
| 2   | R     | 193    | LYS  |
| 1   | S     | 3      | GLN  |
| 1   | S     | 100    | TYR  |
| 1   | S     | 131[A] | ASP  |
| 1   | S     | 131[B] | ASP  |
| 1   | S     | 182    | LEU  |
| 1   | S     | 195    | LEU  |
| 1   | S     | 208    | VAL  |
| 1   | S     | 242    | ASP  |
| 1   | S     | 249    | LYS  |
| 2   | T     | 1      | MET  |
| 2   | T     | 34     | GLU  |
| 2   | T     | 54[A]  | ARG  |
| 2   | T     | 54[B]  | ARG  |
| 2   | T     | 61     | PHE  |
| 2   | T     | 62     | MET  |
| 2   | T     | 67     | GLU  |
| 2   | T     | 85     | LEU  |
| 2   | T     | 127    | GLU  |
| 1   | U     | 32     | LYS  |
| 1   | U     | 100    | TYR  |
| 1   | U     | 117    | ASN  |
| 1   | U     | 131[A] | ASP  |
| 1   | U     | 131[B] | ASP  |
| 1   | U     | 271    | LEU  |
| 2   | V     | 1      | MET  |
| 2   | V     | 63     | GLU  |
| 2   | V     | 67     | GLU  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 2   | V     | 85     | LEU  |
| 2   | V     | 125    | LEU  |
| 2   | V     | 126    | ASP  |
| 2   | V     | 189    | GLU  |
| 1   | W     | 100    | TYR  |
| 1   | W     | 117    | ASN  |
| 1   | W     | 131[A] | ASP  |
| 1   | W     | 131[B] | ASP  |
| 1   | W     | 182    | LEU  |
| 1   | W     | 195    | LEU  |
| 1   | W     | 249    | LYS  |
| 1   | W     | 271    | LEU  |
| 2   | X     | 34     | GLU  |
| 2   | X     | 54[A]  | ARG  |
| 2   | X     | 54[B]  | ARG  |
| 2   | X     | 63     | GLU  |
| 2   | X     | 67     | GLU  |
| 2   | X     | 85     | LEU  |
| 2   | X     | 87     | LYS  |
| 2   | X     | 126    | ASP  |
| 2   | X     | 144    | GLU  |
| 2   | X     | 190    | TYR  |
| 2   | X     | 195    | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 3   | GLN  |
| 1   | A     | 72  | ASN  |
| 1   | A     | 117 | ASN  |
| 2   | B     | 96  | HIS  |
| 2   | B     | 153 | ASN  |
| 2   | B     | 192 | GLN  |
| 1   | C     | 115 | HIS  |
| 1   | C     | 117 | ASN  |
| 2   | D     | 96  | HIS  |
| 2   | D     | 153 | ASN  |
| 2   | D     | 181 | GLN  |
| 1   | E     | 115 | HIS  |
| 1   | E     | 117 | ASN  |
| 1   | E     | 257 | HIS  |
| 2   | F     | 96  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | F     | 138 | HIS  |
| 2   | F     | 153 | ASN  |
| 2   | F     | 181 | GLN  |
| 1   | G     | 115 | HIS  |
| 1   | G     | 117 | ASN  |
| 2   | H     | 96  | HIS  |
| 2   | H     | 138 | HIS  |
| 1   | I     | 115 | HIS  |
| 1   | I     | 117 | ASN  |
| 1   | I     | 257 | HIS  |
| 1   | K     | 115 | HIS  |
| 2   | L     | 96  | HIS  |
| 2   | L     | 153 | ASN  |
| 1   | M     | 115 | HIS  |
| 1   | M     | 117 | ASN  |
| 2   | N     | 96  | HIS  |
| 2   | N     | 153 | ASN  |
| 2   | P     | 96  | HIS  |
| 2   | P     | 138 | HIS  |
| 1   | Q     | 117 | ASN  |
| 2   | R     | 153 | ASN  |
| 1   | S     | 115 | HIS  |
| 2   | T     | 96  | HIS  |
| 2   | T     | 153 | ASN  |
| 1   | U     | 117 | ASN  |
| 2   | V     | 96  | HIS  |
| 2   | V     | 138 | HIS  |
| 2   | V     | 153 | ASN  |
| 2   | V     | 181 | GLN  |
| 1   | W     | 117 | ASN  |
| 2   | X     | 96  | HIS  |
| 2   | X     | 153 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 42 ligands modelled in this entry, 12 are monoatomic - leaving 30 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 4   | EDO  | E     | 6010 | -    | 3,3,3        | 0.39 | 0           | 2,2,2       | 0.30 | 0           |
| 4   | EDO  | Q     | 6035 | -    | 3,3,3        | 1.03 | 0           | 2,2,2       | 0.88 | 0           |
| 4   | EDO  | I     | 6039 | -    | 3,3,3        | 0.67 | 0           | 2,2,2       | 0.13 | 0           |
| 4   | EDO  | E     | 6047 | -    | 3,3,3        | 0.77 | 0           | 2,2,2       | 0.27 | 0           |
| 4   | EDO  | A     | 6031 | -    | 3,3,3        | 0.61 | 0           | 2,2,2       | 0.21 | 0           |
| 5   | GLN  | R     | 6036 | -    | 5,9,9        | 1.05 | 0           | 5,11,11     | 0.16 | 0           |
| 5   | GLN  | V     | 6044 | -    | 5,9,9        | 0.73 | 0           | 5,11,11     | 0.37 | 0           |
| 4   | EDO  | W     | 6046 | -    | 3,3,3        | 0.24 | 0           | 2,2,2       | 0.05 | 0           |
| 4   | EDO  | M     | 6007 | -    | 3,3,3        | 0.91 | 0           | 2,2,2       | 0.50 | 0           |
| 5   | GLN  | X     | 6048 | -    | 7,8,9        | 0.78 | 0           | 4,9,11      | 0.08 | 0           |
| 5   | GLN  | H     | 6016 | -    | 5,9,9        | 0.53 | 0           | 5,11,11     | 0.29 | 0           |
| 4   | EDO  | U     | 6042 | -    | 3,3,3        | 0.46 | 0           | 2,2,2       | 0.16 | 0           |
| 5   | GLN  | P     | 6032 | -    | 5,9,9        | 0.84 | 0           | 5,11,11     | 0.33 | 0           |
| 4   | EDO  | A     | 6030 | -    | 3,3,3        | 0.27 | 0           | 2,2,2       | 0.76 | 0           |
| 4   | EDO  | I     | 6018 | -    | 3,3,3        | 0.29 | 0           | 2,2,2       | 0.88 | 0           |
| 5   | GLN  | D     | 6008 | -    | 5,9,9        | 0.62 | 0           | 5,11,11     | 0.27 | 0           |
| 4   | EDO  | K     | 6022 | -    | 3,3,3        | 0.27 | 0           | 2,2,2       | 0.27 | 0           |
| 4   | EDO  | A     | 6002 | -    | 3,3,3        | 0.62 | 0           | 2,2,2       | 0.55 | 0           |
| 4   | EDO  | U     | 6014 | -    | 3,3,3        | 0.22 | 0           | 2,2,2       | 0.41 | 0           |
| 5   | GLN  | L     | 6024 | -    | 5,9,9        | 1.01 | 1 (20%)     | 5,11,11     | 0.08 | 0           |
| 5   | GLN  | J     | 6020 | -    | 5,9,9        | 0.59 | 0           | 5,11,11     | 0.57 | 0           |
| 4   | EDO  | I     | 6038 | -    | 3,3,3        | 0.26 | 0           | 2,2,2       | 0.30 | 0           |
| 5   | GLN  | T     | 6040 | -    | 5,9,9        | 0.64 | 0           | 5,11,11     | 0.20 | 0           |
| 4   | EDO  | C     | 6006 | -    | 3,3,3        | 0.28 | 0           | 2,2,2       | 0.16 | 0           |
| 4   | EDO  | C     | 6026 | -    | 3,3,3        | 0.22 | 0           | 2,2,2       | 0.28 | 0           |
| 5   | GLN  | F     | 6012 | -    | 5,9,9        | 0.70 | 0           | 5,11,11     | 0.37 | 0           |
| 5   | GLN  | B     | 6004 | -    | 5,9,9        | 0.71 | 0           | 5,11,11     | 0.22 | 0           |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | EDO  | Q     | 6034 | -    | 3,3,3        | 0.28 | 0        | 2,2,2       | 0.11 | 0        |
| 5   | GLN  | N     | 6028 | -    | 5,9,9        | 1.01 | 1 (20%)  | 5,11,11     | 0.69 | 0        |
| 4   | EDO  | G     | 6043 | -    | 3,3,3        | 0.61 | 0        | 2,2,2       | 0.09 | 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 |
|-----|------|-------|------|------|---------|----------|-------|
| 4   | EDO  | E     | 6010 | -    | -       | 1/1/1/1  | -     |
| 4   | EDO  | Q     | 6035 | -    | -       | 1/1/1/1  | -     |
| 4   | EDO  | I     | 6039 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | E     | 6047 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | A     | 6031 | -    | -       | 1/1/1/1  | -     |
| 5   | GLN  | R     | 6036 | -    | -       | 0/5/9/9  | -     |
| 5   | GLN  | V     | 6044 | -    | -       | 0/5/9/9  | -     |
| 4   | EDO  | W     | 6046 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | M     | 6007 | -    | -       | 1/1/1/1  | -     |
| 5   | GLN  | X     | 6048 | -    | -       | 0/6/7/9  | -     |
| 5   | GLN  | H     | 6016 | -    | -       | 0/5/9/9  | -     |
| 4   | EDO  | U     | 6042 | -    | -       | 0/1/1/1  | -     |
| 5   | GLN  | P     | 6032 | -    | -       | 0/5/9/9  | -     |
| 4   | EDO  | A     | 6030 | -    | -       | 1/1/1/1  | -     |
| 4   | EDO  | I     | 6018 | -    | -       | 1/1/1/1  | -     |
| 5   | GLN  | D     | 6008 | -    | -       | 0/5/9/9  | -     |
| 4   | EDO  | K     | 6022 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | A     | 6002 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | U     | 6014 | -    | -       | 1/1/1/1  | -     |
| 5   | GLN  | L     | 6024 | -    | -       | 0/5/9/9  | -     |
| 5   | GLN  | J     | 6020 | -    | -       | 0/5/9/9  | -     |
| 4   | EDO  | I     | 6038 | -    | -       | 1/1/1/1  | -     |
| 5   | GLN  | T     | 6040 | -    | -       | 0/5/9/9  | -     |
| 4   | EDO  | C     | 6006 | -    | -       | 0/1/1/1  | -     |
| 4   | EDO  | C     | 6026 | -    | -       | 1/1/1/1  | -     |
| 5   | GLN  | F     | 6012 | -    | -       | 0/5/9/9  | -     |
| 5   | GLN  | B     | 6004 | -    | -       | 0/5/9/9  | -     |
| 4   | EDO  | Q     | 6034 | -    | -       | 0/1/1/1  | -     |
| 5   | GLN  | N     | 6028 | -    | -       | 0/5/9/9  | -     |
| 4   | EDO  | G     | 6043 | -    | -       | 1/1/1/1  | -     |

All (2) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 5   | L     | 6024 | GLN  | CA-N  | 2.24 | 1.52        | 1.47     |
| 5   | N     | 6028 | GLN  | CA-N  | 2.09 | 1.51        | 1.47     |

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 4   | A     | 6030 | EDO  | O1-C1-C2-O2 |
| 4   | E     | 6010 | EDO  | O1-C1-C2-O2 |
| 4   | U     | 6014 | EDO  | O1-C1-C2-O2 |
| 4   | I     | 6038 | EDO  | O1-C1-C2-O2 |
| 4   | Q     | 6035 | EDO  | O1-C1-C2-O2 |
| 4   | A     | 6031 | EDO  | O1-C1-C2-O2 |
| 4   | C     | 6026 | EDO  | O1-C1-C2-O2 |
| 4   | I     | 6018 | EDO  | O1-C1-C2-O2 |
| 4   | M     | 6007 | EDO  | O1-C1-C2-O2 |
| 4   | G     | 6043 | EDO  | O1-C1-C2-O2 |

There are no ring outliers.

9 monomers are involved in 55 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4   | Q     | 6035 | EDO  | 11      | 0            |
| 4   | I     | 6039 | EDO  | 9       | 0            |
| 4   | E     | 6047 | EDO  | 9       | 0            |
| 4   | A     | 6031 | EDO  | 8       | 0            |
| 4   | M     | 6007 | EDO  | 5       | 0            |
| 5   | P     | 6032 | GLN  | 2       | 0            |
| 5   | D     | 6008 | GLN  | 1       | 0            |
| 5   | B     | 6004 | GLN  | 1       | 0            |
| 4   | G     | 6043 | EDO  | 9       | 0            |

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|---------------|-----------------------|-------|
| 1   | A     | 268/294 (91%) | 0.58   | 11 (4%) 37 43 | 29, 38, 55, 83        | 0     |
| 1   | C     | 269/294 (91%) | 0.74   | 12 (4%) 33 38 | 29, 34, 52, 81        | 0     |
| 1   | E     | 269/294 (91%) | 0.58   | 13 (4%) 30 35 | 30, 38, 54, 80        | 0     |
| 1   | G     | 268/294 (91%) | 0.54   | 13 (4%) 29 35 | 30, 36, 55, 87        | 0     |
| 1   | I     | 271/294 (92%) | 0.59   | 12 (4%) 34 40 | 28, 34, 57, 79        | 0     |
| 1   | K     | 270/294 (91%) | 0.65   | 16 (5%) 22 27 | 29, 36, 61, 79        | 0     |
| 1   | M     | 269/294 (91%) | 0.56   | 10 (3%) 41 48 | 28, 34, 52, 74        | 0     |
| 1   | O     | 268/294 (91%) | 0.62   | 13 (4%) 29 35 | 28, 35, 53, 73        | 0     |
| 1   | Q     | 270/294 (91%) | 0.70   | 17 (6%) 20 24 | 28, 36, 58, 76        | 0     |
| 1   | S     | 270/294 (91%) | 0.73   | 16 (5%) 22 27 | 30, 38, 62, 82        | 0     |
| 1   | U     | 271/294 (92%) | 0.62   | 14 (5%) 27 32 | 30, 39, 61, 82        | 0     |
| 1   | W     | 270/294 (91%) | 0.61   | 13 (4%) 30 35 | 28, 34, 53, 83        | 0     |
| 2   | B     | 193/204 (94%) | 1.17   | 38 (19%) 1 1  | 44, 55, 65, 83        | 0     |
| 2   | D     | 194/204 (95%) | 1.08   | 37 (19%) 1 1  | 40, 51, 60, 70        | 0     |
| 2   | F     | 191/204 (93%) | 1.47   | 48 (25%) 0 0  | 46, 60, 69, 78        | 0     |
| 2   | H     | 193/204 (94%) | 0.63   | 18 (9%) 8 11  | 37, 48, 58, 78        | 0     |
| 2   | J     | 196/204 (96%) | 0.48   | 21 (10%) 6 7  | 36, 45, 57, 63        | 0     |
| 2   | L     | 192/204 (94%) | 0.92   | 29 (15%) 2 3  | 40, 51, 60, 74        | 0     |
| 2   | N     | 193/204 (94%) | 0.46   | 10 (5%) 27 32 | 34, 44, 55, 76        | 0     |
| 2   | P     | 193/204 (94%) | 0.62   | 19 (9%) 7 9   | 38, 48, 59, 70        | 0     |
| 2   | R     | 193/204 (94%) | 0.82   | 27 (13%) 2 3  | 39, 49, 60, 82        | 0     |
| 2   | T     | 194/204 (95%) | 1.42   | 51 (26%) 0 0  | 46, 55, 65, 71        | 0     |
| 2   | V     | 194/204 (95%) | 1.97   | 80 (41%) 0 0  | 47, 62, 70, 78        | 0     |
| 2   | X     | 195/204 (95%) | 0.53   | 21 (10%) 5 7  | 35, 44, 57, 67        | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2                     | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|-----------------------------|-----------------------|-------|
| All | All   | 5554/5976 (92%) | 0.77   | 559 (10%) <b>7</b> <b>8</b> | 28, 42, 64, 87        | 0     |

All (559) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 54  | ALA  | 10.1 |
| 1   | S     | 54  | ALA  | 9.6  |
| 1   | K     | 50  | ALA  | 8.5  |
| 1   | I     | 54  | ALA  | 8.5  |
| 1   | A     | 56  | GLY  | 8.3  |
| 2   | T     | 194 | ALA  | 8.1  |
| 2   | L     | 1   | MET  | 7.7  |
| 1   | S     | 50  | ALA  | 7.6  |
| 1   | A     | 54  | ALA  | 7.5  |
| 1   | W     | 54  | ALA  | 7.5  |
| 1   | G     | 56  | GLY  | 7.5  |
| 1   | C     | 52  | ILE  | 7.4  |
| 1   | G     | 52  | ILE  | 7.4  |
| 1   | E     | 54  | ALA  | 7.2  |
| 1   | C     | 55  | ALA  | 7.2  |
| 1   | U     | 54  | ALA  | 7.1  |
| 1   | C     | 48  | VAL  | 7.0  |
| 1   | I     | 50  | ALA  | 7.0  |
| 1   | G     | 51  | ASP  | 7.0  |
| 1   | K     | 54  | ALA  | 6.9  |
| 2   | X     | 195 | LEU  | 6.8  |
| 1   | Q     | 54  | ALA  | 6.7  |
| 2   | J     | 196 | VAL  | 6.6  |
| 2   | V     | 192 | GLN  | 6.6  |
| 1   | E     | 50  | ALA  | 6.6  |
| 2   | D     | 194 | ALA  | 6.5  |
| 1   | C     | 56  | GLY  | 6.2  |
| 2   | V     | 194 | ALA  | 6.2  |
| 2   | V     | 190 | TYR  | 6.2  |
| 1   | S     | 48  | VAL  | 6.1  |
| 2   | F     | 1   | MET  | 6.1  |
| 2   | B     | 191 | LYS  | 6.1  |
| 2   | V     | 100 | LEU  | 6.0  |
| 2   | V     | 41  | GLY  | 6.0  |
| 1   | A     | 55  | ALA  | 6.0  |
| 1   | M     | 54  | ALA  | 5.9  |
| 2   | X     | 194 | ALA  | 5.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | V     | 125 | LEU  | 5.9  |
| 1   | O     | 52  | ILE  | 5.8  |
| 1   | O     | 54  | ALA  | 5.8  |
| 2   | J     | 195 | LEU  | 5.8  |
| 2   | V     | 154 | GLY  | 5.7  |
| 1   | W     | 55  | ALA  | 5.7  |
| 1   | C     | 49  | PRO  | 5.7  |
| 2   | T     | 1   | MET  | 5.7  |
| 1   | U     | 51  | ASP  | 5.7  |
| 2   | V     | 182 | LEU  | 5.7  |
| 2   | B     | 187 | VAL  | 5.7  |
| 1   | I     | 51  | ASP  | 5.6  |
| 1   | G     | 54  | ALA  | 5.6  |
| 1   | S     | 55  | ALA  | 5.6  |
| 1   | G     | 50  | ALA  | 5.6  |
| 2   | F     | 187 | VAL  | 5.5  |
| 1   | W     | 50  | ALA  | 5.5  |
| 2   | V     | 184 | VAL  | 5.5  |
| 2   | T     | 101 | ASN  | 5.5  |
| 2   | T     | 188 | GLU  | 5.4  |
| 2   | T     | 125 | LEU  | 5.4  |
| 2   | T     | 192 | GLN  | 5.4  |
| 1   | O     | 50  | ALA  | 5.4  |
| 1   | U     | 55  | ALA  | 5.4  |
| 2   | B     | 1   | MET  | 5.4  |
| 2   | J     | 194 | ALA  | 5.3  |
| 2   | F     | 162 | GLY  | 5.3  |
| 1   | U     | 52  | ILE  | 5.3  |
| 2   | D     | 192 | GLN  | 5.3  |
| 2   | R     | 67  | GLU  | 5.3  |
| 1   | S     | 56  | GLY  | 5.3  |
| 2   | J     | 192 | GLN  | 5.3  |
| 1   | G     | 55  | ALA  | 5.2  |
| 2   | P     | 2   | LEU  | 5.2  |
| 2   | B     | 189 | GLU  | 5.2  |
| 2   | V     | 144 | GLU  | 5.2  |
| 2   | V     | 187 | VAL  | 5.1  |
| 2   | F     | 190 | TYR  | 5.0  |
| 2   | B     | 125 | LEU  | 5.0  |
| 2   | L     | 128 | PRO  | 5.0  |
| 2   | R     | 1   | MET  | 5.0  |
| 2   | V     | 126 | ASP  | 5.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | U     | 56  | GLY  | 5.0  |
| 1   | M     | 52  | ILE  | 4.9  |
| 2   | D     | 2   | LEU  | 4.9  |
| 2   | B     | 126 | ASP  | 4.9  |
| 2   | B     | 192 | GLN  | 4.9  |
| 2   | R     | 192 | GLN  | 4.9  |
| 1   | S     | 271 | LEU  | 4.9  |
| 2   | D     | 143 | GLY  | 4.9  |
| 2   | T     | 190 | TYR  | 4.8  |
| 2   | T     | 127 | GLU  | 4.8  |
| 2   | L     | 187 | VAL  | 4.8  |
| 1   | E     | 52  | ILE  | 4.8  |
| 2   | L     | 126 | ASP  | 4.7  |
| 1   | A     | 50  | ALA  | 4.7  |
| 2   | V     | 2   | LEU  | 4.7  |
| 2   | D     | 70  | ALA  | 4.7  |
| 1   | O     | 56  | GLY  | 4.6  |
| 2   | D     | 24  | GLY  | 4.6  |
| 1   | I     | 52  | ILE  | 4.6  |
| 1   | C     | 50  | ALA  | 4.6  |
| 1   | U     | 271 | LEU  | 4.6  |
| 2   | T     | 184 | VAL  | 4.6  |
| 1   | W     | 51  | ASP  | 4.6  |
| 2   | H     | 1   | MET  | 4.5  |
| 2   | V     | 143 | GLY  | 4.5  |
| 2   | V     | 122 | ILE  | 4.5  |
| 1   | K     | 56  | GLY  | 4.5  |
| 2   | T     | 126 | ASP  | 4.5  |
| 2   | T     | 128 | PRO  | 4.4  |
| 2   | V     | 191 | LYS  | 4.4  |
| 1   | E     | 53  | ARG  | 4.4  |
| 2   | H     | 192 | GLN  | 4.3  |
| 2   | T     | 40  | ASP  | 4.3  |
| 2   | V     | 24  | GLY  | 4.3  |
| 2   | V     | 72  | GLY  | 4.3  |
| 2   | P     | 1   | MET  | 4.3  |
| 2   | V     | 129 | PHE  | 4.3  |
| 2   | D     | 1   | MET  | 4.3  |
| 2   | T     | 193 | LYS  | 4.3  |
| 1   | I     | 272 | GLY  | 4.3  |
| 2   | V     | 188 | GLU  | 4.3  |
| 2   | V     | 1   | MET  | 4.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | W     | 56  | GLY  | 4.3  |
| 2   | P     | 190 | TYR  | 4.3  |
| 2   | L     | 127 | GLU  | 4.2  |
| 1   | I     | 271 | LEU  | 4.2  |
| 2   | F     | 2   | LEU  | 4.2  |
| 1   | I     | 55  | ALA  | 4.2  |
| 2   | L     | 72  | GLY  | 4.2  |
| 2   | H     | 190 | TYR  | 4.2  |
| 1   | U     | 50  | ALA  | 4.2  |
| 2   | T     | 187 | VAL  | 4.2  |
| 2   | F     | 101 | ASN  | 4.1  |
| 2   | L     | 153 | ASN  | 4.1  |
| 2   | V     | 121 | THR  | 4.1  |
| 2   | R     | 189 | GLU  | 4.1  |
| 2   | V     | 189 | GLU  | 4.1  |
| 1   | Q     | 56  | GLY  | 4.1  |
| 1   | C     | 2   | ALA  | 4.1  |
| 2   | F     | 189 | GLU  | 4.1  |
| 2   | V     | 148 | VAL  | 4.1  |
| 2   | L     | 67  | GLU  | 4.1  |
| 2   | T     | 143 | GLY  | 4.1  |
| 2   | L     | 23  | CYS  | 4.0  |
| 1   | Q     | 55  | ALA  | 4.0  |
| 2   | L     | 190 | TYR  | 4.0  |
| 1   | E     | 51  | ASP  | 4.0  |
| 1   | K     | 55  | ALA  | 4.0  |
| 2   | V     | 67  | GLU  | 4.0  |
| 1   | S     | 2   | ALA  | 4.0  |
| 2   | D     | 191 | LYS  | 4.0  |
| 2   | F     | 67  | GLU  | 4.0  |
| 1   | K     | 52  | ILE  | 4.0  |
| 1   | A     | 51  | ASP  | 3.9  |
| 1   | K     | 51  | ASP  | 3.9  |
| 2   | V     | 23  | CYS  | 3.9  |
| 2   | N     | 190 | TYR  | 3.9  |
| 2   | T     | 162 | GLY  | 3.9  |
| 1   | Q     | 53  | ARG  | 3.9  |
| 1   | G     | 242 | ASP  | 3.9  |
| 2   | T     | 164 | PHE  | 3.9  |
| 1   | Q     | 271 | LEU  | 3.9  |
| 2   | H     | 126 | ASP  | 3.9  |
| 2   | D     | 125 | LEU  | 3.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | F     | 184 | VAL  | 3.8  |
| 1   | G     | 53  | ARG  | 3.8  |
| 1   | W     | 52  | ILE  | 3.8  |
| 2   | R     | 193 | LYS  | 3.8  |
| 2   | B     | 188 | GLU  | 3.8  |
| 2   | P     | 189 | GLU  | 3.8  |
| 2   | X     | 126 | ASP  | 3.8  |
| 2   | T     | 189 | GLU  | 3.8  |
| 2   | B     | 121 | THR  | 3.8  |
| 2   | V     | 149 | LEU  | 3.8  |
| 2   | H     | 187 | VAL  | 3.8  |
| 1   | I     | 56  | GLY  | 3.8  |
| 1   | U     | 48  | VAL  | 3.8  |
| 1   | O     | 55  | ALA  | 3.8  |
| 2   | X     | 190 | TYR  | 3.7  |
| 2   | V     | 127 | GLU  | 3.7  |
| 2   | P     | 192 | GLN  | 3.7  |
| 1   | S     | 51  | ASP  | 3.7  |
| 2   | D     | 145 | ASN  | 3.7  |
| 2   | R     | 191 | LYS  | 3.7  |
| 2   | X     | 24  | GLY  | 3.7  |
| 1   | W     | 49  | PRO  | 3.7  |
| 2   | B     | 190 | TYR  | 3.7  |
| 2   | V     | 65  | LEU  | 3.7  |
| 2   | D     | 128 | PRO  | 3.7  |
| 1   | Q     | 52  | ILE  | 3.7  |
| 1   | S     | 52  | ILE  | 3.7  |
| 2   | F     | 40  | ASP  | 3.7  |
| 2   | B     | 2   | LEU  | 3.7  |
| 2   | B     | 138 | HIS  | 3.6  |
| 2   | V     | 128 | PRO  | 3.6  |
| 2   | T     | 72  | GLY  | 3.6  |
| 1   | W     | 48  | VAL  | 3.6  |
| 2   | V     | 138 | HIS  | 3.5  |
| 2   | L     | 192 | GLN  | 3.5  |
| 2   | V     | 71  | GLN  | 3.5  |
| 2   | F     | 191 | LYS  | 3.5  |
| 2   | F     | 82  | LEU  | 3.5  |
| 1   | Q     | 270 | GLU  | 3.5  |
| 2   | X     | 192 | GLN  | 3.5  |
| 2   | H     | 69  | ALA  | 3.5  |
| 2   | N     | 189 | GLU  | 3.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 242 | ASP  | 3.5  |
| 2   | J     | 1   | MET  | 3.5  |
| 1   | A     | 52  | ILE  | 3.5  |
| 2   | F     | 65  | LEU  | 3.5  |
| 2   | V     | 181 | GLN  | 3.5  |
| 2   | F     | 62  | MET  | 3.4  |
| 2   | V     | 163 | GLN  | 3.4  |
| 2   | V     | 193 | LYS  | 3.4  |
| 2   | V     | 22  | ALA  | 3.4  |
| 1   | E     | 56  | GLY  | 3.4  |
| 2   | F     | 144 | GLU  | 3.4  |
| 2   | R     | 144 | GLU  | 3.4  |
| 2   | T     | 34  | GLU  | 3.4  |
| 2   | T     | 39  | VAL  | 3.4  |
| 2   | D     | 126 | ASP  | 3.4  |
| 2   | T     | 2   | LEU  | 3.4  |
| 1   | M     | 48  | VAL  | 3.4  |
| 2   | H     | 193 | LYS  | 3.4  |
| 2   | R     | 190 | TYR  | 3.4  |
| 2   | H     | 127 | GLU  | 3.4  |
| 2   | V     | 98  | GLY  | 3.4  |
| 2   | X     | 70  | ALA  | 3.4  |
| 2   | D     | 23  | CYS  | 3.4  |
| 2   | N     | 126 | ASP  | 3.3  |
| 2   | L     | 60  | GLN  | 3.3  |
| 2   | B     | 143 | GLY  | 3.3  |
| 2   | D     | 148 | VAL  | 3.3  |
| 2   | V     | 63  | GLU  | 3.3  |
| 2   | F     | 79  | CYS  | 3.3  |
| 2   | X     | 193 | LYS  | 3.3  |
| 2   | V     | 101 | ASN  | 3.3  |
| 2   | V     | 3   | THR  | 3.3  |
| 1   | M     | 55  | ALA  | 3.3  |
| 1   | Q     | 50  | ALA  | 3.3  |
| 2   | V     | 151 | GLU  | 3.3  |
| 2   | R     | 37  | ASN  | 3.3  |
| 2   | V     | 19  | ALA  | 3.3  |
| 1   | Q     | 51  | ASP  | 3.2  |
| 2   | B     | 127 | GLU  | 3.2  |
| 2   | V     | 153 | ASN  | 3.2  |
| 1   | C     | 51  | ASP  | 3.2  |
| 2   | J     | 127 | GLU  | 3.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | K     | 53   | ARG  | 3.2  |
| 1   | U     | 270  | GLU  | 3.2  |
| 1   | M     | 56   | GLY  | 3.2  |
| 2   | D     | 122  | ILE  | 3.2  |
| 2   | L     | 125  | LEU  | 3.2  |
| 2   | V     | 68   | PHE  | 3.2  |
| 2   | V     | 164  | PHE  | 3.2  |
| 2   | T     | 19   | ALA  | 3.2  |
| 1   | A     | 48   | VAL  | 3.2  |
| 2   | D     | 144  | GLU  | 3.2  |
| 2   | X     | 127  | GLU  | 3.2  |
| 2   | F     | 100  | LEU  | 3.2  |
| 2   | V     | 4    | ILE  | 3.2  |
| 2   | B     | 24   | GLY  | 3.2  |
| 2   | F     | 188  | GLU  | 3.2  |
| 2   | R     | 60   | GLN  | 3.2  |
| 1   | C     | 53   | ARG  | 3.1  |
| 2   | R     | 59   | TYR  | 3.1  |
| 2   | D     | 121  | THR  | 3.1  |
| 2   | F     | 93   | ASP  | 3.1  |
| 2   | J     | 67   | GLU  | 3.1  |
| 1   | A     | 49   | PRO  | 3.1  |
| 1   | K     | 57   | GLY  | 3.1  |
| 2   | F     | 24   | GLY  | 3.1  |
| 2   | V     | 180  | THR  | 3.1  |
| 2   | F     | 37   | ASN  | 3.1  |
| 2   | L     | 123  | LYS  | 3.1  |
| 2   | V     | 36   | LEU  | 3.1  |
| 2   | B     | 184  | VAL  | 3.1  |
| 1   | A     | 2    | ALA  | 3.1  |
| 2   | T     | 121  | THR  | 3.1  |
| 1   | U     | 53   | ARG  | 3.1  |
| 2   | D     | 154  | GLY  | 3.0  |
| 2   | L     | 37   | ASN  | 3.0  |
| 2   | H     | 70   | ALA  | 3.0  |
| 1   | E     | 3[A] | GLN  | 3.0  |
| 1   | K     | 242  | ASP  | 3.0  |
| 1   | S     | 47   | ARG  | 3.0  |
| 2   | V     | 40   | ASP  | 3.0  |
| 1   | E     | 55   | ALA  | 3.0  |
| 2   | L     | 122  | ILE  | 3.0  |
| 2   | H     | 144  | GLU  | 3.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | R     | 187 | VAL  | 3.0  |
| 2   | T     | 159 | ALA  | 3.0  |
| 2   | V     | 142 | ALA  | 3.0  |
| 2   | P     | 191 | LYS  | 3.0  |
| 2   | N     | 1   | MET  | 3.0  |
| 2   | D     | 153 | ASN  | 3.0  |
| 2   | F     | 59  | TYR  | 3.0  |
| 1   | M     | 50  | ALA  | 3.0  |
| 2   | T     | 73  | LYS  | 2.9  |
| 1   | S     | 242 | ASP  | 2.9  |
| 2   | F     | 70  | ALA  | 2.9  |
| 2   | D     | 99  | LEU  | 2.9  |
| 2   | F     | 140 | LEU  | 2.9  |
| 2   | R     | 72  | GLY  | 2.9  |
| 2   | V     | 157 | VAL  | 2.9  |
| 2   | D     | 189 | GLU  | 2.9  |
| 2   | F     | 60  | GLN  | 2.9  |
| 2   | T     | 191 | LYS  | 2.9  |
| 1   | M     | 53  | ARG  | 2.9  |
| 1   | A     | 53  | ARG  | 2.9  |
| 2   | J     | 189 | GLU  | 2.9  |
| 1   | K     | 49  | PRO  | 2.9  |
| 2   | V     | 152 | HIS  | 2.9  |
| 2   | V     | 155 | ARG  | 2.9  |
| 2   | V     | 158 | ALA  | 2.9  |
| 2   | T     | 100 | LEU  | 2.9  |
| 2   | V     | 120 | LEU  | 2.9  |
| 2   | F     | 63  | GLU  | 2.9  |
| 1   | O     | 139 | ILE  | 2.8  |
| 2   | T     | 69  | ALA  | 2.8  |
| 2   | T     | 70  | ALA  | 2.8  |
| 2   | T     | 163 | GLN  | 2.8  |
| 2   | V     | 178 | ARG  | 2.8  |
| 2   | P     | 144 | GLU  | 2.8  |
| 2   | T     | 67  | GLU  | 2.8  |
| 2   | X     | 191 | LYS  | 2.8  |
| 2   | J     | 193 | LYS  | 2.8  |
| 2   | V     | 34  | GLU  | 2.8  |
| 2   | T     | 26  | ALA  | 2.8  |
| 2   | P     | 63  | GLU  | 2.8  |
| 2   | T     | 166 | GLY  | 2.8  |
| 2   | P     | 67  | GLU  | 2.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | F     | 66  | ARG  | 2.8  |
| 2   | F     | 128 | PRO  | 2.7  |
| 2   | V     | 162 | GLY  | 2.7  |
| 2   | V     | 166 | GLY  | 2.7  |
| 2   | R     | 34  | GLU  | 2.7  |
| 2   | P     | 126 | ASP  | 2.7  |
| 2   | R     | 2   | LEU  | 2.7  |
| 2   | B     | 70  | ALA  | 2.7  |
| 2   | V     | 177 | HIS  | 2.7  |
| 2   | H     | 191 | LYS  | 2.7  |
| 2   | B     | 193 | LYS  | 2.7  |
| 1   | K     | 271 | LEU  | 2.7  |
| 2   | H     | 100 | LEU  | 2.7  |
| 2   | D     | 72  | GLY  | 2.7  |
| 1   | G     | 48  | VAL  | 2.7  |
| 1   | K     | 48  | VAL  | 2.7  |
| 2   | T     | 139 | ILE  | 2.7  |
| 2   | L     | 188 | GLU  | 2.7  |
| 2   | T     | 63  | GLU  | 2.7  |
| 2   | F     | 103 | VAL  | 2.7  |
| 2   | V     | 124 | GLY  | 2.7  |
| 2   | X     | 128 | PRO  | 2.7  |
| 1   | O     | 51  | ASP  | 2.7  |
| 1   | I     | 53  | ARG  | 2.7  |
| 2   | D     | 182 | LEU  | 2.7  |
| 2   | D     | 186 | MET  | 2.7  |
| 2   | N     | 187 | VAL  | 2.6  |
| 2   | R     | 33  | PRO  | 2.6  |
| 2   | V     | 156 | ILE  | 2.6  |
| 1   | W     | 271 | LEU  | 2.6  |
| 2   | J     | 2   | LEU  | 2.6  |
| 2   | J     | 190 | TYR  | 2.6  |
| 1   | G     | 57  | GLY  | 2.6  |
| 1   | W     | 152 | PRO  | 2.6  |
| 2   | B     | 74  | PRO  | 2.6  |
| 2   | R     | 66  | ARG  | 2.6  |
| 2   | T     | 37  | ASN  | 2.6  |
| 2   | F     | 164 | PHE  | 2.6  |
| 1   | O     | 53  | ARG  | 2.6  |
| 2   | H     | 67  | GLU  | 2.6  |
| 2   | V     | 79  | CYS  | 2.6  |
| 2   | N     | 192 | GLN  | 2.6  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 2   | F     | 141   | GLU  | 2.6  |
| 1   | I     | 49    | PRO  | 2.6  |
| 2   | V     | 174   | THR  | 2.6  |
| 2   | P     | 24    | GLY  | 2.6  |
| 2   | V     | 39    | VAL  | 2.6  |
| 2   | L     | 34    | GLU  | 2.6  |
| 2   | F     | 69    | ALA  | 2.6  |
| 1   | E     | 49    | PRO  | 2.6  |
| 2   | X     | 184   | VAL  | 2.5  |
| 1   | E     | 2     | ALA  | 2.5  |
| 2   | F     | 159   | ALA  | 2.5  |
| 2   | P     | 127   | GLU  | 2.5  |
| 1   | M     | 51    | ASP  | 2.5  |
| 1   | Q     | 242   | ASP  | 2.5  |
| 2   | H     | 93    | ASP  | 2.5  |
| 1   | Q     | 171   | VAL  | 2.5  |
| 1   | S     | 57    | GLY  | 2.5  |
| 2   | B     | 37    | ASN  | 2.5  |
| 1   | S     | 49    | PRO  | 2.5  |
| 2   | D     | 188   | GLU  | 2.5  |
| 2   | J     | 191   | LYS  | 2.5  |
| 2   | L     | 24    | GLY  | 2.5  |
| 2   | P     | 37    | ASN  | 2.5  |
| 2   | B     | 54[A] | ARG  | 2.5  |
| 2   | B     | 128   | PRO  | 2.5  |
| 2   | J     | 34    | GLU  | 2.5  |
| 1   | W     | 47    | ARG  | 2.5  |
| 2   | D     | 190   | TYR  | 2.5  |
| 2   | F     | 83    | ILE  | 2.5  |
| 1   | A     | 242   | ASP  | 2.5  |
| 2   | B     | 176   | ASP  | 2.5  |
| 2   | H     | 68    | PHE  | 2.5  |
| 2   | T     | 87    | LYS  | 2.5  |
| 2   | T     | 155   | ARG  | 2.5  |
| 2   | V     | 54[A] | ARG  | 2.5  |
| 2   | R     | 188   | GLU  | 2.5  |
| 2   | T     | 124   | GLY  | 2.5  |
| 2   | V     | 20    | ILE  | 2.5  |
| 2   | B     | 19    | ALA  | 2.5  |
| 2   | B     | 118   | ALA  | 2.5  |
| 1   | G     | 196   | LEU  | 2.4  |
| 2   | P     | 188   | GLU  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 25  | ALA  | 2.4  |
| 1   | U     | 47  | ARG  | 2.4  |
| 2   | V     | 60  | GLN  | 2.4  |
| 2   | R     | 65  | LEU  | 2.4  |
| 2   | T     | 151 | GLU  | 2.4  |
| 1   | K     | 240 | LYS  | 2.4  |
| 2   | J     | 184 | VAL  | 2.4  |
| 1   | I     | 270 | GLU  | 2.4  |
| 2   | J     | 188 | GLU  | 2.4  |
| 2   | X     | 188 | GLU  | 2.4  |
| 1   | Q     | 2   | ALA  | 2.4  |
| 2   | F     | 180 | THR  | 2.4  |
| 2   | T     | 129 | PHE  | 2.4  |
| 2   | T     | 24  | GLY  | 2.4  |
| 2   | F     | 152 | HIS  | 2.4  |
| 2   | D     | 102 | VAL  | 2.4  |
| 2   | R     | 184 | VAL  | 2.4  |
| 2   | V     | 26  | ALA  | 2.4  |
| 2   | B     | 72  | GLY  | 2.4  |
| 2   | P     | 193 | LYS  | 2.4  |
| 2   | V     | 70  | ALA  | 2.4  |
| 2   | J     | 126 | ASP  | 2.4  |
| 1   | M     | 270 | GLU  | 2.3  |
| 2   | J     | 144 | GLU  | 2.3  |
| 1   | W     | 53  | ARG  | 2.3  |
| 2   | F     | 143 | GLY  | 2.3  |
| 2   | V     | 119 | ASP  | 2.3  |
| 2   | V     | 146 | VAL  | 2.3  |
| 2   | D     | 142 | ALA  | 2.3  |
| 2   | L     | 154 | GLY  | 2.3  |
| 2   | F     | 34  | GLU  | 2.3  |
| 2   | N     | 127 | GLU  | 2.3  |
| 2   | D     | 120 | LEU  | 2.3  |
| 2   | N     | 24  | GLY  | 2.3  |
| 1   | E     | 240 | LYS  | 2.3  |
| 1   | W     | 2   | ALA  | 2.3  |
| 2   | B     | 69  | ALA  | 2.3  |
| 2   | N     | 142 | ALA  | 2.3  |
| 1   | O     | 195 | LEU  | 2.3  |
| 1   | O     | 213 | GLY  | 2.3  |
| 1   | Q     | 132 | LEU  | 2.3  |
| 2   | F     | 87  | LYS  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | T     | 36  | LEU  | 2.3  |
| 2   | R     | 68  | PHE  | 2.3  |
| 2   | F     | 78  | THR  | 2.3  |
| 1   | Q     | 199 | ILE  | 2.3  |
| 2   | V     | 84  | ILE  | 2.3  |
| 2   | B     | 163 | GLN  | 2.3  |
| 2   | V     | 69  | ALA  | 2.3  |
| 1   | I     | 48  | VAL  | 2.3  |
| 1   | O     | 171 | VAL  | 2.3  |
| 1   | U     | 272 | GLY  | 2.3  |
| 2   | B     | 67  | GLU  | 2.3  |
| 2   | R     | 71  | GLN  | 2.3  |
| 2   | T     | 153 | ASN  | 2.3  |
| 2   | J     | 125 | LEU  | 2.2  |
| 2   | R     | 69  | ALA  | 2.2  |
| 2   | V     | 99  | LEU  | 2.2  |
| 2   | R     | 164 | PHE  | 2.2  |
| 1   | E     | 48  | VAL  | 2.2  |
| 2   | F     | 179 | VAL  | 2.2  |
| 2   | T     | 146 | VAL  | 2.2  |
| 2   | F     | 145 | ASN  | 2.2  |
| 2   | X     | 1   | MET  | 2.2  |
| 1   | M     | 92  | VAL  | 2.2  |
| 1   | C     | 270 | GLU  | 2.2  |
| 2   | J     | 18  | HIS  | 2.2  |
| 2   | L     | 73  | LYS  | 2.2  |
| 2   | L     | 182 | LEU  | 2.2  |
| 1   | K     | 67  | VAL  | 2.2  |
| 1   | K     | 241 | SER  | 2.2  |
| 2   | B     | 41  | GLY  | 2.2  |
| 2   | H     | 184 | VAL  | 2.2  |
| 2   | X     | 187 | VAL  | 2.2  |
| 2   | X     | 67  | GLU  | 2.2  |
| 1   | K     | 153 | GLY  | 2.2  |
| 1   | O     | 242 | ASP  | 2.2  |
| 2   | L     | 40  | ASP  | 2.2  |
| 2   | D     | 155 | ARG  | 2.2  |
| 1   | S     | 53  | ARG  | 2.2  |
| 2   | B     | 181 | GLN  | 2.2  |
| 1   | Q     | 48  | VAL  | 2.2  |
| 2   | F     | 109 | PHE  | 2.2  |
| 2   | D     | 67  | GLU  | 2.2  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 2   | F     | 75    | MET  | 2.2  |
| 2   | P     | 70    | ALA  | 2.2  |
| 2   | V     | 64    | PRO  | 2.2  |
| 2   | B     | 20    | ILE  | 2.1  |
| 2   | V     | 97    | LEU  | 2.1  |
| 2   | R     | 141   | GLU  | 2.1  |
| 2   | P     | 23    | CYS  | 2.1  |
| 2   | V     | 123   | LYS  | 2.1  |
| 2   | H     | 128   | PRO  | 2.1  |
| 2   | X     | 144   | GLU  | 2.1  |
| 2   | B     | 183   | PHE  | 2.1  |
| 2   | D     | 151   | GLU  | 2.1  |
| 2   | N     | 63    | GLU  | 2.1  |
| 1   | C     | 227   | LEU  | 2.1  |
| 1   | S     | 146   | LEU  | 2.1  |
| 2   | F     | 42    | LEU  | 2.1  |
| 2   | F     | 110   | GLY  | 2.1  |
| 2   | L     | 121   | THR  | 2.1  |
| 2   | T     | 23    | CYS  | 2.1  |
| 2   | T     | 20    | ILE  | 2.1  |
| 2   | B     | 28    | LEU  | 2.1  |
| 2   | L     | 145   | ASN  | 2.1  |
| 2   | X     | 37    | ASN  | 2.1  |
| 2   | F     | 54[A] | ARG  | 2.1  |
| 2   | X     | 23    | CYS  | 2.1  |
| 1   | U     | 57    | GLY  | 2.1  |
| 1   | U     | 242   | ASP  | 2.1  |
| 2   | B     | 142   | ALA  | 2.1  |
| 2   | B     | 59    | TYR  | 2.1  |
| 2   | B     | 34    | GLU  | 2.0  |
| 1   | G     | 76    | ILE  | 2.0  |
| 1   | O     | 199   | ILE  | 2.0  |
| 1   | Q     | 195   | LEU  | 2.0  |
| 2   | H     | 20    | ILE  | 2.0  |
| 2   | J     | 54[A] | ARG  | 2.0  |
| 2   | T     | 182   | LEU  | 2.0  |
| 2   | D     | 152   | HIS  | 2.0  |
| 2   | L     | 138   | HIS  | 2.0  |
| 2   | L     | 177   | HIS  | 2.0  |
| 2   | V     | 25    | ALA  | 2.0  |
| 2   | D     | 34    | GLU  | 2.0  |
| 2   | P     | 41    | GLY  | 2.0  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 2   | T     | 38    | GLU  | 2.0  |
| 2   | D     | 101   | ASN  | 2.0  |
| 2   | L     | 54[A] | ARG  | 2.0  |
| 2   | T     | 122   | ILE  | 2.0  |
| 2   | X     | 121   | THR  | 2.0  |
| 1   | S     | 174   | VAL  | 2.0  |
| 2   | D     | 184   | VAL  | 2.0  |
| 2   | L     | 146   | VAL  | 2.0  |
| 2   | R     | 63    | GLU  | 2.0  |
| 2   | P     | 162   | GLY  | 2.0  |
| 2   | V     | 183   | PHE  | 2.0  |
| 2   | F     | 163   | GLN  | 2.0  |
| 2   | D     | 123   | LYS  | 2.0  |
| 1   | Q     | 49    | PRO  | 2.0  |
| 2   | J     | 69    | ALA  | 2.0  |
| 2   | X     | 2     | LEU  | 2.0  |
| 2   | R     | 14[A] | ARG  | 2.0  |
| 1   | G     | 153   | GLY  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 3   | CL   | A     | 6001 | 1/1   | 0.75 | 0.08 | 73,73,73,73                 | 0     |
| 3   | CL   | U     | 6041 | 1/1   | 0.79 | 0.08 | 80,80,80,80                 | 0     |
| 3   | CL   | O     | 6029 | 1/1   | 0.81 | 0.13 | 83,83,83,83                 | 0     |
| 3   | CL   | C     | 6005 | 1/1   | 0.85 | 0.08 | 75,75,75,75                 | 0     |
| 3   | CL   | G     | 6013 | 1/1   | 0.85 | 0.11 | 74,74,74,74                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 4   | EDO  | A     | 6030 | 4/4   | 0.91 | 0.18 | 35,43,46,51                 | 0     |
| 4   | EDO  | G     | 6043 | 4/4   | 0.91 | 0.25 | 31,37,44,50                 | 0     |
| 4   | EDO  | M     | 6007 | 4/4   | 0.91 | 0.20 | 28,37,41,43                 | 0     |
| 5   | GLN  | R     | 6036 | 10/10 | 0.91 | 0.17 | 36,37,39,40                 | 0     |
| 3   | CL   | W     | 6045 | 1/1   | 0.92 | 0.05 | 65,65,65,65                 | 0     |
| 4   | EDO  | A     | 6002 | 4/4   | 0.92 | 0.16 | 37,43,45,51                 | 0     |
| 5   | GLN  | B     | 6004 | 10/10 | 0.92 | 0.12 | 43,44,45,46                 | 0     |
| 3   | CL   | I     | 6017 | 1/1   | 0.92 | 0.09 | 65,65,65,65                 | 0     |
| 5   | GLN  | T     | 6040 | 10/10 | 0.92 | 0.13 | 41,42,43,43                 | 0     |
| 5   | GLN  | V     | 6044 | 10/10 | 0.92 | 0.12 | 45,46,47,49                 | 0     |
| 4   | EDO  | I     | 6039 | 4/4   | 0.93 | 0.22 | 34,39,46,49                 | 0     |
| 3   | CL   | S     | 6037 | 1/1   | 0.93 | 0.07 | 72,72,72,72                 | 0     |
| 4   | EDO  | Q     | 6035 | 4/4   | 0.93 | 0.19 | 32,34,43,46                 | 0     |
| 3   | CL   | M     | 6025 | 1/1   | 0.93 | 0.07 | 65,65,65,65                 | 0     |
| 5   | GLN  | L     | 6024 | 10/10 | 0.93 | 0.13 | 39,41,42,43                 | 0     |
| 4   | EDO  | A     | 6031 | 4/4   | 0.93 | 0.19 | 32,39,44,49                 | 0     |
| 4   | EDO  | E     | 6047 | 4/4   | 0.93 | 0.19 | 30,40,44,47                 | 0     |
| 3   | CL   | E     | 6009 | 1/1   | 0.93 | 0.07 | 67,67,67,67                 | 0     |
| 5   | GLN  | F     | 6012 | 10/10 | 0.94 | 0.17 | 43,46,47,49                 | 0     |
| 5   | GLN  | H     | 6016 | 10/10 | 0.94 | 0.13 | 34,36,36,38                 | 0     |
| 4   | EDO  | I     | 6018 | 4/4   | 0.94 | 0.14 | 35,40,44,49                 | 0     |
| 4   | EDO  | I     | 6038 | 4/4   | 0.94 | 0.13 | 37,42,43,46                 | 0     |
| 4   | EDO  | U     | 6042 | 4/4   | 0.94 | 0.12 | 38,43,46,51                 | 0     |
| 4   | EDO  | C     | 6026 | 4/4   | 0.94 | 0.14 | 37,43,44,51                 | 0     |
| 4   | EDO  | U     | 6014 | 4/4   | 0.95 | 0.13 | 38,42,44,46                 | 0     |
| 3   | CL   | Q     | 6033 | 1/1   | 0.95 | 0.13 | 79,79,79,79                 | 0     |
| 5   | GLN  | N     | 6028 | 10/10 | 0.95 | 0.10 | 32,32,34,34                 | 0     |
| 5   | GLN  | X     | 6048 | 9/10  | 0.95 | 0.10 | 32,34,36,37                 | 0     |
| 5   | GLN  | D     | 6008 | 10/10 | 0.96 | 0.10 | 33,35,35,35                 | 0     |
| 5   | GLN  | P     | 6032 | 10/10 | 0.96 | 0.07 | 37,38,39,40                 | 0     |
| 4   | EDO  | C     | 6006 | 4/4   | 0.96 | 0.12 | 38,41,43,50                 | 0     |
| 4   | EDO  | W     | 6046 | 4/4   | 0.96 | 0.13 | 36,42,43,45                 | 0     |
| 5   | GLN  | J     | 6020 | 10/10 | 0.96 | 0.07 | 33,34,35,35                 | 0     |
| 4   | EDO  | E     | 6010 | 4/4   | 0.96 | 0.12 | 35,43,44,48                 | 0     |
| 3   | CL   | K     | 6021 | 1/1   | 0.97 | 0.08 | 70,70,70,70                 | 0     |
| 4   | EDO  | Q     | 6034 | 4/4   | 0.97 | 0.09 | 35,39,39,48                 | 0     |
| 4   | EDO  | K     | 6022 | 4/4   | 0.97 | 0.10 | 33,39,39,45                 | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.