



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:00 PM UTC

PDB ID : 7DR7 / pdb\_00007dr7  
EMDB ID : EMD-30825  
Title : bovine 20S immunoproteasome  
Authors : Xu, C.; Cong, Y.  
Deposited on : 2020-12-26  
Resolution : 3.30 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

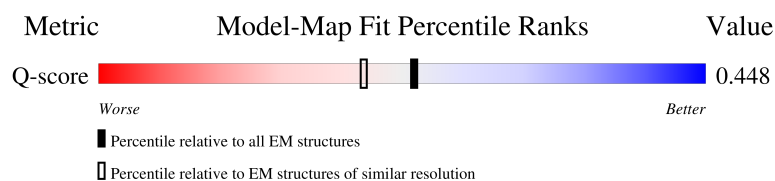
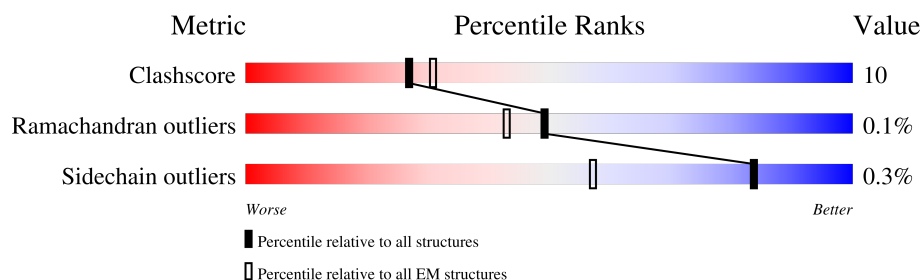
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 15087 ( 2.80 - 3.80 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                        |
|-----|-------|--------|-------------------------------------------------------------------------|
| 1   | A     | 248    | <div> <div>28%</div> <div>75%</div> <div>18%</div> <div>6%</div> </div> |
| 1   | O     | 248    | <div> <div>27%</div> <div>75%</div> <div>19%</div> <div>6%</div> </div> |
| 2   | B     | 241    | <div> <div>24%</div> <div>73%</div> <div>24%</div> <div>.</div> </div>  |
| 2   | P     | 241    | <div> <div>28%</div> <div>73%</div> <div>24%</div> <div>.</div> </div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | C     | 263    |                  |
| 3   | Q     | 263    |                  |
| 4   | D     | 255    |                  |
| 4   | R     | 255    |                  |
| 5   | E     | 246    |                  |
| 5   | L     | 246    |                  |
| 6   | F     | 234    |                  |
| 6   | M     | 234    |                  |
| 7   | G     | 261    |                  |
| 7   | N     | 261    |                  |
| 8   | H     | 205    |                  |
| 8   | S     | 205    |                  |
| 9   | I     | 201    |                  |
| 9   | T     | 201    |                  |
| 10  | J     | 241    |                  |
| 10  | U     | 241    |                  |
| 11  | K     | 264    |                  |
| 11  | V     | 264    |                  |
| 12  | W     | 219    |                  |
| 12  | Z     | 219    |                  |
| 13  | 1     | 273    |                  |
| 13  | X     | 273    |                  |
| 14  | 2     | 276    |                  |
| 14  | Y     | 276    |                  |

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 48304 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Proteasome subunit alpha type-7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | A     | 232      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1824  | 1149 | 322 | 348 | 5 |         |       |
| 1   | O     | 232      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1824  | 1149 | 322 | 348 | 5 |         |       |

- Molecule 2 is a protein called Proteasome subunit alpha type-5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | B     | 234      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1790  | 1125 | 295 | 359 | 11 |         |       |
| 2   | P     | 234      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1790  | 1125 | 295 | 359 | 11 |         |       |

- Molecule 3 is a protein called Proteasome subunit alpha type-1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | C     | 235      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1846  | 1156 | 330 | 349 | 11 |         |       |
| 3   | Q     | 235      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1846  | 1156 | 330 | 349 | 11 |         |       |

- Molecule 4 is a protein called Proteasome subunit alpha type-3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | D     | 240      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1879  | 1191 | 321 | 356 | 11 |         |       |
| 4   | R     | 240      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1879  | 1191 | 321 | 356 | 11 |         |       |

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | E     | 244      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1903  | 1206 | 320 | 364 | 13 |         |       |
| 5   | L     | 243      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1892  | 1200 | 316 | 363 | 13 |         |       |

- Molecule 6 is a protein called Proteasome subunit alpha type-2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | F     | 231      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1804  | 1153 | 306 | 339 | 6 |         |       |
| 6   | M     | 229      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1790  | 1144 | 304 | 336 | 6 |         |       |

- Molecule 7 is a protein called Proteasome subunit alpha type-4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | G     | 246      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1936  | 1225 | 331 | 369 | 11 |         |       |
| 7   | N     | 246      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1936  | 1225 | 331 | 369 | 11 |         |       |

- Molecule 8 is a protein called Proteasome subunit beta type-3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8   | H     | 204      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1594  | 1015 | 265 | 295 | 19 |         |       |
| 8   | S     | 204      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1594  | 1015 | 265 | 295 | 19 |         |       |

- Molecule 9 is a protein called Proteasome subunit beta type-2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9   | I     | 198      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1593  | 1023 | 270 | 292 | 8 |         |       |
| 9   | T     | 197      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1584  | 1017 | 268 | 291 | 8 |         |       |

- Molecule 10 is a protein called Proteasome subunit beta type-1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 10  | J     | 213      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1645  | 1042 | 282 | 311 | 10 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 10  | U     | 213      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1645  | 1042 | 282 | 311 | 10 |         |       |

- Molecule 11 is a protein called Proteasome subunit beta type-4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 11  | K     | 216      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1685  | 1065 | 289 | 319 | 12 |         |       |
| 11  | V     | 216      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1682  | 1063 | 289 | 318 | 12 |         |       |

- Molecule 12 is a protein called Proteasome subunit beta type-9.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 12  | W     | 199      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1499  | 942 | 257 | 290 | 10 |         |       |
| 12  | Z     | 199      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1500  | 942 | 257 | 291 | 10 |         |       |

- Molecule 13 is a protein called Proteasome subunit beta type-10.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 13  | X     | 219      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1611  | 1010 | 281 | 309 | 11 |         |       |
| 13  | 1     | 219      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1611  | 1010 | 281 | 309 | 11 |         |       |

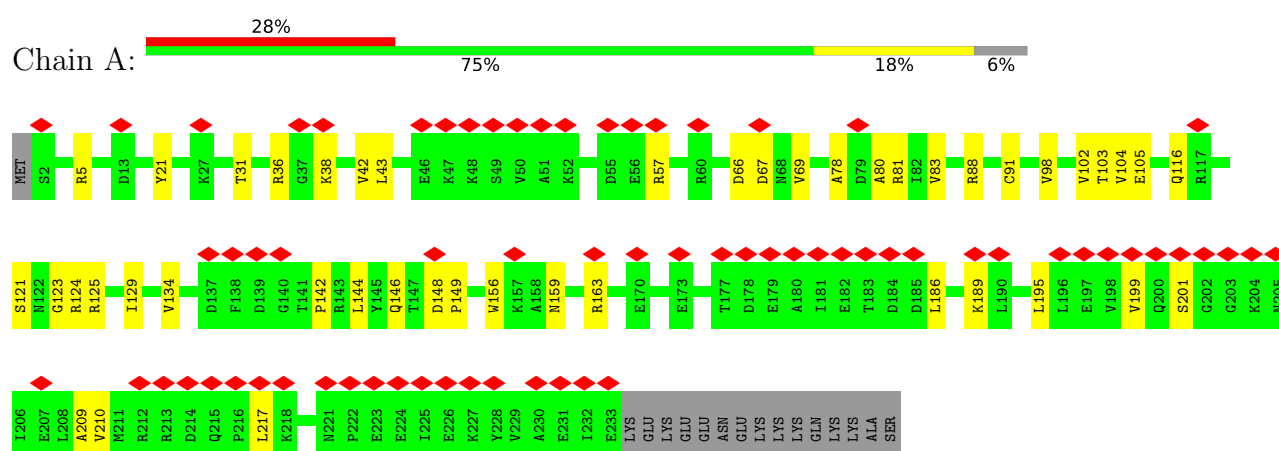
- Molecule 14 is a protein called Proteasome subunit beta type-8.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 14  | Y     | 201      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1561  | 975 | 273 | 297 | 16 |         |       |
| 14  | 2     | 201      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1561  | 975 | 273 | 297 | 16 |         |       |

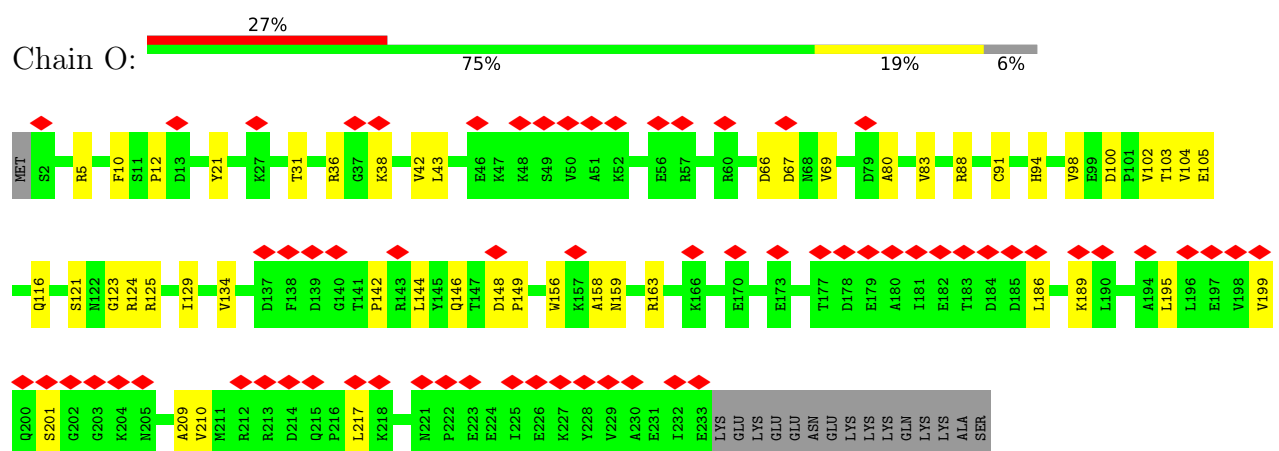
### 3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

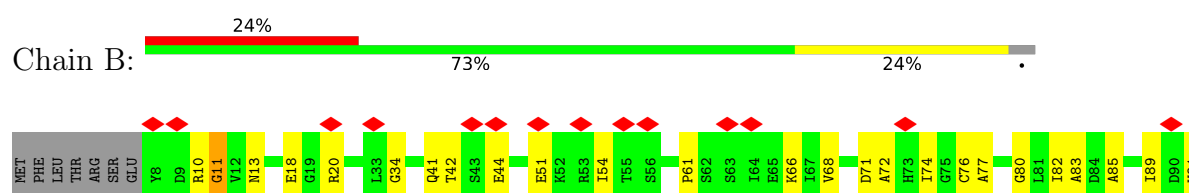
#### • Molecule 1: Proteasome subunit alpha type-7

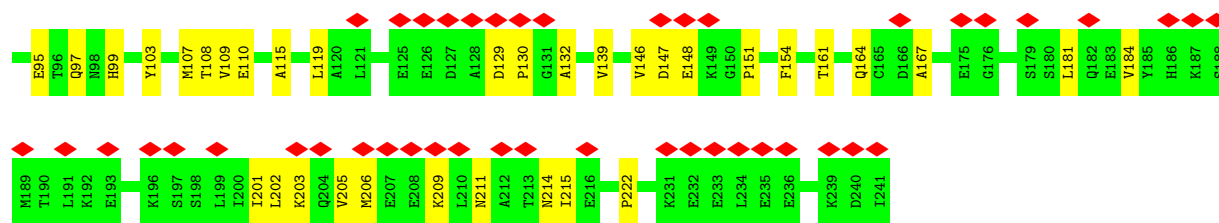


#### • Molecule 1: Proteasome subunit alpha type-7

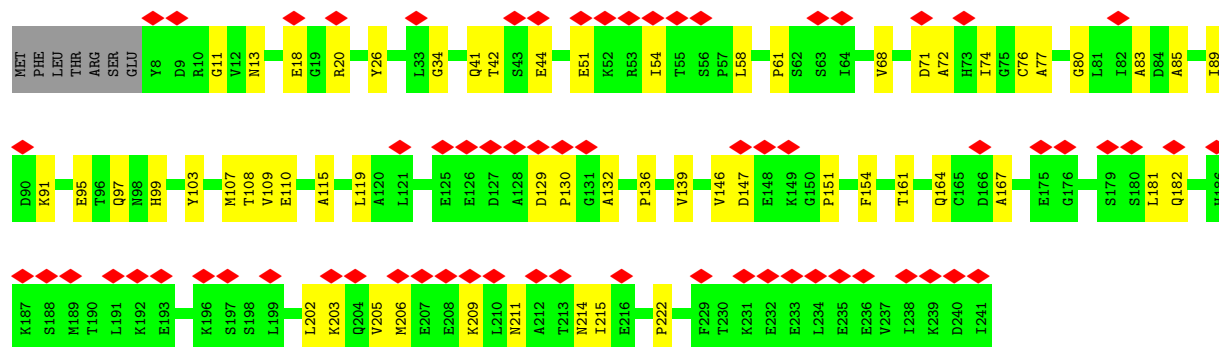
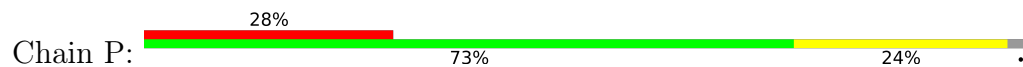


#### • Molecule 2: Proteasome subunit alpha type-5

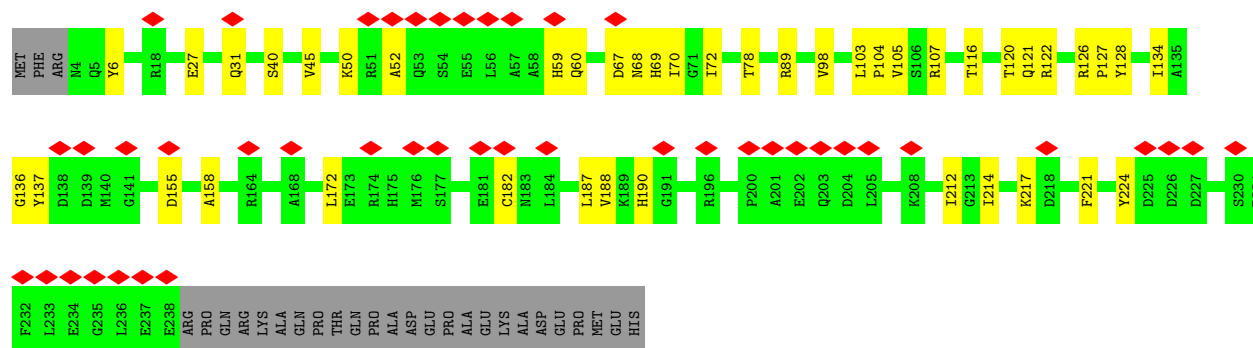
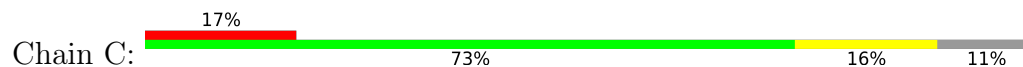




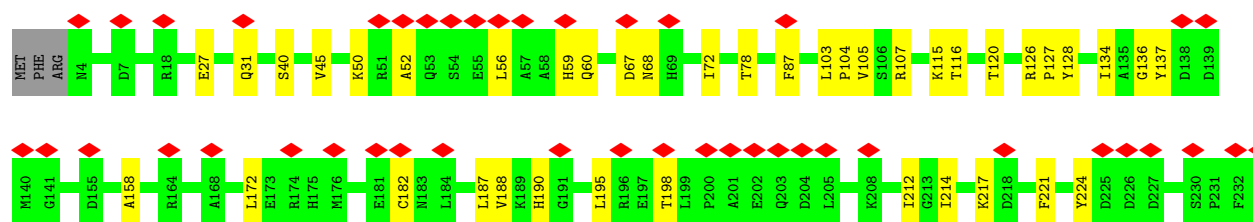
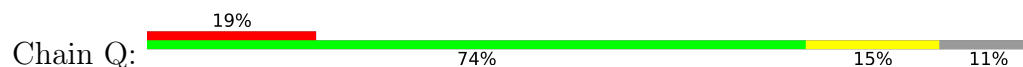
• Molecule 2: Proteasome subunit alpha type-5

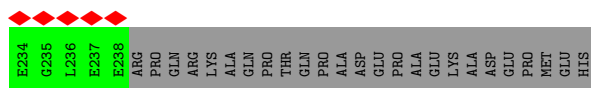


• Molecule 3: Proteasome subunit alpha type-1

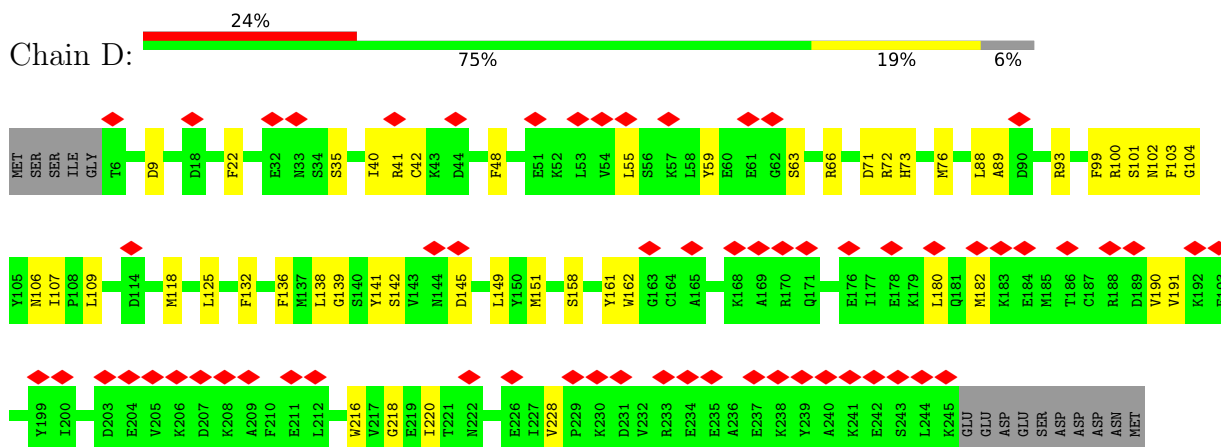


• Molecule 3: Proteasome subunit alpha type-1

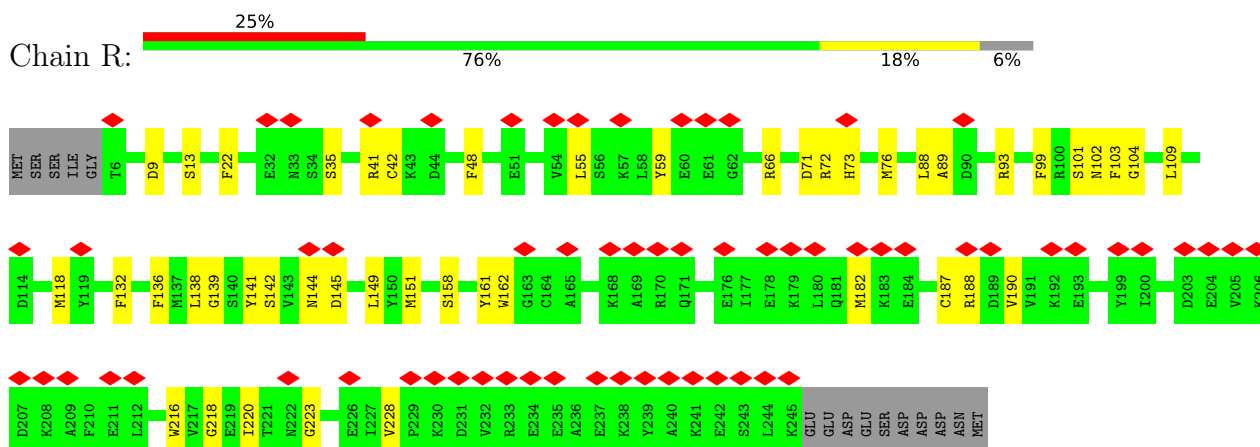




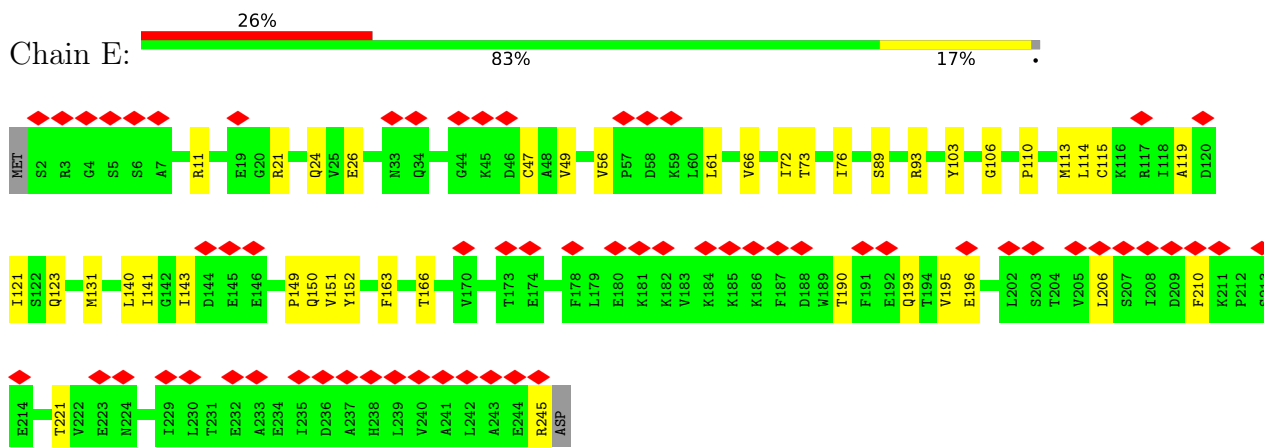
• Molecule 4: Proteasome subunit alpha type-3



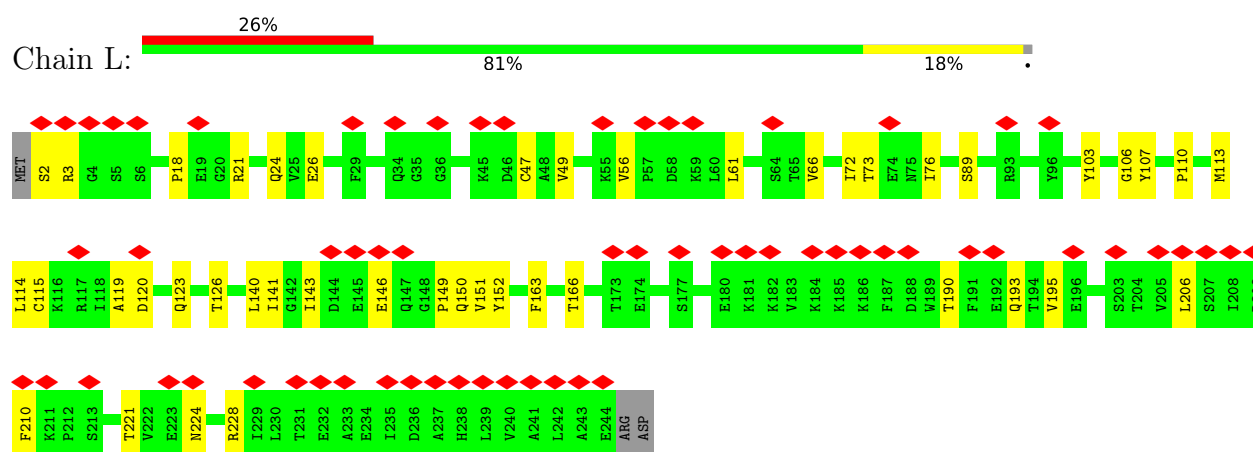
• Molecule 4: Proteasome subunit alpha type-3



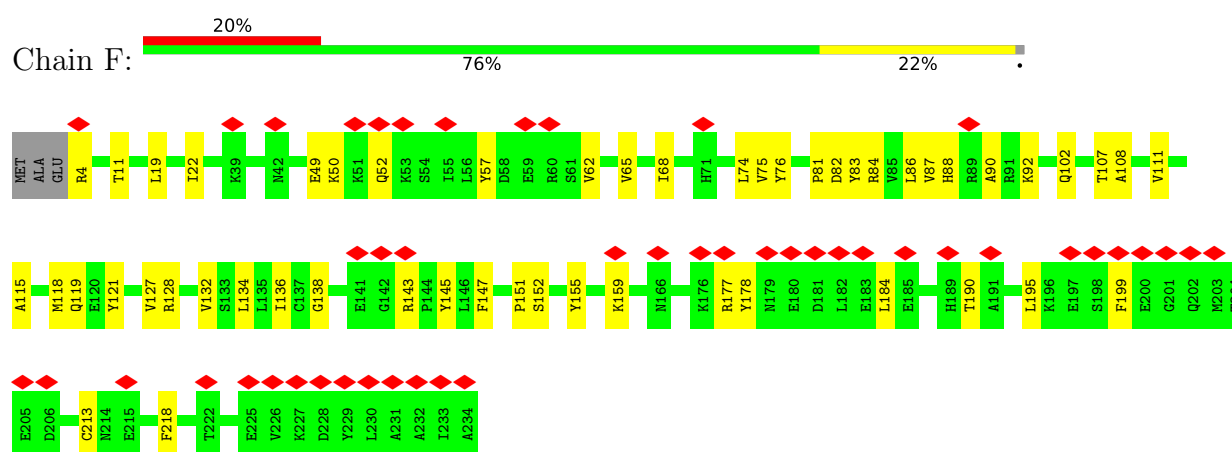
• Molecule 5: Proteasome subunit alpha type-6



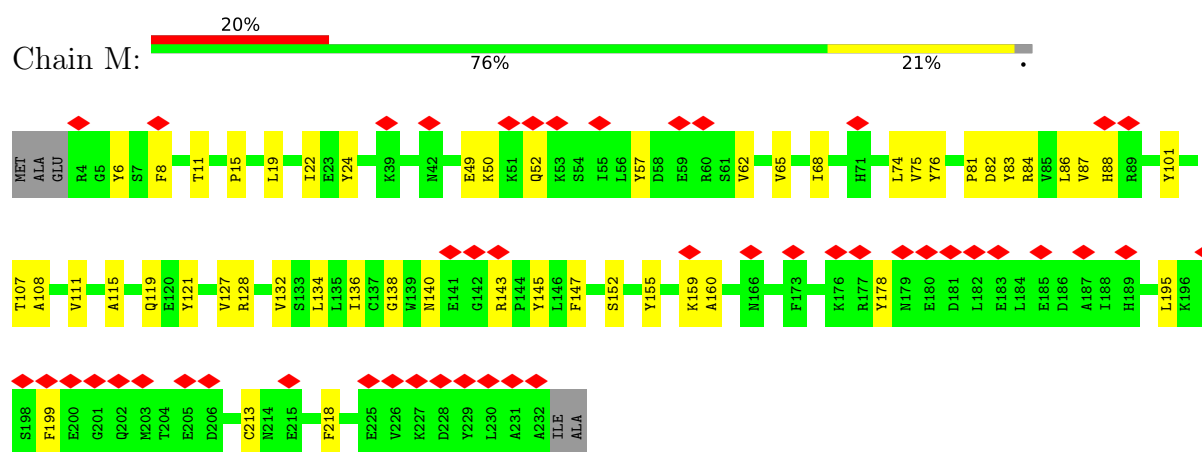
• Molecule 5: Proteasome subunit alpha type-6



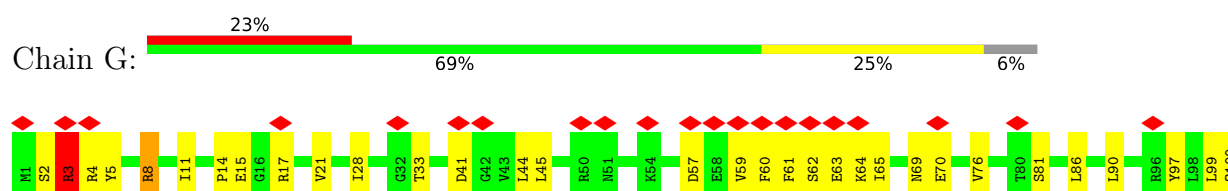
• Molecule 6: Proteasome subunit alpha type-2

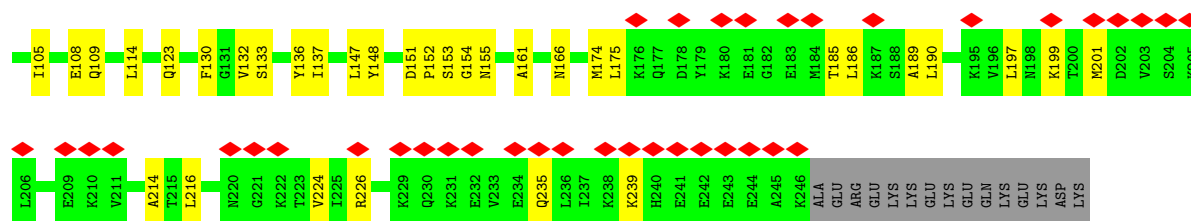


• Molecule 6: Proteasome subunit alpha type-2

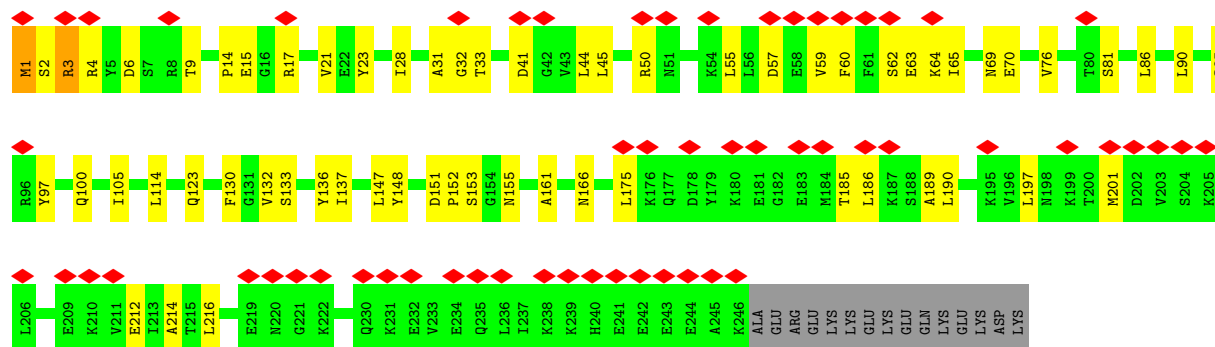


• Molecule 7: Proteasome subunit alpha type-4

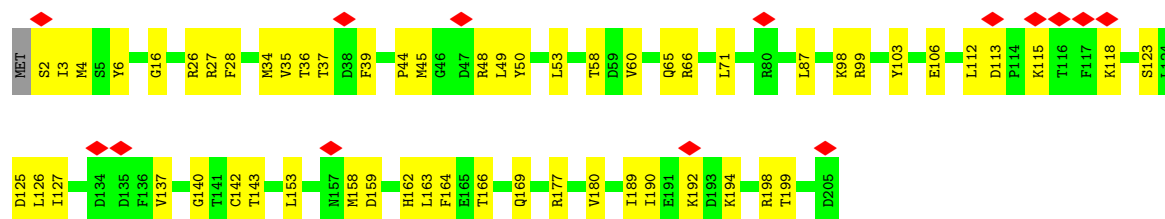




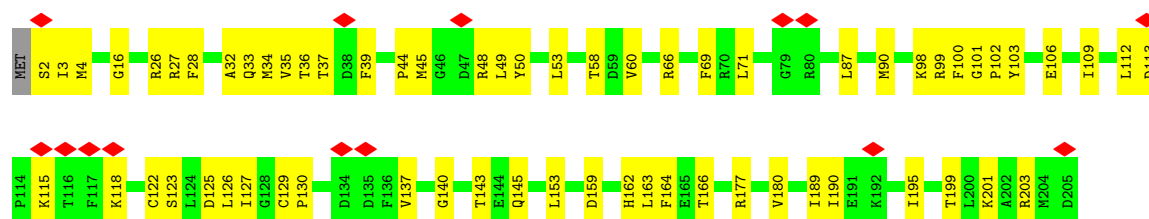
• Molecule 7: Proteasome subunit alpha type-4



• Molecule 8: Proteasome subunit beta type-3

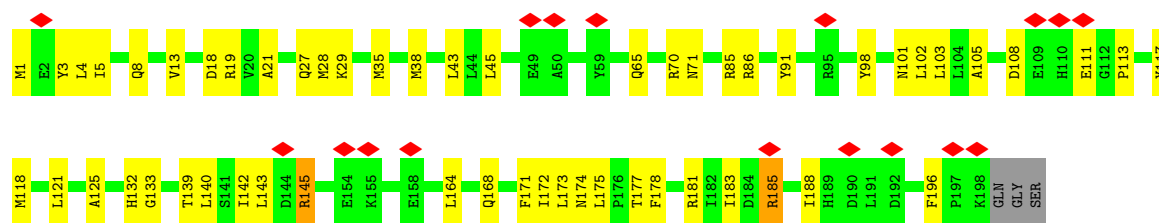


• Molecule 8: Proteasome subunit beta type-3

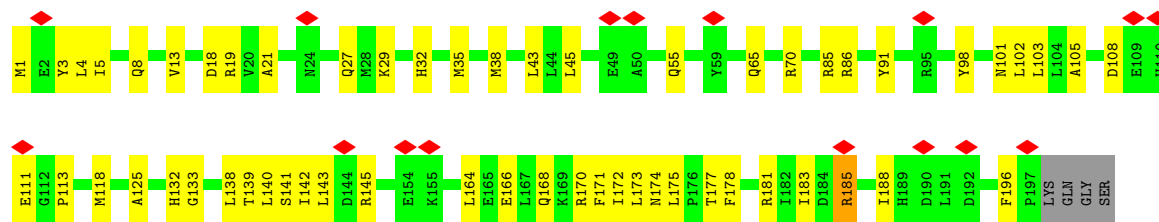


• Molecule 9: Proteasome subunit beta type-2

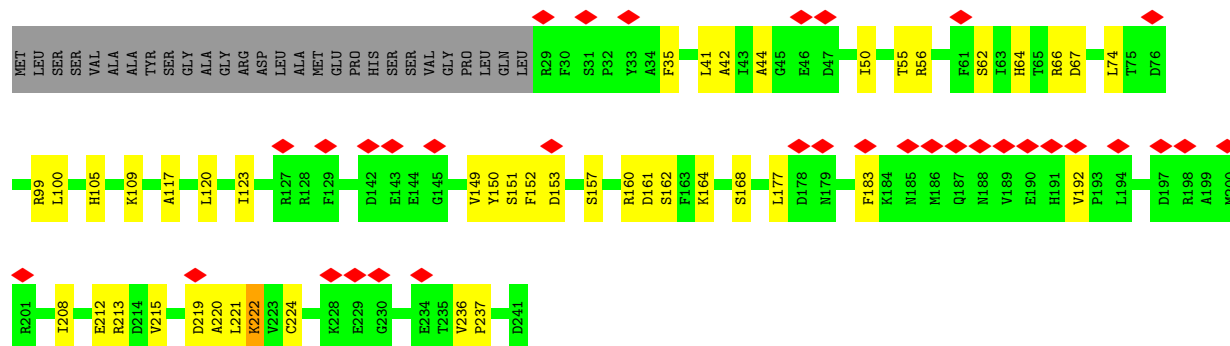




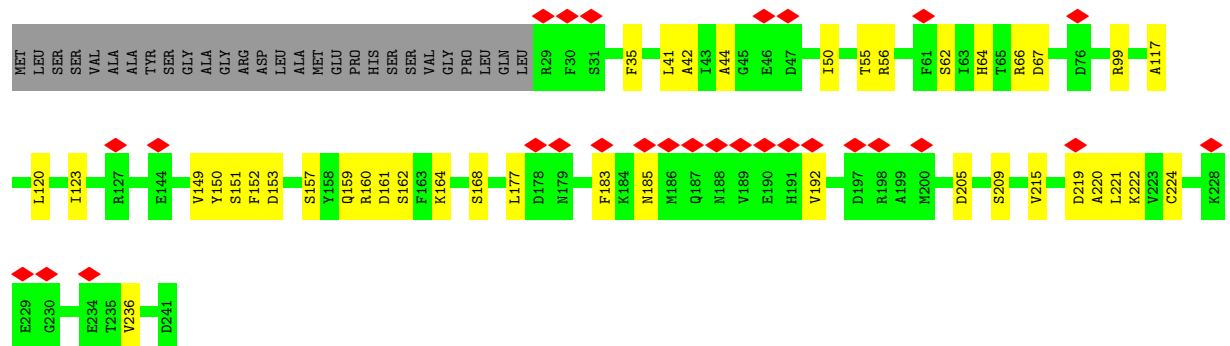
- Molecule 9: Proteasome subunit beta type-2



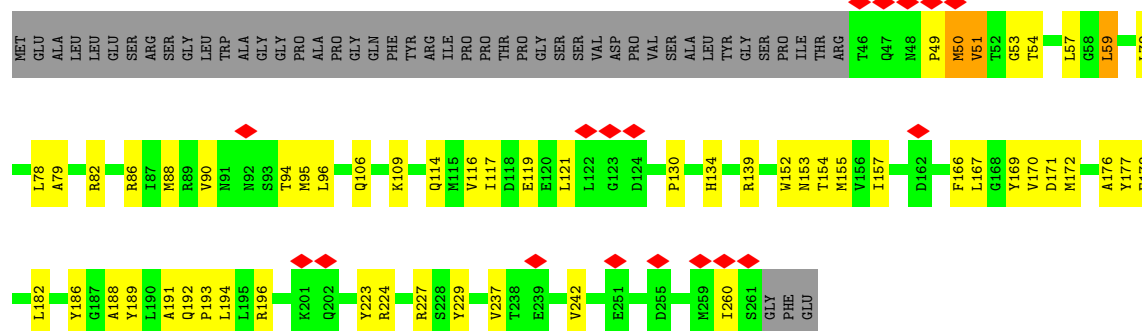
- Molecule 10: Proteasome subunit beta type-1



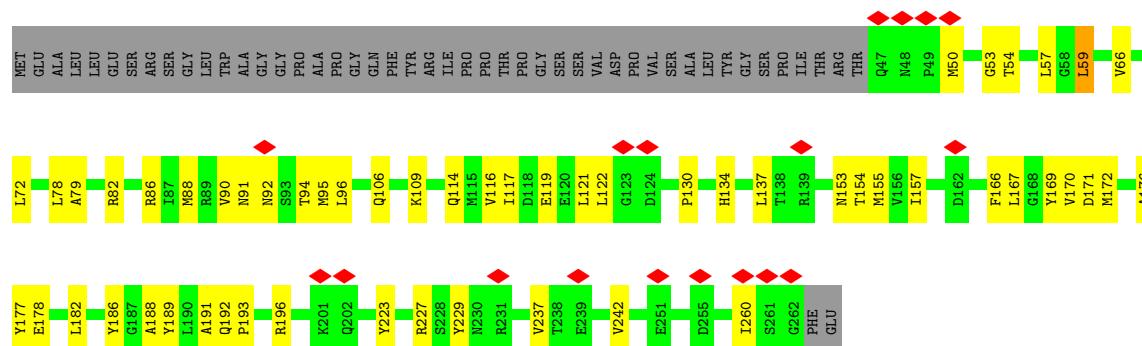
- Molecule 10: Proteasome subunit beta type-1



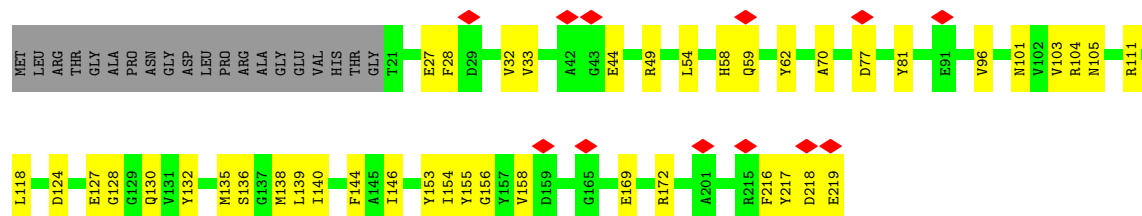
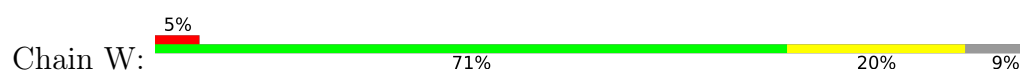
- Molecule 11: Proteasome subunit beta type-4



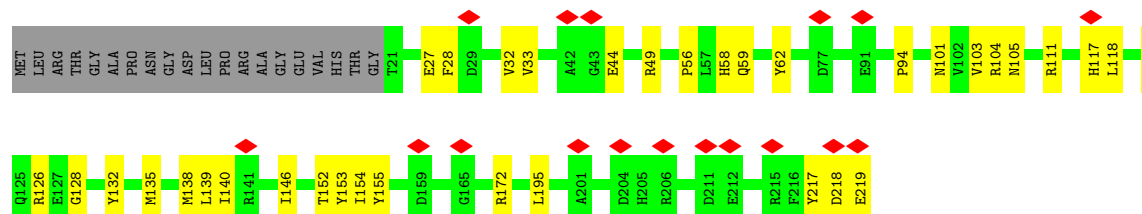
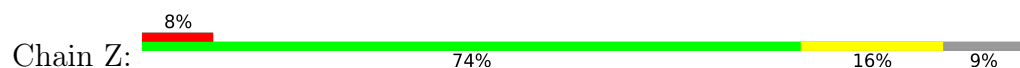
• Molecule 11: Proteasome subunit beta type-4



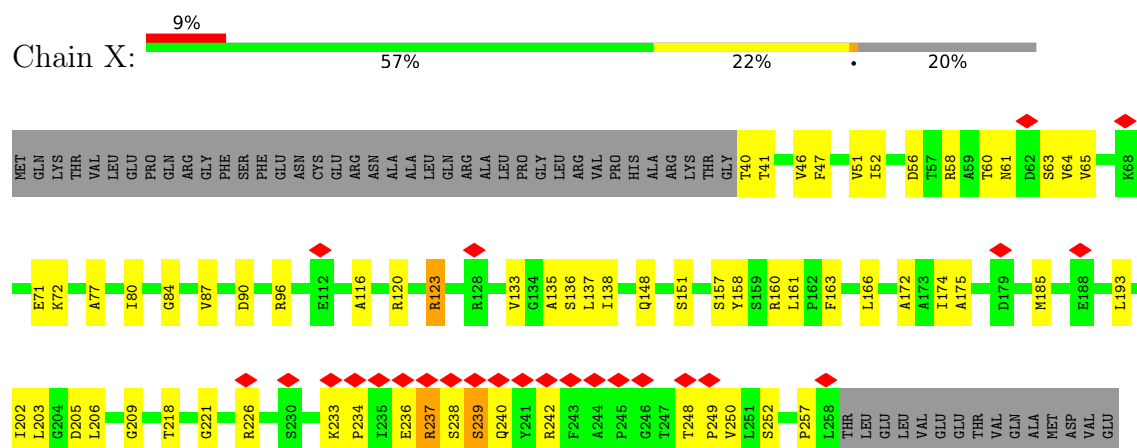
• Molecule 12: Proteasome subunit beta type-9



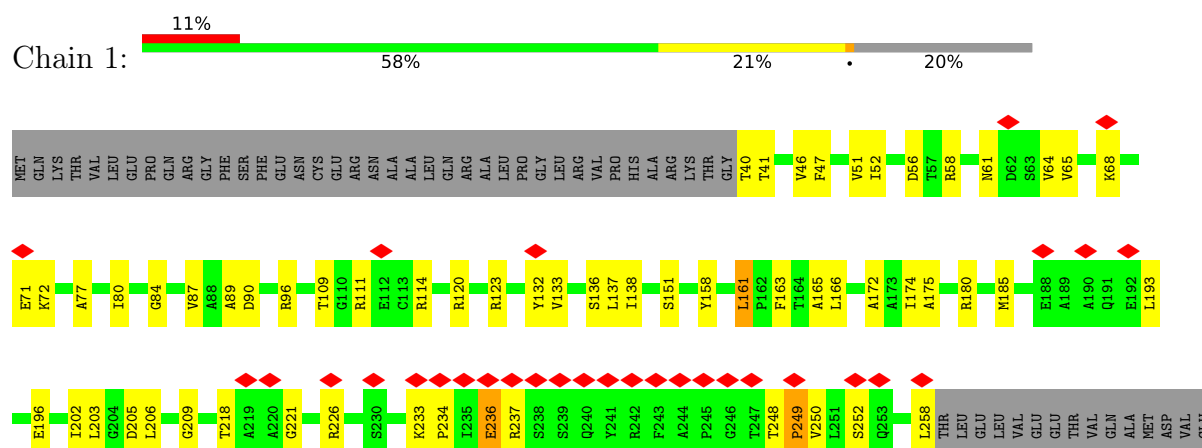
• Molecule 12: Proteasome subunit beta type-9



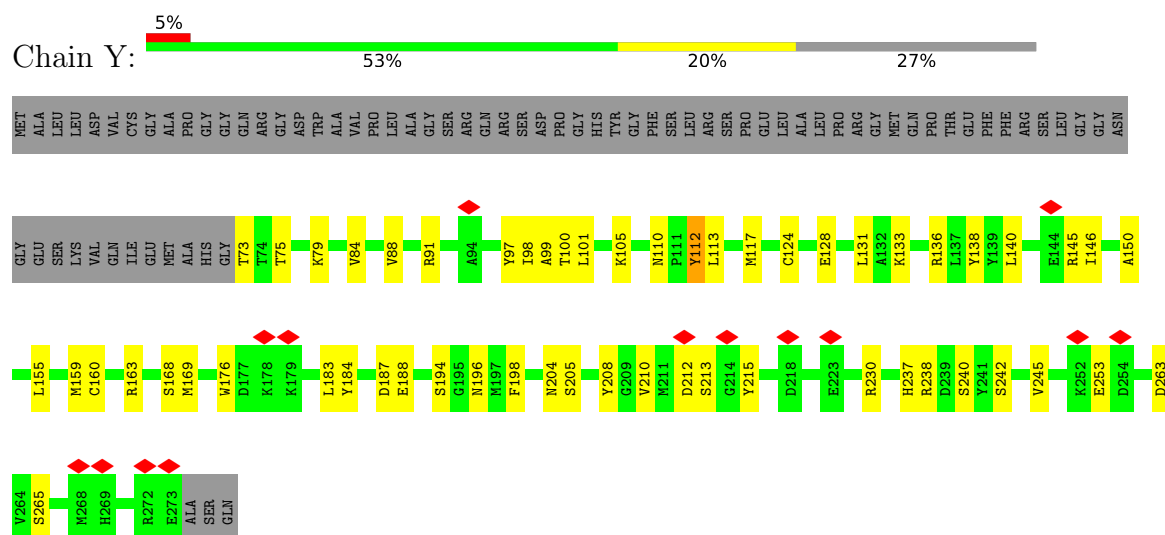
- Molecule 13: Proteasome subunit beta type-10



- Molecule 13: Proteasome subunit beta type-10

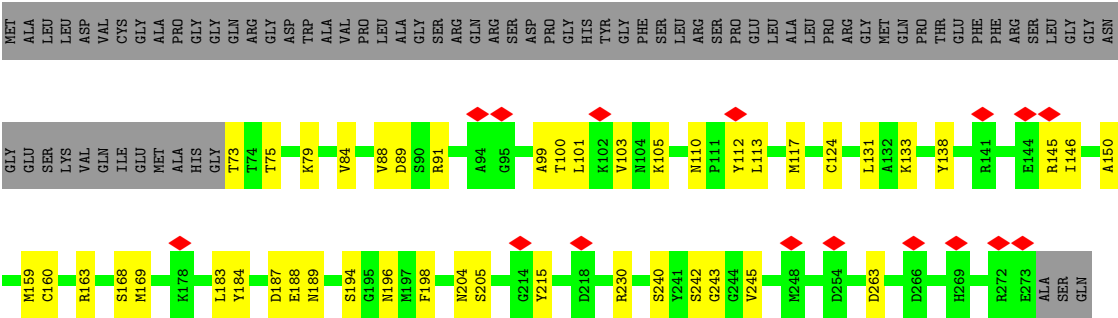


- Molecule 14: Proteasome subunit beta type-8



- Molecule 14: Proteasome subunit beta type-8





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 56663                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 38                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.171                                   | Depositor |
| Minimum map value                    | -0.110                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.005                                   | Depositor |
| Recommended contour level            | 0.03                                    | Depositor |
| Map size (Å)                         | 337.408, 337.408, 337.408               | wwPDB     |
| Map dimensions                       | 256, 256, 256                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.318, 1.318, 1.318                     | Depositor |

## 5 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 1   | A     | 0.15         | 0/1851  | 0.40        | 0/2501         |
| 1   | O     | 0.15         | 0/1851  | 0.39        | 0/2501         |
| 2   | B     | 0.15         | 0/1818  | 0.33        | 0/2455         |
| 2   | P     | 0.14         | 0/1818  | 0.32        | 0/2455         |
| 3   | C     | 0.14         | 0/1880  | 0.35        | 0/2541         |
| 3   | Q     | 0.14         | 0/1880  | 0.35        | 0/2541         |
| 4   | D     | 0.16         | 0/1914  | 0.35        | 0/2578         |
| 4   | R     | 0.15         | 0/1914  | 0.34        | 0/2578         |
| 5   | E     | 0.17         | 0/1937  | 0.37        | 0/2617         |
| 5   | L     | 0.16         | 0/1926  | 0.37        | 0/2603         |
| 6   | F     | 0.17         | 0/1843  | 0.35        | 0/2495         |
| 6   | M     | 0.17         | 0/1829  | 0.35        | 0/2477         |
| 7   | G     | 0.20         | 0/1966  | 0.42        | 2/2648 (0.1%)  |
| 7   | N     | 0.20         | 0/1966  | 0.45        | 0/2648         |
| 8   | H     | 0.20         | 0/1623  | 0.38        | 0/2188         |
| 8   | S     | 0.20         | 0/1623  | 0.38        | 0/2188         |
| 9   | I     | 0.19         | 0/1627  | 0.38        | 1/2201 (0.0%)  |
| 9   | T     | 0.18         | 0/1618  | 0.35        | 0/2190         |
| 10  | J     | 0.18         | 0/1676  | 0.35        | 0/2258         |
| 10  | U     | 0.18         | 0/1676  | 0.36        | 0/2258         |
| 11  | K     | 0.20         | 0/1718  | 0.40        | 0/2324         |
| 11  | V     | 0.20         | 0/1715  | 0.40        | 0/2319         |
| 12  | W     | 0.23         | 0/1528  | 0.44        | 0/2071         |
| 12  | Z     | 0.19         | 0/1529  | 0.40        | 0/2071         |
| 13  | 1     | 0.19         | 0/1637  | 0.48        | 1/2225 (0.0%)  |
| 13  | X     | 0.24         | 0/1637  | 0.54        | 2/2225 (0.1%)  |
| 14  | 2     | 0.19         | 0/1592  | 0.40        | 0/2145         |
| 14  | Y     | 0.20         | 0/1592  | 0.42        | 0/2145         |
| All | All   | 0.18         | 0/49184 | 0.39        | 6/66446 (0.0%) |

There are no bond length outliers.

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 9   | I     | 145 | ARG  | N-CA-C | 6.38  | 120.27      | 112.23   |
| 13  | X     | 123 | ARG  | N-CA-C | 5.60  | 117.47      | 111.36   |
| 7   | G     | 3   | ARG  | N-CA-C | -5.56 | 105.22      | 111.28   |
| 13  | X     | 236 | GLU  | N-CA-C | 5.54  | 118.52      | 110.42   |
| 7   | G     | 8   | ARG  | N-CA-C | 5.54  | 118.75      | 111.28   |
| 13  | 1     | 161 | LEU  | N-CA-C | 5.03  | 112.55      | 108.07   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1824  | 0        | 1851     | 31      | 0            |
| 1   | O     | 1824  | 0        | 1851     | 33      | 0            |
| 2   | B     | 1790  | 0        | 1773     | 45      | 0            |
| 2   | P     | 1790  | 0        | 1773     | 41      | 0            |
| 3   | C     | 1846  | 0        | 1832     | 29      | 0            |
| 3   | Q     | 1846  | 0        | 1832     | 25      | 0            |
| 4   | D     | 1879  | 0        | 1864     | 38      | 0            |
| 4   | R     | 1879  | 0        | 1864     | 37      | 0            |
| 5   | E     | 1903  | 0        | 1911     | 32      | 0            |
| 5   | L     | 1892  | 0        | 1898     | 36      | 0            |
| 6   | F     | 1804  | 0        | 1800     | 36      | 0            |
| 6   | M     | 1790  | 0        | 1784     | 43      | 0            |
| 7   | G     | 1936  | 0        | 1961     | 44      | 0            |
| 7   | N     | 1936  | 0        | 1961     | 53      | 0            |
| 8   | H     | 1594  | 0        | 1613     | 40      | 0            |
| 8   | S     | 1594  | 0        | 1613     | 50      | 0            |
| 9   | I     | 1593  | 0        | 1597     | 52      | 0            |
| 9   | T     | 1584  | 0        | 1584     | 50      | 0            |
| 10  | J     | 1645  | 0        | 1644     | 33      | 0            |
| 10  | U     | 1645  | 0        | 1644     | 29      | 0            |
| 11  | K     | 1685  | 0        | 1665     | 47      | 0            |
| 11  | V     | 1682  | 0        | 1661     | 42      | 0            |
| 12  | W     | 1499  | 0        | 1459     | 33      | 0            |
| 12  | Z     | 1500  | 0        | 1459     | 28      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 13  | 1     | 1611  | 0        | 1624     | 55      | 0            |
| 13  | X     | 1611  | 0        | 1624     | 70      | 0            |
| 14  | 2     | 1561  | 0        | 1516     | 36      | 0            |
| 14  | Y     | 1561  | 0        | 1516     | 44      | 0            |
| All | All   | 48304 | 0        | 48174    | 954     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (954) 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) |
|-------------------|------------------|--------------------------|-------------------|
| 8:S:100:PHE:HE1   | 13:1:132:TYR:CD2 | 1.47                     | 1.32              |
| 8:S:100:PHE:CE1   | 13:1:132:TYR:CE2 | 2.23                     | 1.26              |
| 8:S:100:PHE:HE1   | 13:1:132:TYR:CE2 | 1.54                     | 1.25              |
| 8:S:100:PHE:CE1   | 13:1:132:TYR:CD2 | 2.40                     | 1.08              |
| 13:X:123:ARG:CD   | 13:X:158:TYR:HD2 | 1.71                     | 1.03              |
| 5:E:106:GLY:HA3   | 13:X:120:ARG:HD2 | 1.41                     | 1.02              |
| 6:M:6:TYR:CE1     | 7:N:1:MET:HA     | 1.99                     | 0.98              |
| 8:H:140:GLY:O     | 8:H:143:THR:HG23 | 1.68                     | 0.92              |
| 12:W:146:ILE:HD11 | 12:W:155:TYR:CE1 | 2.05                     | 0.91              |
| 13:X:123:ARG:CD   | 13:X:158:TYR:CD2 | 2.53                     | 0.91              |
| 6:M:6:TYR:CD1     | 7:N:1:MET:HA     | 2.06                     | 0.90              |
| 13:X:237:ARG:HB2  | 13:X:237:ARG:NH1 | 1.86                     | 0.88              |
| 14:2:112:TYR:HE2  | 14:2:145:ARG:HD2 | 1.43                     | 0.83              |
| 8:S:100:PHE:CD1   | 13:1:132:TYR:CE2 | 2.67                     | 0.83              |
| 5:L:123:GLN:HE22  | 6:M:84:ARG:HB2   | 1.43                     | 0.82              |
| 10:U:205:ASP:OD2  | 13:X:239:SER:HB2 | 1.78                     | 0.82              |
| 13:X:233:LYS:HB3  | 13:X:234:PRO:HD3 | 1.59                     | 0.82              |
| 8:S:140:GLY:O     | 8:S:143:THR:HG23 | 1.78                     | 0.82              |
| 10:U:222:LYS:HE2  | 10:U:224:CYS:SG  | 2.21                     | 0.81              |
| 14:Y:124:CYS:O    | 14:Y:128:GLU:HG3 | 1.81                     | 0.80              |
| 9:I:43:LEU:HD11   | 9:I:188:ILE:HD12 | 1.63                     | 0.79              |
| 9:T:43:LEU:HD11   | 9:T:188:ILE:HD12 | 1.63                     | 0.79              |
| 13:X:123:ARG:NE   | 13:X:158:TYR:CD2 | 2.51                     | 0.78              |
| 8:H:158:MET:SD    | 13:X:242:ARG:NH2 | 2.57                     | 0.77              |
| 9:I:91:TYR:CD2    | 9:I:98:TYR:CD2   | 2.73                     | 0.77              |
| 5:E:106:GLY:HA3   | 13:X:120:ARG:CD  | 2.15                     | 0.77              |
| 11:V:186:TYR:HE2  | 12:W:44:GLU:HB2  | 1.52                     | 0.75              |
| 1:A:81:ARG:NH2    | 7:G:154:GLY:O    | 2.20                     | 0.75              |
| 4:R:216:TRP:CZ3   | 4:R:220:ILE:HD12 | 2.22                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 9:I:91:TYR:CE2   | 9:I:98:TYR:HE2   | 2.05                     | 0.74              |
| 7:N:1:MET:HE3    | 1:O:5:ARG:HD2    | 1.69                     | 0.74              |
| 2:B:99:HIS:HB2   | 2:B:107:MET:HE3  | 1.71                     | 0.73              |
| 10:J:222:LYS:HE2 | 10:J:224:CYS:SG  | 2.29                     | 0.73              |
| 13:X:71:GLU:OE1  | 13:X:226:ARG:NH1 | 2.22                     | 0.73              |
| 13:X:123:ARG:HD3 | 13:X:158:TYR:CD2 | 2.24                     | 0.73              |
| 4:D:101:SER:OG   | 11:K:114:GLN:NE2 | 2.22                     | 0.73              |
| 2:P:99:HIS:HB2   | 2:P:107:MET:HE3  | 1.71                     | 0.73              |
| 6:M:6:TYR:CE1    | 7:N:1:MET:CA     | 2.72                     | 0.72              |
| 10:J:222:LYS:CE  | 10:J:224:CYS:SG  | 2.77                     | 0.72              |
| 11:K:49:PRO:HG3  | 11:K:152:TRP:CD1 | 2.24                     | 0.72              |
| 2:B:41:GLN:NE2   | 2:B:151:PRO:O    | 2.23                     | 0.71              |
| 5:E:93:ARG:HE    | 5:E:121:ILE:HD13 | 1.53                     | 0.71              |
| 8:S:203:ARG:NH1  | 14:Y:263:ASP:OD2 | 2.22                     | 0.71              |
| 2:P:41:GLN:NE2   | 2:P:151:PRO:O    | 2.23                     | 0.71              |
| 3:Q:107:ARG:HH22 | 11:V:119:GLU:HG3 | 1.55                     | 0.71              |
| 13:X:123:ARG:HD2 | 13:X:158:TYR:HD2 | 1.53                     | 0.71              |
| 1:A:125:ARG:HE   | 7:G:123:GLN:HA   | 1.55                     | 0.71              |
| 1:A:209:ALA:HB1  | 1:A:217:LEU:HD11 | 1.72                     | 0.71              |
| 4:R:101:SER:OG   | 11:V:114:GLN:NE2 | 2.22                     | 0.71              |
| 1:O:209:ALA:HB1  | 1:O:217:LEU:HD11 | 1.72                     | 0.70              |
| 9:I:91:TYR:CE2   | 9:I:98:TYR:CE2   | 2.80                     | 0.70              |
| 11:K:59:LEU:C    | 11:K:59:LEU:HD12 | 2.15                     | 0.70              |
| 5:L:21:ARG:NE    | 5:L:26:GLU:OE2   | 2.21                     | 0.69              |
| 10:J:66:ARG:HH22 | 13:1:203:LEU:HB3 | 1.57                     | 0.69              |
| 3:C:107:ARG:HH22 | 11:K:119:GLU:HG3 | 1.56                     | 0.69              |
| 4:D:100:ARG:NH2  | 4:D:106:ASN:OD1  | 2.25                     | 0.69              |
| 6:M:74:LEU:HD11  | 6:M:134:LEU:HD22 | 1.75                     | 0.69              |
| 12:W:144:PHE:CE1 | 12:W:158:VAL:HB  | 2.27                     | 0.69              |
| 6:F:74:LEU:HD11  | 6:F:134:LEU:HD22 | 1.74                     | 0.69              |
| 6:M:119:GLN:NE2  | 7:N:81:SER:O     | 2.26                     | 0.68              |
| 11:V:59:LEU:O    | 11:V:59:LEU:HD23 | 1.93                     | 0.68              |
| 4:D:125:LEU:HD23 | 5:E:131:MET:HE1  | 1.75                     | 0.68              |
| 13:1:236:GLU:HA  | 13:1:236:GLU:OE1 | 1.94                     | 0.68              |
| 8:H:140:GLY:O    | 8:H:143:THR:CG2  | 2.42                     | 0.67              |
| 8:S:100:PHE:CE1  | 13:1:132:TYR:HE2 | 2.04                     | 0.67              |
| 5:E:106:GLY:CA   | 13:X:120:ARG:HD2 | 2.21                     | 0.67              |
| 9:I:181:ARG:HD3  | 9:I:188:ILE:HD11 | 1.75                     | 0.67              |
| 4:D:40:ILE:HD11  | 4:D:182:MET:HG3  | 1.75                     | 0.67              |
| 9:T:181:ARG:HD3  | 9:T:188:ILE:HD11 | 1.75                     | 0.67              |
| 4:D:118:MET:HE1  | 5:E:89:SER:HA    | 1.75                     | 0.67              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 10:J:41:LEU:HD11 | 10:J:177:LEU:HD11 | 1.77                     | 0.67              |
| 6:F:52:GLN:HB3   | 6:F:57:TYR:HD2    | 1.59                     | 0.67              |
| 8:S:113:ASP:HB3  | 8:S:118:LYS:HB3   | 1.77                     | 0.67              |
| 14:Y:73:THR:N    | 14:Y:242:SER:HG   | 1.92                     | 0.67              |
| 8:S:45:MET:HE3   | 8:S:71:LEU:HD22   | 1.77                     | 0.66              |
| 10:U:41:LEU:HD11 | 10:U:177:LEU:HD11 | 1.77                     | 0.66              |
| 11:V:82:ARG:NH1  | 12:W:218:ASP:O    | 2.28                     | 0.66              |
| 12:Z:135:MET:O   | 12:Z:138:MET:HG2  | 1.95                     | 0.66              |
| 1:A:42:VAL:HG22  | 1:A:210:VAL:HG12  | 1.77                     | 0.66              |
| 6:M:52:GLN:HB3   | 6:M:57:TYR:HD2    | 1.59                     | 0.66              |
| 12:W:135:MET:O   | 12:W:138:MET:HG2  | 1.95                     | 0.66              |
| 9:I:185:ARG:HH11 | 9:I:185:ARG:HB2   | 1.59                     | 0.66              |
| 8:H:45:MET:HE3   | 8:H:71:LEU:HD22   | 1.77                     | 0.66              |
| 8:H:113:ASP:HB3  | 8:H:118:LYS:HB3   | 1.77                     | 0.66              |
| 14:2:73:THR:N    | 14:2:242:SER:HG   | 1.92                     | 0.66              |
| 8:S:140:GLY:O    | 8:S:143:THR:CG2   | 2.44                     | 0.66              |
| 10:U:209:SER:OG  | 13:X:237:ARG:NH2  | 2.29                     | 0.66              |
| 13:1:218:THR:H   | 13:1:221:GLY:HA2  | 1.61                     | 0.65              |
| 11:V:50:MET:SD   | 12:Z:111:ARG:NH2  | 2.68                     | 0.65              |
| 1:O:42:VAL:HG22  | 1:O:210:VAL:HG12  | 1.77                     | 0.65              |
| 13:X:237:ARG:O   | 13:X:237:ARG:HG3  | 1.96                     | 0.65              |
| 5:L:123:GLN:NE2  | 6:M:81:PRO:O      | 2.30                     | 0.65              |
| 12:W:77:ASP:OD2  | 13:X:123:ARG:NH1  | 2.26                     | 0.65              |
| 11:K:50:MET:SD   | 12:W:111:ARG:NH2  | 2.69                     | 0.65              |
| 10:U:66:ARG:NH2  | 13:X:203:LEU:O    | 2.30                     | 0.65              |
| 4:R:188:ARG:HG3  | 4:R:220:ILE:HD11  | 1.78                     | 0.65              |
| 12:W:169:GLU:OE1 | 12:W:172:ARG:NH2  | 2.30                     | 0.65              |
| 2:B:10:ARG:O     | 2:B:11:GLY:O      | 2.15                     | 0.65              |
| 5:E:21:ARG:NE    | 5:E:26:GLU:OE2    | 2.21                     | 0.65              |
| 9:I:91:TYR:CD2   | 9:I:98:TYR:HD2    | 2.14                     | 0.65              |
| 9:I:140:LEU:HD23 | 9:I:143:LEU:HD12  | 1.78                     | 0.65              |
| 13:X:218:THR:H   | 13:X:221:GLY:HA2  | 1.61                     | 0.65              |
| 8:H:164:PHE:CE2  | 13:X:248:THR:HG21 | 2.32                     | 0.64              |
| 11:K:186:TYR:HE2 | 12:Z:44:GLU:HB2   | 1.62                     | 0.64              |
| 9:T:140:LEU:HD23 | 9:T:143:LEU:HD12  | 1.78                     | 0.64              |
| 8:S:164:PHE:HB2  | 8:S:189:ILE:HD11  | 1.80                     | 0.64              |
| 4:R:55:LEU:HB2   | 4:R:59:TYR:HE2    | 1.63                     | 0.64              |
| 4:D:55:LEU:HB2   | 4:D:59:TYR:HE2    | 1.63                     | 0.64              |
| 5:E:11:ARG:O     | 5:E:24:GLN:NE2    | 2.31                     | 0.63              |
| 8:H:164:PHE:HB2  | 8:H:189:ILE:HD11  | 1.80                     | 0.63              |
| 3:Q:87:PHE:HB3   | 3:Q:115:LYS:HE2   | 1.79                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 7:N:1:MET:CE     | 1:O:5:ARG:HD2     | 2.28                     | 0.62              |
| 6:F:50:LYS:NZ    | 6:F:62:VAL:O      | 2.31                     | 0.62              |
| 5:E:123:GLN:HE22 | 6:F:84:ARG:HB2    | 1.65                     | 0.62              |
| 9:I:38:MET:O     | 9:I:65:GLN:NE2    | 2.32                     | 0.62              |
| 13:X:40:THR:HG23 | 13:X:72:LYS:HE2   | 1.81                     | 0.62              |
| 3:C:116:THR:HG22 | 3:C:128:TYR:HD2   | 1.64                     | 0.62              |
| 6:M:50:LYS:NZ    | 6:M:62:VAL:O      | 2.31                     | 0.62              |
| 4:R:187:CYS:SG   | 4:R:220:ILE:CD1   | 2.87                     | 0.62              |
| 6:F:65:VAL:HG22  | 6:F:75:VAL:HG12   | 1.81                     | 0.62              |
| 10:J:66:ARG:NH2  | 13:1:203:LEU:O    | 2.32                     | 0.62              |
| 8:S:177:ARG:NH2  | 14:Y:99:ALA:O     | 2.31                     | 0.62              |
| 8:H:177:ARG:NH2  | 14:2:99:ALA:O     | 2.31                     | 0.62              |
| 11:K:50:MET:SD   | 12:W:136:SER:HB3  | 2.40                     | 0.61              |
| 9:I:28:MET:HE3   | 14:Y:198:PHE:HD1  | 1.66                     | 0.61              |
| 9:T:185:ARG:HG2  | 9:T:185:ARG:HH21  | 1.64                     | 0.61              |
| 3:Q:45:VAL:HG11  | 3:Q:188:VAL:HG22  | 1.83                     | 0.61              |
| 13:1:71:GLU:OE1  | 13:1:226:ARG:NH1  | 2.33                     | 0.61              |
| 7:G:69:ASN:OD1   | 7:G:70:GLU:N      | 2.34                     | 0.61              |
| 6:M:65:VAL:HG22  | 6:M:75:VAL:HG12   | 1.81                     | 0.61              |
| 7:N:69:ASN:OD1   | 7:N:70:GLU:N      | 2.34                     | 0.61              |
| 13:1:40:THR:HG23 | 13:1:72:LYS:HE2   | 1.81                     | 0.61              |
| 5:L:146:GLU:OE1  | 13:1:111:ARG:NH1  | 2.34                     | 0.61              |
| 7:G:44:LEU:HD22  | 7:G:190:LEU:HD23  | 1.82                     | 0.60              |
| 3:Q:116:THR:HG22 | 3:Q:128:TYR:HD2   | 1.64                     | 0.60              |
| 8:S:159:ASP:OD1  | 8:S:162:HIS:ND1   | 2.34                     | 0.60              |
| 9:T:185:ARG:HH21 | 9:T:185:ARG:CG    | 2.14                     | 0.60              |
| 8:H:159:ASP:OD1  | 8:H:162:HIS:ND1   | 2.35                     | 0.60              |
| 1:O:116:GLN:NE2  | 2:P:83:ALA:O      | 2.35                     | 0.60              |
| 5:E:196:GLU:OE1  | 5:E:245:ARG:NH2   | 2.34                     | 0.60              |
| 10:J:44:ALA:HB2  | 10:J:149:VAL:HG23 | 1.82                     | 0.60              |
| 2:P:203:LYS:HA   | 2:P:206:MET:HE3   | 1.84                     | 0.60              |
| 13:X:123:ARG:NE  | 13:X:158:TYR:CE2  | 2.69                     | 0.60              |
| 2:B:10:ARG:HH11  | 2:B:10:ARG:HB3    | 1.66                     | 0.60              |
| 10:U:44:ALA:HB2  | 10:U:149:VAL:HG23 | 1.82                     | 0.60              |
| 7:N:3:ARG:HH22   | 2:P:11:GLY:HA3    | 1.66                     | 0.60              |
| 3:C:45:VAL:HG11  | 3:C:188:VAL:HG22  | 1.83                     | 0.60              |
| 9:I:91:TYR:CD2   | 9:I:98:TYR:CE2    | 2.89                     | 0.60              |
| 8:H:194:LYS:HG2  | 13:X:257:PRO:HA   | 1.84                     | 0.60              |
| 10:J:208:ILE:CG2 | 13:1:237:ARG:HG2  | 2.32                     | 0.60              |
| 1:A:116:GLN:NE2  | 2:B:83:ALA:O      | 2.35                     | 0.59              |
| 7:G:151:ASP:HB2  | 7:G:152:PRO:HD2   | 1.83                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:N:44:LEU:HD22   | 7:N:190:LEU:HD23  | 1.82                     | 0.59              |
| 11:K:90:VAL:HB    | 11:K:94:THR:HG23  | 1.85                     | 0.59              |
| 13:X:237:ARG:HB2  | 13:X:237:ARG:CZ   | 2.33                     | 0.59              |
| 13:X:237:ARG:HB2  | 13:X:237:ARG:HH11 | 1.62                     | 0.59              |
| 14:Y:117:MET:HG3  | 14:Y:124:CYS:SG   | 2.43                     | 0.59              |
| 7:N:151:ASP:HB2   | 7:N:152:PRO:HD2   | 1.83                     | 0.59              |
| 9:T:43:LEU:HD13   | 9:T:183:ILE:HD11  | 1.85                     | 0.59              |
| 14:2:79:LYS:O     | 14:2:215:TYR:OH   | 2.21                     | 0.59              |
| 4:R:187:CYS:SG    | 4:R:220:ILE:HD12  | 2.43                     | 0.59              |
| 1:A:31:THR:OG1    | 1:A:163:ARG:O     | 2.21                     | 0.58              |
| 1:A:146:GLN:OE1   | 1:A:159:ASN:ND2   | 2.35                     | 0.58              |
| 14:Y:79:LYS:O     | 14:Y:215:TYR:OH   | 2.21                     | 0.58              |
| 14:2:112:TYR:CE2  | 14:2:145:ARG:HD2  | 2.31                     | 0.58              |
| 2:B:203:LYS:HA    | 2:B:206:MET:HE3   | 1.84                     | 0.58              |
| 6:F:119:GLN:NE2   | 7:G:81:SER:O      | 2.35                     | 0.58              |
| 14:2:117:MET:HG3  | 14:2:124:CYS:SG   | 2.43                     | 0.58              |
| 14:2:124:CYS:HB3  | 14:2:169:MET:HB2  | 1.85                     | 0.58              |
| 12:W:28:PHE:HE2   | 12:W:33:VAL:HG23  | 1.69                     | 0.58              |
| 13:1:58:ARG:NH2   | 13:1:206:LEU:O    | 2.37                     | 0.58              |
| 2:P:211:ASN:HB2   | 2:P:214:ASN:HB2   | 1.85                     | 0.58              |
| 13:X:161:LEU:HD13 | 13:X:163:PHE:O    | 2.04                     | 0.58              |
| 13:1:90:ASP:HB3   | 13:1:133:VAL:HG13 | 1.85                     | 0.58              |
| 2:B:211:ASN:HB2   | 2:B:214:ASN:HB2   | 1.85                     | 0.58              |
| 14:2:75:THR:HG23  | 14:2:88:VAL:HG12  | 1.86                     | 0.58              |
| 9:I:168:GLN:NE2   | 9:I:175:LEU:O     | 2.35                     | 0.58              |
| 11:K:153:ASN:OD1  | 11:K:154:THR:N    | 2.37                     | 0.58              |
| 11:V:153:ASN:OD1  | 11:V:154:THR:N    | 2.37                     | 0.58              |
| 14:Y:100:THR:HG22 | 14:Y:101:LEU:H    | 1.69                     | 0.58              |
| 14:2:100:THR:HG22 | 14:2:101:LEU:H    | 1.69                     | 0.58              |
| 12:W:154:ILE:O    | 12:W:154:ILE:HG13 | 2.02                     | 0.58              |
| 13:1:165:ALA:HB3  | 13:1:174:ILE:HG13 | 1.85                     | 0.58              |
| 7:G:8:ARG:O       | 7:G:11:ILE:HG12   | 2.03                     | 0.58              |
| 9:I:43:LEU:HD13   | 9:I:183:ILE:HD11  | 1.84                     | 0.58              |
| 1:O:36:ARG:NH2    | 1:O:142:PRO:O     | 2.34                     | 0.58              |
| 11:K:171:ASP:OD1  | 11:K:172:MET:N    | 2.36                     | 0.58              |
| 6:M:6:TYR:HE1     | 7:N:1:MET:HA      | 1.63                     | 0.58              |
| 10:U:120:LEU:HD23 | 10:U:152:PHE:HE2  | 1.69                     | 0.58              |
| 11:V:171:ASP:OD1  | 11:V:172:MET:N    | 2.36                     | 0.58              |
| 13:X:133:VAL:HG12 | 13:X:135:ALA:H    | 1.69                     | 0.58              |
| 4:D:9:ASP:HB3     | 4:D:22:PHE:HD2    | 1.69                     | 0.57              |
| 4:R:9:ASP:HB3     | 4:R:22:PHE:HD2    | 1.69                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:S:199:THR:HB    | 13:1:252:SER:HB2  | 1.87                     | 0.57              |
| 12:Z:28:PHE:HE2   | 12:Z:33:VAL:HG23  | 1.69                     | 0.57              |
| 11:V:90:VAL:HB    | 11:V:94:THR:HG23  | 1.85                     | 0.57              |
| 10:J:120:LEU:HD23 | 10:J:152:PHE:HE2  | 1.69                     | 0.57              |
| 10:J:151:SER:HB2  | 10:J:164:LYS:HG3  | 1.86                     | 0.57              |
| 7:N:100:GLN:HG2   | 9:T:86:ARG:HD3    | 1.87                     | 0.57              |
| 13:X:58:ARG:NH2   | 13:X:206:LEU:O    | 2.37                     | 0.57              |
| 13:X:248:THR:O    | 13:X:250:VAL:N    | 2.37                     | 0.57              |
| 10:U:99:ARG:HD2   | 10:U:123:ILE:HD11 | 1.87                     | 0.57              |
| 14:Y:124:CYS:HB3  | 14:Y:169:MET:HB2  | 1.85                     | 0.57              |
| 14:2:160:CYS:SG   | 14:2:163:ARG:NH2  | 2.73                     | 0.57              |
| 5:L:24:GLN:NE2    | 4:R:13:SER:O      | 2.37                     | 0.57              |
| 7:N:32:GLY:HA2    | 7:N:50:ARG:CZ     | 2.35                     | 0.57              |
| 2:B:108:THR:OG1   | 2:B:147:ASP:OD2   | 2.22                     | 0.57              |
| 2:B:110:GLU:HA    | 2:B:154:PHE:HE2   | 1.70                     | 0.57              |
| 8:S:195:ILE:HG13  | 13:1:258:LEU:HD11 | 1.87                     | 0.57              |
| 9:T:38:MET:O      | 9:T:65:GLN:NE2    | 2.33                     | 0.57              |
| 6:M:6:TYR:HE1     | 7:N:1:MET:CA      | 2.14                     | 0.57              |
| 1:O:199:VAL:HG12  | 1:O:201:SER:H     | 1.70                     | 0.57              |
| 3:Q:50:LYS:HB3    | 3:Q:59:HIS:HB3    | 1.87                     | 0.57              |
| 10:J:99:ARG:HD2   | 10:J:123:ILE:HD11 | 1.87                     | 0.56              |
| 14:Y:75:THR:HG23  | 14:Y:88:VAL:HG12  | 1.86                     | 0.56              |
| 11:K:155:MET:HE3  | 11:K:170:VAL:HG21 | 1.87                     | 0.56              |
| 10:U:66:ARG:HH22  | 13:X:203:LEU:HB3  | 1.70                     | 0.56              |
| 1:A:199:VAL:HG12  | 1:A:201:SER:H     | 1.70                     | 0.56              |
| 6:F:52:GLN:HB3    | 6:F:57:TYR:CD2    | 2.40                     | 0.56              |
| 9:I:185:ARG:HB2   | 9:I:185:ARG:NH1   | 2.19                     | 0.56              |
| 1:O:146:GLN:OE1   | 1:O:159:ASN:ND2   | 2.35                     | 0.56              |
| 11:V:155:MET:HE3  | 11:V:170:VAL:HG21 | 1.87                     | 0.56              |
| 13:1:248:THR:O    | 13:1:250:VAL:N    | 2.37                     | 0.56              |
| 4:R:42:CYS:HB3    | 4:R:190:VAL:HG21  | 1.87                     | 0.56              |
| 4:D:42:CYS:HB3    | 4:D:190:VAL:HG21  | 1.87                     | 0.56              |
| 7:G:3:ARG:O       | 7:G:4:ARG:C       | 2.49                     | 0.56              |
| 11:K:96:LEU:HD13  | 11:K:157:ILE:HG13 | 1.88                     | 0.56              |
| 2:P:42:THR:HG22   | 2:P:44:GLU:H      | 1.70                     | 0.56              |
| 6:F:86:LEU:HD13   | 6:F:134:LEU:HD11  | 1.88                     | 0.56              |
| 10:U:151:SER:HB2  | 10:U:164:LYS:HG3  | 1.86                     | 0.56              |
| 14:2:105:LYS:HB3  | 14:2:117:MET:HB3  | 1.88                     | 0.56              |
| 2:B:76:CYS:SG     | 2:B:77:ALA:N      | 2.79                     | 0.56              |
| 7:N:31:ALA:O      | 7:N:50:ARG:NH2    | 2.39                     | 0.56              |
| 2:P:76:CYS:SG     | 2:P:77:ALA:N      | 2.79                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:V:96:LEU:HD13  | 11:V:157:ILE:HG13 | 1.88                     | 0.56              |
| 2:P:110:GLU:HA    | 2:P:154:PHE:HE2   | 1.70                     | 0.55              |
| 13:1:180:ARG:NH1  | 13:1:196:GLU:OE1  | 2.39                     | 0.55              |
| 7:N:123:GLN:HA    | 1:O:125:ARG:HE    | 1.71                     | 0.55              |
| 8:S:33:GLN:HE22   | 14:Y:238:ARG:HB3  | 1.72                     | 0.55              |
| 8:S:44:PRO:HA     | 8:S:50:TYR:HD1    | 1.71                     | 0.55              |
| 6:M:195:LEU:O     | 6:M:199:PHE:N     | 2.38                     | 0.55              |
| 1:O:121:SER:HB2   | 1:O:124:ARG:HG3   | 1.89                     | 0.55              |
| 2:P:108:THR:OG1   | 2:P:147:ASP:OD2   | 2.22                     | 0.55              |
| 10:U:55:THR:HB    | 10:U:67:ASP:HA    | 1.89                     | 0.55              |
| 7:N:3:ARG:NH2     | 2:P:11:GLY:HA3    | 2.21                     | 0.55              |
| 9:T:168:GLN:NE2   | 9:T:175:LEU:O     | 2.35                     | 0.55              |
| 2:B:42:THR:HG22   | 2:B:44:GLU:H      | 1.70                     | 0.55              |
| 5:E:93:ARG:NE     | 5:E:121:ILE:HD13  | 2.21                     | 0.55              |
| 6:M:86:LEU:HD13   | 6:M:134:LEU:HD11  | 1.88                     | 0.55              |
| 8:S:58:THR:O      | 9:T:85:ARG:NH2    | 2.40                     | 0.55              |
| 3:C:50:LYS:HB3    | 3:C:59:HIS:HB3    | 1.87                     | 0.55              |
| 11:K:88:MET:SD    | 11:K:109:LYS:HG3  | 2.47                     | 0.55              |
| 2:B:13:ASN:HB3    | 3:C:126:ARG:HB3   | 1.90                     | 0.54              |
| 2:B:74:ILE:HG12   | 2:B:109:VAL:HG22  | 1.90                     | 0.54              |
| 12:W:156:GLY:HA3  | 12:Z:154:ILE:HG22 | 1.89                     | 0.54              |
| 14:Y:176:TRP:CE2  | 14:Y:253:GLU:HG2  | 2.42                     | 0.54              |
| 1:A:36:ARG:NH2    | 1:A:142:PRO:O     | 2.34                     | 0.54              |
| 8:H:44:PRO:HA     | 8:H:50:TYR:HD1    | 1.72                     | 0.54              |
| 1:O:31:THR:OG1    | 1:O:163:ARG:O     | 2.21                     | 0.54              |
| 12:W:216:PHE:O    | 12:W:217:TYR:C    | 2.50                     | 0.54              |
| 14:Y:187:ASP:OD1  | 14:Y:188:GLU:N    | 2.36                     | 0.54              |
| 9:I:172:ILE:HG22  | 9:T:173:LEU:HD22  | 1.89                     | 0.54              |
| 10:J:208:ILE:HG21 | 13:1:237:ARG:HG2  | 1.89                     | 0.54              |
| 2:P:34:GLY:HA3    | 2:P:80:GLY:H      | 1.72                     | 0.54              |
| 9:T:185:ARG:HB3   | 9:T:185:ARG:NH2   | 2.22                     | 0.54              |
| 11:V:88:MET:SD    | 11:V:109:LYS:HG3  | 2.47                     | 0.54              |
| 10:J:153:ASP:OD1  | 10:J:157:SER:N    | 2.41                     | 0.54              |
| 11:K:82:ARG:NH1   | 12:Z:218:ASP:O    | 2.40                     | 0.54              |
| 6:M:52:GLN:HB3    | 6:M:57:TYR:CD2    | 2.40                     | 0.54              |
| 6:M:68:ILE:HD11   | 6:M:74:LEU:HD22   | 1.89                     | 0.54              |
| 7:N:15:GLU:OE1    | 7:N:17:ARG:NH2    | 2.41                     | 0.54              |
| 9:T:45:LEU:HB2    | 9:T:103:LEU:HB2   | 1.90                     | 0.54              |
| 8:H:169:GLN:NE2   | 10:U:185:ASN:O    | 2.38                     | 0.54              |
| 11:K:223:TYR:HB3  | 12:Z:49:ARG:HD3   | 1.89                     | 0.54              |
| 12:W:138:MET:HE2  | 12:W:140:ILE:HD11 | 1.89                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 13:X:158:TYR:CD1 | 13:X:158:TYR:C    | 2.85                     | 0.54              |
| 13:X:163:PHE:C   | 13:X:163:PHE:CD1  | 2.85                     | 0.54              |
| 1:A:121:SER:HB2  | 1:A:124:ARG:HG3   | 1.89                     | 0.54              |
| 5:E:110:PRO:HG2  | 5:E:113:MET:HB2   | 1.90                     | 0.54              |
| 4:R:48:PHE:HZ    | 4:R:139:GLY:H     | 1.56                     | 0.54              |
| 8:H:153:LEU:HB3  | 8:H:166:THR:HG23  | 1.90                     | 0.53              |
| 8:S:99:ARG:NH1   | 13:1:132:TYR:OH   | 2.40                     | 0.53              |
| 12:W:70:ALA:HB2  | 13:X:157:SER:OG   | 2.08                     | 0.53              |
| 8:H:58:THR:O     | 9:I:85:ARG:NH2    | 2.41                     | 0.53              |
| 10:J:55:THR:HB   | 10:J:67:ASP:HA    | 1.89                     | 0.53              |
| 10:J:62:SER:HB2  | 11:K:189:TYR:HE1  | 1.73                     | 0.53              |
| 2:P:74:ILE:HG12  | 2:P:109:VAL:HG22  | 1.90                     | 0.53              |
| 13:X:237:ARG:CZ  | 13:X:237:ARG:CB   | 2.86                     | 0.53              |
| 11:V:95:MET:HE3  | 11:V:237:VAL:HB   | 1.91                     | 0.53              |
| 13:X:116:ALA:O   | 13:X:120:ARG:HG3  | 2.09                     | 0.53              |
| 6:F:68:ILE:HD11  | 6:F:74:LEU:HD22   | 1.89                     | 0.53              |
| 9:T:185:ARG:CZ   | 9:T:185:ARG:CB    | 2.87                     | 0.53              |
| 5:L:224:ASN:HD21 | 5:L:228:ARG:HE    | 1.56                     | 0.53              |
| 3:Q:158:ALA:HB1  | 3:Q:172:LEU:HD13  | 1.90                     | 0.53              |
| 10:U:153:ASP:OD1 | 10:U:157:SER:N    | 2.41                     | 0.53              |
| 9:I:45:LEU:HB2   | 9:I:103:LEU:HB2   | 1.90                     | 0.53              |
| 8:S:153:LEU:HB3  | 8:S:166:THR:HG23  | 1.90                     | 0.53              |
| 12:Z:117:HIS:HB3 | 12:Z:135:MET:SD   | 2.48                     | 0.53              |
| 4:D:216:TRP:CD1  | 4:D:228:VAL:HG22  | 2.44                     | 0.53              |
| 7:G:15:GLU:OE1   | 7:G:17:ARG:NH2    | 2.41                     | 0.53              |
| 5:L:110:PRO:HG2  | 5:L:113:MET:HB2   | 1.90                     | 0.53              |
| 1:O:69:VAL:HG22  | 1:O:104:VAL:HG22  | 1.90                     | 0.53              |
| 13:1:46:VAL:HG22 | 13:1:51:VAL:HG12  | 1.91                     | 0.53              |
| 1:A:69:VAL:HG22  | 1:A:104:VAL:HG22  | 1.90                     | 0.53              |
| 2:B:34:GLY:HA3   | 2:B:80:GLY:H      | 1.72                     | 0.53              |
| 6:F:111:VAL:HG22 | 6:F:136:ILE:HD12  | 1.91                     | 0.53              |
| 6:M:111:VAL:HG22 | 6:M:136:ILE:HD12  | 1.91                     | 0.53              |
| 2:B:54:ILE:HD11  | 2:B:61:PRO:HB3    | 1.91                     | 0.53              |
| 7:N:3:ARG:NH2    | 2:P:11:GLY:CA     | 2.72                     | 0.53              |
| 4:R:216:TRP:CD1  | 4:R:228:VAL:HG22  | 2.44                     | 0.53              |
| 8:S:4:MET:HE1    | 8:S:106:GLU:HG3   | 1.91                     | 0.53              |
| 12:Z:172:ARG:HG3 | 12:Z:195:LEU:HD13 | 1.90                     | 0.53              |
| 7:N:151:ASP:OD1  | 7:N:155:ASN:N     | 2.36                     | 0.52              |
| 1:A:21:TYR:CE1   | 7:G:14:PRO:HA     | 2.44                     | 0.52              |
| 1:A:148:ASP:OD1  | 1:A:149:PRO:HD2   | 2.10                     | 0.52              |
| 3:C:105:VAL:HG21 | 3:C:136:GLY:HA3   | 1.92                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:158:ALA:HB1  | 3:C:172:LEU:HD13  | 1.90                     | 0.52              |
| 4:D:142:SER:HB3  | 4:D:145:ASP:HB2   | 1.91                     | 0.52              |
| 6:F:111:VAL:HG21 | 6:F:147:PHE:HD2   | 1.74                     | 0.52              |
| 4:D:48:PHE:HZ    | 4:D:139:GLY:H     | 1.56                     | 0.52              |
| 6:F:22:ILE:HG21  | 6:F:152:SER:HB3   | 1.91                     | 0.52              |
| 2:P:13:ASN:HB3   | 3:Q:126:ARG:HB3   | 1.91                     | 0.52              |
| 2:P:54:ILE:HD11  | 2:P:61:PRO:HB3    | 1.91                     | 0.52              |
| 13:X:160:ARG:HG2 | 13:X:160:ARG:HH11 | 1.74                     | 0.52              |
| 9:I:171:PHE:CE2  | 9:I:173:LEU:HB2   | 2.44                     | 0.52              |
| 6:M:111:VAL:HG21 | 6:M:147:PHE:HD2   | 1.74                     | 0.52              |
| 14:Y:112:TYR:CZ  | 14:Y:145:ARG:HD2  | 2.44                     | 0.52              |
| 2:P:161:THR:HG1  | 3:Q:78:THR:HG1    | 1.57                     | 0.52              |
| 9:T:170:ARG:HG3  | 14:Y:208:TYR:HB3  | 1.91                     | 0.52              |
| 9:T:171:PHE:CE2  | 9:T:173:LEU:HB2   | 2.44                     | 0.52              |
| 8:H:4:MET:HE1    | 8:H:106:GLU:HG3   | 1.91                     | 0.52              |
| 9:I:185:ARG:NH1  | 9:I:185:ARG:CB    | 2.73                     | 0.52              |
| 9:T:145:ARG:HG3  | 14:Y:230:ARG:HD3  | 1.91                     | 0.52              |
| 10:U:64:HIS:HB3  | 11:V:177:TYR:CZ   | 2.44                     | 0.52              |
| 14:2:187:ASP:OD1 | 14:2:188:GLU:N    | 2.36                     | 0.52              |
| 2:B:10:ARG:NH1   | 2:B:10:ARG:CB     | 2.73                     | 0.52              |
| 2:B:146:VAL:HG11 | 2:B:222:PRO:HA    | 1.92                     | 0.52              |
| 2:B:148:GLU:OE2  | 10:J:109:LYS:NZ   | 2.41                     | 0.52              |
| 8:H:123:SER:HB3  | 8:H:137:VAL:HB    | 1.92                     | 0.52              |
| 2:B:99:HIS:CE1   | 2:B:103:TYR:HD2   | 2.28                     | 0.52              |
| 2:P:146:VAL:HG11 | 2:P:222:PRO:HA    | 1.92                     | 0.52              |
| 13:X:46:VAL:HG22 | 13:X:51:VAL:HG12  | 1.91                     | 0.52              |
| 14:Y:138:TYR:CD2 | 14:Y:146:ILE:HB   | 2.45                     | 0.52              |
| 5:E:106:GLY:CA   | 13:X:120:ARG:CD   | 2.84                     | 0.51              |
| 9:T:55:GLN:OE1   | 14:2:163:ARG:NH1  | 2.42                     | 0.51              |
| 3:C:6:TYR:OH     | 4:D:9:ASP:OD2     | 2.28                     | 0.51              |
| 4:R:216:TRP:CD1  | 4:R:228:VAL:HA    | 2.45                     | 0.51              |
| 8:S:123:SER:HB3  | 8:S:137:VAL:HB    | 1.92                     | 0.51              |
| 12:W:104:ARG:HD3 | 12:W:139:LEU:HB2  | 1.92                     | 0.51              |
| 1:O:148:ASP:OD1  | 1:O:149:PRO:HD2   | 2.10                     | 0.51              |
| 4:R:142:SER:HB3  | 4:R:145:ASP:HB2   | 1.91                     | 0.51              |
| 8:S:2:SER:OG     | 8:S:3:ILE:N       | 2.43                     | 0.51              |
| 9:T:164:LEU:HB3  | 9:T:178:PHE:CD2   | 2.46                     | 0.51              |
| 11:V:72:LEU:HD11 | 11:V:79:ALA:HB1   | 1.92                     | 0.51              |
| 13:X:84:GLY:HA2  | 13:X:137:LEU:HD23 | 1.93                     | 0.51              |
| 12:Z:104:ARG:HD3 | 12:Z:139:LEU:HB2  | 1.92                     | 0.51              |
| 11:K:95:MET:HE3  | 11:K:237:VAL:HB   | 1.91                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:V:95:MET:HE2   | 11:V:242:VAL:HG13 | 1.93                     | 0.51              |
| 5:L:89:SER:HA     | 4:R:118:MET:HE1   | 1.92                     | 0.51              |
| 6:M:155:TYR:HE1   | 7:N:60:PHE:HE2    | 1.56                     | 0.51              |
| 13:X:138:ILE:HG13 | 13:X:166:LEU:HD12 | 1.93                     | 0.51              |
| 1:A:43:LEU:HD11   | 1:A:134:VAL:HG21  | 1.93                     | 0.51              |
| 7:N:3:ARG:O       | 7:N:6:ASP:HB3     | 2.10                     | 0.51              |
| 2:P:99:HIS:CE1    | 2:P:103:TYR:HD2   | 2.28                     | 0.51              |
| 13:1:84:GLY:HA2   | 13:1:137:LEU:HD23 | 1.93                     | 0.51              |
| 13:1:138:ILE:HG13 | 13:1:166:LEU:HD12 | 1.92                     | 0.51              |
| 14:2:138:TYR:CD2  | 14:2:146:ILE:HB   | 2.45                     | 0.51              |
| 7:G:2:SER:O       | 7:G:3:ARG:C       | 2.54                     | 0.51              |
| 9:I:164:LEU:HB3   | 9:I:178:PHE:CD2   | 2.46                     | 0.51              |
| 1:O:43:LEU:HD11   | 1:O:134:VAL:HG21  | 1.93                     | 0.51              |
| 3:Q:105:VAL:HG21  | 3:Q:136:GLY:HA3   | 1.91                     | 0.51              |
| 2:B:161:THR:HG1   | 3:C:78:THR:HG1    | 1.54                     | 0.51              |
| 4:D:180:LEU:HB2   | 4:D:182:MET:HE2   | 1.93                     | 0.51              |
| 7:G:60:PHE:HB3    | 7:G:61:PHE:CD2    | 2.46                     | 0.51              |
| 8:H:2:SER:OG      | 8:H:3:ILE:N       | 2.43                     | 0.51              |
| 11:K:95:MET:HE2   | 11:K:242:VAL:HG13 | 1.93                     | 0.51              |
| 14:Y:73:THR:HA    | 14:Y:105:LYS:HE2  | 1.93                     | 0.51              |
| 7:G:57:ASP:HB3    | 7:G:59:VAL:HG13   | 1.93                     | 0.51              |
| 8:H:26:ARG:HB3    | 8:H:37:THR:O      | 2.11                     | 0.51              |
| 6:M:22:ILE:HG21   | 6:M:152:SER:HB3   | 1.91                     | 0.51              |
| 8:S:28:PHE:HB2    | 8:S:39:PHE:HB2    | 1.92                     | 0.51              |
| 4:D:216:TRP:CD1   | 4:D:228:VAL:HA    | 2.45                     | 0.51              |
| 4:D:216:TRP:HE1   | 4:D:228:VAL:HG13  | 1.76                     | 0.51              |
| 7:N:21:VAL:HG11   | 7:N:153:SER:HB3   | 1.93                     | 0.51              |
| 10:U:161:ASP:OD1  | 10:U:162:SER:N    | 2.44                     | 0.51              |
| 14:Y:160:CYS:HA   | 14:Y:163:ARG:HG3  | 1.93                     | 0.51              |
| 4:D:216:TRP:HD1   | 4:D:228:VAL:HA    | 1.76                     | 0.50              |
| 7:G:21:VAL:HG11   | 7:G:153:SER:HB3   | 1.93                     | 0.50              |
| 8:H:198:ARG:HD3   | 13:X:250:VAL:HG21 | 1.92                     | 0.50              |
| 11:K:72:LEU:HD11  | 11:K:79:ALA:HB1   | 1.92                     | 0.50              |
| 8:S:26:ARG:HB3    | 8:S:37:THR:O      | 2.11                     | 0.50              |
| 9:I:8:GLN:HE21    | 9:I:113:PRO:HG2   | 1.76                     | 0.50              |
| 7:N:57:ASP:HB3    | 7:N:59:VAL:HG13   | 1.93                     | 0.50              |
| 7:N:76:VAL:HG13   | 7:N:132:VAL:HG13  | 1.94                     | 0.50              |
| 3:Q:72:ILE:HG22   | 3:Q:134:ILE:HG13  | 1.94                     | 0.50              |
| 12:W:103:VAL:HG13 | 12:W:118:LEU:HD12 | 1.93                     | 0.50              |
| 1:A:5:ARG:HH12    | 7:G:8:ARG:HD3     | 1.75                     | 0.50              |
| 3:C:45:VAL:HG22   | 3:C:214:ILE:HG12  | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:74:LEU:HD13   | 6:F:136:ILE:HG12  | 1.94                     | 0.50              |
| 7:G:33:THR:OG1    | 7:G:166:ASN:O     | 2.26                     | 0.50              |
| 7:G:151:ASP:OD1   | 7:G:155:ASN:N     | 2.36                     | 0.50              |
| 7:N:62:SER:OG     | 7:N:212:GLU:OE1   | 2.22                     | 0.50              |
| 9:T:185:ARG:CG    | 9:T:185:ARG:NH2   | 2.73                     | 0.50              |
| 10:U:215:VAL:HG22 | 13:X:63:SER:HB2   | 1.94                     | 0.50              |
| 2:B:129:ASP:HB2   | 2:B:130:PRO:HD2   | 1.94                     | 0.50              |
| 3:C:72:ILE:HG22   | 3:C:134:ILE:HG13  | 1.94                     | 0.50              |
| 8:H:28:PHE:HB2    | 8:H:39:PHE:HB2    | 1.92                     | 0.50              |
| 11:K:72:LEU:HD22  | 11:K:229:TYR:HB2  | 1.94                     | 0.50              |
| 11:K:78:LEU:HD13  | 12:Z:153:TYR:CE1  | 2.47                     | 0.50              |
| 5:L:56:VAL:HG13   | 5:L:61:LEU:HD23   | 1.94                     | 0.50              |
| 1:O:5:ARG:O       | 1:O:123:GLY:N     | 2.44                     | 0.50              |
| 9:I:145:ARG:NE    | 14:2:230:ARG:CD   | 2.75                     | 0.50              |
| 13:X:151:SER:O    | 13:X:158:TYR:HA   | 2.11                     | 0.50              |
| 13:X:60:THR:HB    | 13:X:64:VAL:O     | 2.12                     | 0.50              |
| 14:2:79:LYS:HE2   | 14:2:196:ASN:HA   | 1.94                     | 0.50              |
| 1:A:195:LEU:O     | 1:A:199:VAL:HG23  | 2.12                     | 0.50              |
| 2:B:97:GLN:HB3    | 14:Y:133:LYS:HG3  | 1.94                     | 0.50              |
| 7:G:235:GLN:HE21  | 7:G:239:LYS:HE3   | 1.77                     | 0.50              |
| 5:L:115:CYS:SG    | 5:L:140:LEU:HD12  | 2.52                     | 0.50              |
| 14:Y:79:LYS:HE2   | 14:Y:196:ASN:HA   | 1.94                     | 0.50              |
| 11:V:72:LEU:HD22  | 11:V:229:TYR:HB2  | 1.94                     | 0.49              |
| 3:C:67:ASP:OD1    | 3:C:68:ASN:N      | 2.42                     | 0.49              |
| 5:E:115:CYS:SG    | 5:E:140:LEU:HD12  | 2.52                     | 0.49              |
| 5:E:163:PHE:HB2   | 5:E:166:THR:HG22  | 1.94                     | 0.49              |
| 1:O:195:LEU:O     | 1:O:199:VAL:HG23  | 2.12                     | 0.49              |
| 3:Q:45:VAL:HG22   | 3:Q:214:ILE:HG12  | 1.93                     | 0.49              |
| 4:R:216:TRP:HD1   | 4:R:228:VAL:HA    | 1.76                     | 0.49              |
| 2:B:167:ALA:HB3   | 2:B:181:LEU:HD21  | 1.94                     | 0.49              |
| 2:P:167:ALA:HB3   | 2:P:181:LEU:HD21  | 1.94                     | 0.49              |
| 14:Y:110:ASN:OD1  | 14:Y:113:LEU:HD12 | 2.13                     | 0.49              |
| 5:E:56:VAL:HG13   | 5:E:61:LEU:HD23   | 1.94                     | 0.49              |
| 5:L:163:PHE:HB2   | 5:L:166:THR:HG22  | 1.94                     | 0.49              |
| 3:Q:120:THR:HG22  | 3:Q:127:PRO:HB3   | 1.94                     | 0.49              |
| 12:Z:103:VAL:HG13 | 12:Z:118:LEU:HD12 | 1.93                     | 0.49              |
| 3:C:122:ARG:HH21  | 6:F:4:ARG:HH22    | 1.60                     | 0.49              |
| 4:D:73:HIS:HE1    | 4:D:107:ILE:O     | 1.94                     | 0.49              |
| 14:2:110:ASN:OD1  | 14:2:113:LEU:HD12 | 2.13                     | 0.49              |
| 11:K:88:MET:HE2   | 11:K:96:LEU:HD23  | 1.95                     | 0.49              |
| 1:O:83:VAL:HG21   | 1:O:129:ILE:HD11  | 1.95                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:R:73:HIS:ND1    | 4:R:223:GLY:O     | 2.39                     | 0.49              |
| 4:R:216:TRP:HE1   | 4:R:228:VAL:HG13  | 1.76                     | 0.49              |
| 14:Y:169:MET:H    | 14:Y:188:GLU:HB3  | 1.78                     | 0.49              |
| 6:F:195:LEU:O     | 6:F:199:PHE:N     | 2.38                     | 0.49              |
| 7:G:76:VAL:HG13   | 7:G:132:VAL:HG13  | 1.94                     | 0.49              |
| 9:T:8:GLN:HE21    | 9:T:113:PRO:HG2   | 1.76                     | 0.49              |
| 7:G:3:ARG:O       | 7:G:5:TYR:N       | 2.46                     | 0.49              |
| 6:M:74:LEU:HD13   | 6:M:136:ILE:HG12  | 1.94                     | 0.49              |
| 8:S:130:PRO:HG3   | 13:1:96:ARG:HH22  | 1.78                     | 0.49              |
| 12:W:146:ILE:HD11 | 12:W:155:TYR:CD1  | 2.46                     | 0.49              |
| 13:X:87:VAL:HB    | 13:X:90:ASP:HB2   | 1.93                     | 0.49              |
| 14:Y:91:ARG:HH11  | 14:Y:98:ILE:HD13  | 1.77                     | 0.49              |
| 13:1:161:LEU:HD13 | 13:1:163:PHE:O    | 2.12                     | 0.49              |
| 5:L:103:TYR:C     | 13:1:120:ARG:HH12 | 2.20                     | 0.49              |
| 2:P:129:ASP:HB2   | 2:P:130:PRO:HD2   | 1.94                     | 0.49              |
| 9:T:166:GLU:OE1   | 14:Y:212:ASP:HB3  | 2.11                     | 0.49              |
| 3:C:121:GLN:NE2   | 4:D:132:PHE:HE1   | 2.11                     | 0.49              |
| 6:F:177:ARG:HE    | 6:F:190:THR:HG22  | 1.78                     | 0.49              |
| 7:G:161:ALA:HB1   | 7:G:175:LEU:HD13  | 1.95                     | 0.49              |
| 9:I:145:ARG:HG3   | 14:2:230:ARG:HD3  | 1.95                     | 0.49              |
| 10:J:161:ASP:OD1  | 10:J:162:SER:N    | 2.44                     | 0.49              |
| 14:2:169:MET:H    | 14:2:188:GLU:HB3  | 1.78                     | 0.49              |
| 1:A:5:ARG:O       | 1:A:123:GLY:N     | 2.44                     | 0.48              |
| 1:A:81:ARG:CZ     | 7:G:154:GLY:O     | 2.61                     | 0.48              |
| 2:B:85:ALA:HB2    | 2:B:139:VAL:HG21  | 1.94                     | 0.48              |
| 2:P:85:ALA:HB2    | 2:P:139:VAL:HG21  | 1.94                     | 0.48              |
| 9:T:145:ARG:NH1   | 14:Y:213:SER:OG   | 2.46                     | 0.48              |
| 10:U:55:THR:OG1   | 10:U:220:ALA:HB3  | 2.13                     | 0.48              |
| 13:X:238:SER:O    | 13:X:240:GLN:N    | 2.46                     | 0.48              |
| 7:G:100:GLN:HG2   | 9:I:86:ARG:HD3    | 1.94                     | 0.48              |
| 9:I:5:ILE:HD12    | 9:I:139:THR:HG21  | 1.95                     | 0.48              |
| 11:K:169:TYR:HB2  | 11:K:182:LEU:HD13 | 1.95                     | 0.48              |
| 9:T:175:LEU:HB3   | 9:T:178:PHE:CE1   | 2.49                     | 0.48              |
| 11:V:88:MET:HE2   | 11:V:96:LEU:HD23  | 1.95                     | 0.48              |
| 12:Z:58:HIS:CG    | 12:Z:59:GLN:H     | 2.31                     | 0.48              |
| 13:1:61:ASN:O     | 13:1:64:VAL:HG22  | 2.13                     | 0.48              |
| 3:C:107:ARG:NH2   | 11:K:119:GLU:HG3  | 2.26                     | 0.48              |
| 7:G:3:ARG:H       | 7:G:3:ARG:HD2     | 1.78                     | 0.48              |
| 8:S:16:GLY:HA3    | 8:S:163:LEU:HD11  | 1.95                     | 0.48              |
| 9:T:185:ARG:NH2   | 9:T:185:ARG:CB    | 2.76                     | 0.48              |
| 10:U:205:ASP:OD2  | 13:X:239:SER:CB   | 2.57                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:1:87:VAL:HB    | 13:1:90:ASP:HB2   | 1.93                     | 0.48              |
| 7:G:185:THR:O     | 7:G:189:ALA:N     | 2.45                     | 0.48              |
| 2:P:71:ASP:OD1    | 2:P:72:ALA:N      | 2.43                     | 0.48              |
| 8:S:101:GLY:N     | 8:S:102:PRO:HD3   | 2.29                     | 0.48              |
| 3:C:120:THR:HG22  | 3:C:127:PRO:HB3   | 1.94                     | 0.48              |
| 3:Q:195:LEU:O     | 3:Q:198:THR:OG1   | 2.30                     | 0.48              |
| 5:L:143:ILE:HG12  | 5:L:149:PRO:HA    | 1.95                     | 0.48              |
| 3:Q:182:CYS:SG    | 3:Q:190:HIS:NE2   | 2.86                     | 0.48              |
| 11:V:59:LEU:HD23  | 11:V:66:VAL:CG1   | 2.44                     | 0.48              |
| 11:V:223:TYR:HB3  | 12:W:49:ARG:HD3   | 1.96                     | 0.48              |
| 11:V:169:TYR:HB2  | 11:V:182:LEU:HD13 | 1.95                     | 0.48              |
| 1:A:83:VAL:HG21   | 1:A:129:ILE:HD11  | 1.95                     | 0.48              |
| 2:B:91:LYS:HG2    | 2:B:119:LEU:HD11  | 1.95                     | 0.48              |
| 9:I:175:LEU:HB3   | 9:I:178:PHE:CE1   | 2.49                     | 0.48              |
| 2:P:91:LYS:HG2    | 2:P:119:LEU:HD11  | 1.95                     | 0.48              |
| 13:X:61:ASN:O     | 13:X:64:VAL:HG22  | 2.13                     | 0.48              |
| 5:E:143:ILE:HG12  | 5:E:149:PRO:HA    | 1.95                     | 0.48              |
| 5:L:224:ASN:HD21  | 5:L:228:ARG:NE    | 2.12                     | 0.48              |
| 7:N:185:THR:O     | 7:N:189:ALA:N     | 2.45                     | 0.48              |
| 12:W:54:LEU:HD12  | 12:W:54:LEU:N     | 2.29                     | 0.48              |
| 13:X:174:ILE:HG23 | 13:X:175:ALA:N    | 2.28                     | 0.48              |
| 12:Z:217:TYR:CZ   | 12:Z:219:GLU:HB2  | 2.49                     | 0.48              |
| 8:H:44:PRO:HA     | 8:H:50:TYR:CD1    | 2.49                     | 0.47              |
| 8:H:125:ASP:OD1   | 8:H:126:LEU:N     | 2.44                     | 0.47              |
| 10:J:55:THR:OG1   | 10:J:220:ALA:HB3  | 2.13                     | 0.47              |
| 12:W:124:ASP:OD1  | 12:W:128:GLY:N    | 2.46                     | 0.47              |
| 13:X:90:ASP:HB3   | 13:X:133:VAL:HG13 | 1.95                     | 0.47              |
| 4:D:149:LEU:HD22  | 4:D:161:TYR:HB2   | 1.96                     | 0.47              |
| 8:H:16:GLY:HA3    | 8:H:163:LEU:HD11  | 1.95                     | 0.47              |
| 8:S:44:PRO:HA     | 8:S:50:TYR:CD1    | 2.48                     | 0.47              |
| 5:E:206:LEU:HD12  | 5:E:210:PHE:HZ    | 1.79                     | 0.47              |
| 3:C:182:CYS:SG    | 3:C:190:HIS:NE2   | 2.86                     | 0.47              |
| 4:D:71:ASP:OD1    | 4:D:72:ARG:N      | 2.45                     | 0.47              |
| 5:E:93:ARG:HE     | 5:E:121:ILE:HG21  | 1.79                     | 0.47              |
| 1:O:144:LEU:HD22  | 1:O:156:TRP:HB2   | 1.97                     | 0.47              |
| 9:T:141:SER:HB3   | 14:Y:210:VAL:HG23 | 1.96                     | 0.47              |
| 12:Z:152:THR:HA   | 12:Z:155:TYR:HE2  | 1.79                     | 0.47              |
| 8:H:199:THR:HB    | 13:X:252:SER:HB2  | 1.97                     | 0.47              |
| 7:N:161:ALA:HB1   | 7:N:175:LEU:HD13  | 1.95                     | 0.47              |
| 8:S:125:ASP:OD1   | 8:S:126:LEU:N     | 2.44                     | 0.47              |
| 8:S:145:GLN:NE2   | 14:Y:97:TYR:HD1   | 2.12                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:Z:124:ASP:OD1  | 12:Z:128:GLY:N    | 2.46                     | 0.47              |
| 13:1:185:MET:HE1  | 13:1:193:LEU:HD13 | 1.96                     | 0.47              |
| 5:E:47:CYS:HB3    | 5:E:221:THR:HG22  | 1.97                     | 0.47              |
| 6:F:143:ARG:NH2   | 6:F:145:TYR:OH    | 2.32                     | 0.47              |
| 3:Q:52:ALA:HB2    | 3:Q:59:HIS:NE2    | 2.30                     | 0.47              |
| 8:S:129:CYS:HB2   | 13:1:89:ALA:HB2   | 1.97                     | 0.47              |
| 9:T:5:ILE:HD12    | 9:T:139:THR:HG21  | 1.95                     | 0.47              |
| 10:U:120:LEU:HD23 | 10:U:152:PHE:CE2  | 2.49                     | 0.47              |
| 14:Y:131:LEU:HD22 | 14:Y:155:LEU:HB2  | 1.96                     | 0.47              |
| 14:2:91:ARG:NH2   | 14:2:240:SER:O    | 2.48                     | 0.47              |
| 11:K:106:GLN:HA   | 11:K:109:LYS:HB3  | 1.97                     | 0.47              |
| 4:R:73:HIS:HD1    | 4:R:223:GLY:C     | 2.22                     | 0.47              |
| 13:X:148:GLN:HG2  | 13:X:160:ARG:HH21 | 1.80                     | 0.47              |
| 2:P:97:GLN:HB3    | 14:2:133:LYS:HG3  | 1.95                     | 0.47              |
| 12:W:96:VAL:HB    | 12:W:130:GLN:OE1  | 2.14                     | 0.47              |
| 12:W:217:TYR:CZ   | 12:W:219:GLU:HB2  | 2.49                     | 0.47              |
| 4:D:41:ARG:HE     | 4:D:162:TRP:HA    | 1.80                     | 0.47              |
| 4:D:88:LEU:HD13   | 4:D:136:PHE:CE2   | 2.50                     | 0.47              |
| 9:I:4:LEU:HD22    | 9:I:45:LEU:HB3    | 1.97                     | 0.47              |
| 3:Q:67:ASP:OD1    | 3:Q:68:ASN:N      | 2.42                     | 0.47              |
| 8:H:98:LYS:HG3    | 8:H:103:TYR:CE2   | 2.50                     | 0.46              |
| 8:S:98:LYS:HG3    | 8:S:103:TYR:CE2   | 2.51                     | 0.46              |
| 9:T:27:GLN:HE22   | 9:T:174:ASN:HB3   | 1.81                     | 0.46              |
| 10:U:56:ARG:HH21  | 10:U:219:ASP:CG   | 2.23                     | 0.46              |
| 4:R:144:ASN:ND2   | 12:Z:126:ARG:HH21 | 2.13                     | 0.46              |
| 4:R:149:LEU:HD22  | 4:R:161:TYR:HB2   | 1.96                     | 0.46              |
| 8:S:32:ALA:HA     | 14:Y:240:SER:OG   | 2.16                     | 0.46              |
| 9:T:19:ARG:HD3    | 9:T:177:THR:HG22  | 1.97                     | 0.46              |
| 12:Z:56:PRO:HB3   | 12:Z:62:TYR:CE1   | 2.49                     | 0.46              |
| 9:I:19:ARG:HD3    | 9:I:177:THR:HG22  | 1.97                     | 0.46              |
| 9:T:4:LEU:HD22    | 9:T:45:LEU:HB3    | 1.97                     | 0.46              |
| 12:Z:154:ILE:HG13 | 12:Z:154:ILE:O    | 2.15                     | 0.46              |
| 14:2:131:LEU:HD22 | 14:2:155:LEU:HB2  | 1.96                     | 0.46              |
| 1:A:78:ALA:HA     | 1:A:81:ARG:CZ     | 2.45                     | 0.46              |
| 3:C:52:ALA:HB2    | 3:C:59:HIS:NE2    | 2.30                     | 0.46              |
| 4:D:104:GLY:HA3   | 12:W:101:ASN:ND2  | 2.31                     | 0.46              |
| 11:K:260:ILE:HG12 | 13:1:161:LEU:HA   | 1.98                     | 0.46              |
| 5:L:47:CYS:HB3    | 5:L:221:THR:HG22  | 1.97                     | 0.46              |
| 7:N:137:ILE:HD12  | 7:N:216:LEU:HB2   | 1.97                     | 0.46              |
| 4:R:88:LEU:HD13   | 4:R:136:PHE:CE2   | 2.50                     | 0.46              |
| 10:U:150:TYR:HE1  | 10:U:160:ARG:HB2  | 1.81                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:V:117:ILE:O    | 11:V:121:LEU:HG   | 2.16                     | 0.46              |
| 13:X:185:MET:HE1  | 13:X:193:LEU:HD13 | 1.96                     | 0.46              |
| 5:E:141:ILE:HG22  | 5:E:151:VAL:HG22  | 1.98                     | 0.46              |
| 11:K:82:ARG:NH2   | 12:Z:219:GLU:O    | 2.48                     | 0.46              |
| 5:L:106:GLY:HA3   | 13:1:120:ARG:HD3  | 1.97                     | 0.46              |
| 5:L:206:LEU:HD12  | 5:L:210:PHE:HZ    | 1.79                     | 0.46              |
| 6:M:108:ALA:HA    | 6:M:147:PHE:HE2   | 1.80                     | 0.46              |
| 2:P:95:GLU:HG3    | 2:P:115:ALA:HB1   | 1.98                     | 0.46              |
| 13:X:136:SER:OG   | 13:X:166:LEU:HD13 | 2.16                     | 0.46              |
| 14:2:163:ARG:NH2  | 14:2:189:ASN:O    | 2.42                     | 0.46              |
| 6:F:11:THR:HG22   | 6:F:19:LEU:HD22   | 1.97                     | 0.46              |
| 7:G:28:ILE:HD13   | 7:G:133:SER:HB2   | 1.97                     | 0.46              |
| 7:G:90:LEU:HD21   | 7:G:114:LEU:HB2   | 1.98                     | 0.46              |
| 10:J:64:HIS:HB3   | 11:K:177:TYR:CZ   | 2.50                     | 0.46              |
| 10:J:221:LEU:HB3  | 10:J:236:VAL:HB   | 1.98                     | 0.46              |
| 5:L:126:THR:HG22  | 6:M:128:ARG:HH21  | 1.81                     | 0.46              |
| 6:M:11:THR:HG22   | 6:M:19:LEU:HD22   | 1.97                     | 0.46              |
| 7:N:4:ARG:C       | 7:N:6:ASP:H       | 2.23                     | 0.46              |
| 2:P:51:GLU:HA     | 2:P:215:ILE:HG22  | 1.97                     | 0.46              |
| 2:B:51:GLU:HA     | 2:B:215:ILE:HG22  | 1.97                     | 0.46              |
| 6:F:108:ALA:HA    | 6:F:147:PHE:HE2   | 1.80                     | 0.46              |
| 7:G:86:LEU:HD21   | 7:G:130:PHE:CD2   | 2.51                     | 0.46              |
| 5:L:141:ILE:HG22  | 5:L:151:VAL:HG22  | 1.98                     | 0.46              |
| 7:N:86:LEU:HD21   | 7:N:130:PHE:CD2   | 2.50                     | 0.46              |
| 10:U:117:ALA:HA   | 10:U:152:PHE:HZ   | 1.81                     | 0.46              |
| 12:W:54:LEU:N     | 12:W:54:LEU:CD1   | 2.78                     | 0.46              |
| 2:B:10:ARG:HB3    | 2:B:10:ARG:NH1    | 2.29                     | 0.46              |
| 7:G:62:SER:HB3    | 7:G:65:ILE:HB     | 1.98                     | 0.46              |
| 8:H:162:HIS:HD2   | 13:X:242:ARG:HD2  | 1.81                     | 0.46              |
| 2:P:129:ASP:OD1   | 2:P:132:ALA:N     | 2.49                     | 0.46              |
| 13:X:202:ILE:HG23 | 13:X:209:GLY:HA2  | 1.98                     | 0.46              |
| 1:A:144:LEU:HD22  | 1:A:156:TRP:HB2   | 1.97                     | 0.46              |
| 2:B:95:GLU:HG3    | 2:B:115:ALA:HB1   | 1.98                     | 0.46              |
| 1:O:88:ARG:HH11   | 9:T:70:ARG:HA     | 1.80                     | 0.46              |
| 1:A:98:VAL:HG13   | 14:Y:150:ALA:HB2  | 1.98                     | 0.45              |
| 2:B:18:GLU:OE1    | 2:B:20:ARG:NH2    | 2.46                     | 0.45              |
| 2:B:129:ASP:OD1   | 2:B:132:ALA:N     | 2.49                     | 0.45              |
| 9:I:145:ARG:NE    | 14:2:230:ARG:HD2  | 2.31                     | 0.45              |
| 4:R:41:ARG:HE     | 4:R:162:TRP:HA    | 1.80                     | 0.45              |
| 11:V:260:ILE:HG12 | 13:X:161:LEU:HA   | 1.98                     | 0.45              |
| 13:1:136:SER:OG   | 13:1:166:LEU:HD13 | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:2:79:LYS:HB3   | 14:2:84:VAL:HG22  | 1.99                     | 0.45              |
| 5:E:61:LEU:HD11   | 5:E:66:VAL:HG21   | 1.99                     | 0.45              |
| 6:F:102:GLN:HE22  | 13:X:96:ARG:HD3   | 1.81                     | 0.45              |
| 9:I:27:GLN:HE22   | 9:I:174:ASN:HB3   | 1.81                     | 0.45              |
| 10:J:150:TYR:HE1  | 10:J:160:ARG:HB2  | 1.81                     | 0.45              |
| 7:N:62:SER:HB3    | 7:N:65:ILE:HB     | 1.98                     | 0.45              |
| 7:N:197:LEU:O     | 7:N:201:MET:HG2   | 2.16                     | 0.45              |
| 5:E:163:PHE:CD2   | 5:E:166:THR:HG22  | 2.52                     | 0.45              |
| 6:F:155:TYR:HE1   | 7:G:60:PHE:HE2    | 1.63                     | 0.45              |
| 9:I:91:TYR:CZ     | 9:I:98:TYR:HE2    | 2.34                     | 0.45              |
| 11:V:106:GLN:HA   | 11:V:109:LYS:HB3  | 1.97                     | 0.45              |
| 13:1:58:ARG:HD2   | 13:1:65:VAL:HG22  | 1.98                     | 0.45              |
| 6:F:115:ALA:O     | 6:F:119:GLN:HG3   | 2.17                     | 0.45              |
| 11:K:117:ILE:O    | 11:K:121:LEU:HG   | 2.16                     | 0.45              |
| 5:L:163:PHE:CD2   | 5:L:166:THR:HG22  | 2.52                     | 0.45              |
| 6:M:115:ALA:O     | 6:M:119:GLN:HG3   | 2.17                     | 0.45              |
| 4:R:109:LEU:HD11  | 4:R:138:LEU:HB3   | 1.98                     | 0.45              |
| 8:S:99:ARG:HD3    | 8:S:127:ILE:HG23  | 1.99                     | 0.45              |
| 10:U:62:SER:HB2   | 11:V:189:TYR:HE1  | 1.82                     | 0.45              |
| 1:A:88:ARG:HH11   | 9:I:70:ARG:HA     | 1.80                     | 0.45              |
| 4:D:9:ASP:HB3     | 4:D:22:PHE:CD2    | 2.51                     | 0.45              |
| 7:G:137:ILE:HD12  | 7:G:216:LEU:HB2   | 1.97                     | 0.45              |
| 6:M:121:TYR:CD1   | 6:M:127:VAL:HG21  | 2.52                     | 0.45              |
| 7:N:4:ARG:C       | 7:N:6:ASP:N       | 2.74                     | 0.45              |
| 4:R:35:SER:HB3    | 4:R:66:ARG:HH12   | 1.82                     | 0.45              |
| 13:1:202:ILE:HG23 | 13:1:209:GLY:HA2  | 1.98                     | 0.45              |
| 1:A:88:ARG:NH1    | 9:I:70:ARG:HA     | 2.32                     | 0.45              |
| 6:F:121:TYR:HD1   | 6:F:127:VAL:HG21  | 1.82                     | 0.45              |
| 10:J:56:ARG:HH21  | 10:J:219:ASP:CG   | 2.23                     | 0.45              |
| 5:L:150:GLN:HB3   | 5:L:152:TYR:HE2   | 1.82                     | 0.45              |
| 7:N:28:ILE:HD13   | 7:N:133:SER:HB2   | 1.97                     | 0.45              |
| 11:V:167:LEU:HG   | 11:V:182:LEU:HD12 | 1.99                     | 0.45              |
| 12:Z:27:GLU:HA    | 12:Z:32:VAL:HG12  | 1.98                     | 0.45              |
| 9:I:21:ALA:HB3    | 9:I:29:LYS:HB3    | 1.98                     | 0.45              |
| 10:J:117:ALA:HA   | 10:J:152:PHE:HZ   | 1.81                     | 0.45              |
| 10:U:159:GLN:HG3  | 14:2:103:VAL:HG22 | 1.99                     | 0.45              |
| 13:X:58:ARG:HD2   | 13:X:65:VAL:HG22  | 1.98                     | 0.45              |
| 9:I:145:ARG:NE    | 14:2:230:ARG:HD3  | 2.32                     | 0.45              |
| 11:K:57:LEU:HD21  | 11:K:191:ALA:HB3  | 1.99                     | 0.45              |
| 11:K:167:LEU:HG   | 11:K:182:LEU:HD12 | 1.99                     | 0.45              |
| 5:L:113:MET:SD    | 13:1:109:THR:HA   | 2.57                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:109:LEU:HD11  | 4:D:138:LEU:HB3   | 1.98                     | 0.45              |
| 4:D:141:TYR:CG    | 4:D:218:GLY:HA2   | 2.52                     | 0.45              |
| 6:F:88:HIS:CE1    | 6:F:92:LYS:HE3    | 2.52                     | 0.45              |
| 9:I:18:ASP:HB2    | 9:I:175:LEU:HD22  | 1.99                     | 0.45              |
| 7:N:90:LEU:HD21   | 7:N:114:LEU:HB2   | 1.98                     | 0.45              |
| 11:V:57:LEU:HD21  | 11:V:191:ALA:HB3  | 1.99                     | 0.45              |
| 12:W:27:GLU:HA    | 12:W:32:VAL:HG12  | 1.98                     | 0.45              |
| 5:E:190:THR:H     | 5:E:193:GLN:HB3   | 1.82                     | 0.45              |
| 5:L:113:MET:HG3   | 13:1:109:THR:HG22 | 1.99                     | 0.45              |
| 6:M:121:TYR:HD1   | 6:M:127:VAL:HG21  | 1.82                     | 0.45              |
| 7:N:14:PRO:HA     | 1:O:21:TYR:CE1    | 2.52                     | 0.45              |
| 4:R:99:PHE:CE1    | 4:R:103:PHE:HD2   | 2.35                     | 0.45              |
| 13:X:233:LYS:CB   | 13:X:234:PRO:HD3  | 2.39                     | 0.45              |
| 14:2:184:TYR:CE1  | 14:2:194:SER:HB3  | 2.52                     | 0.45              |
| 5:L:73:THR:HG22   | 5:L:76:ILE:HB     | 1.98                     | 0.44              |
| 8:S:34:MET:HE1    | 14:Y:237:HIS:NE2  | 2.32                     | 0.44              |
| 9:T:21:ALA:HB3    | 9:T:29:LYS:HB3    | 1.98                     | 0.44              |
| 10:U:221:LEU:HB3  | 10:U:236:VAL:HB   | 1.98                     | 0.44              |
| 12:W:58:HIS:O     | 12:W:59:GLN:C     | 2.58                     | 0.44              |
| 2:B:10:ARG:O      | 2:B:11:GLY:C      | 2.60                     | 0.44              |
| 8:H:99:ARG:HD3    | 8:H:127:ILE:HG23  | 1.98                     | 0.44              |
| 10:J:183:PHE:HE2  | 10:J:192:VAL:H    | 1.64                     | 0.44              |
| 11:K:53:GLY:O     | 11:K:227:ARG:NH1  | 2.49                     | 0.44              |
| 4:R:141:TYR:CG    | 4:R:218:GLY:HA2   | 2.52                     | 0.44              |
| 9:T:18:ASP:HB2    | 9:T:175:LEU:HD22  | 1.98                     | 0.44              |
| 14:Y:136:ARG:NH2  | 14:Y:140:LEU:HD21 | 2.33                     | 0.44              |
| 3:C:69:HIS:CD2    | 3:C:70:ILE:HG13   | 2.52                     | 0.44              |
| 6:F:121:TYR:CD1   | 6:F:127:VAL:HG21  | 2.52                     | 0.44              |
| 2:P:209:LYS:O     | 2:P:214:ASN:ND2   | 2.51                     | 0.44              |
| 3:Q:40:SER:HB3    | 3:Q:187:LEU:HD12  | 2.00                     | 0.44              |
| 14:Y:79:LYS:HB3   | 14:Y:84:VAL:HG22  | 1.98                     | 0.44              |
| 14:Y:100:THR:HG22 | 14:Y:101:LEU:N    | 2.31                     | 0.44              |
| 7:G:197:LEU:O     | 7:G:201:MET:HG2   | 2.16                     | 0.44              |
| 8:H:34:MET:HG2    | 8:H:35:VAL:N      | 2.33                     | 0.44              |
| 8:S:203:ARG:HA    | 14:Y:265:SER:OG   | 2.17                     | 0.44              |
| 13:X:233:LYS:HB3  | 13:X:234:PRO:CD   | 2.41                     | 0.44              |
| 5:E:72:ILE:HG21   | 5:E:114:LEU:HD21  | 2.00                     | 0.44              |
| 5:E:123:GLN:NE2   | 6:F:81:PRO:O      | 2.50                     | 0.44              |
| 5:E:150:GLN:HB3   | 5:E:152:TYR:HE2   | 1.82                     | 0.44              |
| 5:L:190:THR:H     | 5:L:193:GLN:HB3   | 1.82                     | 0.44              |
| 1:O:158:ALA:HB3   | 2:P:58:LEU:HD13   | 1.99                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:80:ALA:HA     | 1:A:129:ILE:HD13 | 2.00                     | 0.44              |
| 4:D:35:SER:HB3    | 4:D:66:ARG:HH12  | 1.82                     | 0.44              |
| 4:D:99:PHE:CE1    | 4:D:103:PHE:HD2  | 2.35                     | 0.44              |
| 7:G:41:ASP:O      | 7:G:186:LEU:HB2  | 2.18                     | 0.44              |
| 11:K:54:THR:H     | 11:K:86:ARG:NH2  | 2.15                     | 0.44              |
| 5:L:61:LEU:HD11   | 5:L:66:VAL:HG21  | 1.99                     | 0.44              |
| 4:R:9:ASP:HB3     | 4:R:22:PHE:CD2   | 2.51                     | 0.44              |
| 10:U:183:PHE:HE2  | 10:U:192:VAL:H   | 1.64                     | 0.44              |
| 11:V:130:PRO:HB2  | 11:V:166:PHE:CD2 | 2.53                     | 0.44              |
| 11:V:167:LEU:O    | 11:V:178:GLU:HG3 | 2.18                     | 0.44              |
| 14:Y:184:TYR:CE1  | 14:Y:194:SER:HB3 | 2.52                     | 0.44              |
| 4:D:191:VAL:HG21  | 4:D:216:TRP:CZ2  | 2.53                     | 0.44              |
| 8:H:49:LEU:HD21   | 8:H:87:LEU:HD22  | 2.00                     | 0.44              |
| 8:H:140:GLY:N     | 8:H:143:THR:HG22 | 2.33                     | 0.44              |
| 10:J:212:GLU:HB3  | 13:1:68:LYS:HE3  | 2.00                     | 0.44              |
| 12:Z:58:HIS:CD2   | 12:Z:94:PRO:HD2  | 2.53                     | 0.44              |
| 12:Z:152:THR:HA   | 12:Z:155:TYR:CE2 | 2.53                     | 0.44              |
| 10:J:120:LEU:HD23 | 10:J:152:PHE:CE2 | 2.49                     | 0.44              |
| 8:S:34:MET:HG2    | 8:S:35:VAL:N     | 2.33                     | 0.44              |
| 2:B:71:ASP:OD1    | 2:B:72:ALA:N     | 2.43                     | 0.44              |
| 3:C:40:SER:HB3    | 3:C:187:LEU:HD12 | 1.99                     | 0.44              |
| 5:E:73:THR:HG22   | 5:E:76:ILE:HB    | 1.98                     | 0.44              |
| 7:N:41:ASP:O      | 7:N:186:LEU:HB2  | 2.18                     | 0.44              |
| 2:P:68:VAL:HG21   | 2:P:89:ILE:HD13  | 1.99                     | 0.44              |
| 11:V:54:THR:H     | 11:V:86:ARG:NH2  | 2.15                     | 0.44              |
| 14:Y:124:CYS:O    | 14:Y:128:GLU:CG  | 2.61                     | 0.44              |
| 3:C:89:ARG:NH1    | 10:J:105:HIS:HB3 | 2.31                     | 0.43              |
| 4:D:76:MET:HE3    | 4:D:136:PHE:CD1  | 2.53                     | 0.43              |
| 11:K:59:LEU:C     | 11:K:59:LEU:CD1  | 2.86                     | 0.43              |
| 11:K:130:PRO:HB2  | 11:K:166:PHE:CD2 | 2.53                     | 0.43              |
| 11:K:167:LEU:O    | 11:K:178:GLU:HG3 | 2.18                     | 0.43              |
| 4:R:151:MET:O     | 4:R:158:SER:HA   | 2.18                     | 0.43              |
| 11:V:53:GLY:O     | 11:V:227:ARG:NH1 | 2.49                     | 0.43              |
| 14:2:204:ASN:OD1  | 14:2:205:SER:N   | 2.52                     | 0.43              |
| 1:A:57:ARG:NH1    | 7:G:108:GLU:OE2  | 2.41                     | 0.43              |
| 2:B:161:THR:HG21  | 3:C:60:GLN:HE21  | 1.83                     | 0.43              |
| 7:G:174:MET:SD    | 7:G:199:LYS:HD3  | 2.58                     | 0.43              |
| 4:R:76:MET:HE3    | 4:R:136:PHE:CD1  | 2.53                     | 0.43              |
| 13:X:77:ALA:HB3   | 13:X:80:ILE:HB   | 2.00                     | 0.43              |
| 13:1:77:ALA:HB3   | 13:1:80:ILE:HB   | 2.01                     | 0.43              |
| 3:C:103:LEU:HD12  | 3:C:104:PRO:HD2  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 8:H:53:LEU:HB2    | 8:H:60:VAL:HG13  | 2.00                     | 0.43              |
| 11:K:192:GLN:HE21 | 11:K:196:ARG:HG3 | 1.84                     | 0.43              |
| 6:M:15:PRO:HA     | 7:N:23:TYR:CE1   | 2.54                     | 0.43              |
| 11:V:78:LEU:HG    | 12:W:153:TYR:CE1 | 2.53                     | 0.43              |
| 14:Y:204:ASN:OD1  | 14:Y:205:SER:N   | 2.52                     | 0.43              |
| 1:O:10:PHE:HE2    | 2:P:136:PRO:HG2  | 1.83                     | 0.43              |
| 1:O:98:VAL:HG13   | 14:2:150:ALA:HB2 | 2.01                     | 0.43              |
| 9:T:139:THR:O     | 9:T:142:ILE:N    | 2.50                     | 0.43              |
| 13:X:158:TYR:O    | 13:X:158:TYR:CG  | 2.70                     | 0.43              |
| 4:D:35:SER:HB3    | 4:D:66:ARG:NH1   | 2.33                     | 0.43              |
| 4:D:88:LEU:HD21   | 4:D:132:PHE:CE2  | 2.54                     | 0.43              |
| 4:D:151:MET:O     | 4:D:158:SER:HA   | 2.17                     | 0.43              |
| 11:K:88:MET:HE3   | 11:K:90:VAL:HG22 | 2.00                     | 0.43              |
| 6:M:8:PHE:CZ      | 7:N:9:THR:HG23   | 2.53                     | 0.43              |
| 7:N:136:TYR:HB2   | 7:N:148:TYR:HB2  | 2.00                     | 0.43              |
| 7:N:136:TYR:O     | 7:N:147:LEU:HD12 | 2.19                     | 0.43              |
| 9:T:13:VAL:HG11   | 9:T:105:ALA:HB1  | 2.01                     | 0.43              |
| 14:2:100:THR:HG22 | 14:2:101:LEU:N   | 2.32                     | 0.43              |
| 2:B:209:LYS:O     | 2:B:214:ASN:ND2  | 2.51                     | 0.43              |
| 7:G:136:TYR:O     | 7:G:147:LEU:HD12 | 2.19                     | 0.43              |
| 5:L:72:ILE:HG21   | 5:L:114:LEU:HD21 | 2.00                     | 0.43              |
| 2:P:18:GLU:OE1    | 2:P:20:ARG:NH2   | 2.47                     | 0.43              |
| 4:R:71:ASP:OD1    | 4:R:72:ARG:N     | 2.46                     | 0.43              |
| 4:R:88:LEU:HD21   | 4:R:132:PHE:CE2  | 2.54                     | 0.43              |
| 8:S:49:LEU:HD21   | 8:S:87:LEU:HD22  | 2.00                     | 0.43              |
| 12:W:132:TYR:HA   | 12:W:140:ILE:O   | 2.18                     | 0.43              |
| 2:B:68:VAL:HG21   | 2:B:89:ILE:HD13  | 1.99                     | 0.43              |
| 10:J:222:LYS:HE3  | 10:J:224:CYS:SG  | 2.57                     | 0.43              |
| 7:N:33:THR:OG1    | 7:N:166:ASN:O    | 2.26                     | 0.43              |
| 1:O:66:ASP:OD1    | 1:O:67:ASP:N     | 2.45                     | 0.43              |
| 1:O:80:ALA:HA     | 1:O:129:ILE:HD13 | 2.00                     | 0.43              |
| 1:O:103:THR:HG22  | 1:O:105:GLU:H    | 1.84                     | 0.43              |
| 13:X:47:PHE:HE2   | 13:X:52:ILE:HG13 | 1.84                     | 0.43              |
| 12:Z:146:ILE:HD11 | 12:Z:155:TYR:CE1 | 2.54                     | 0.43              |
| 1:A:66:ASP:OD1    | 1:A:67:ASP:N     | 2.45                     | 0.43              |
| 7:G:136:TYR:HB2   | 7:G:148:TYR:HB2  | 2.00                     | 0.43              |
| 7:G:224:VAL:HG12  | 7:G:226:ARG:HG3  | 2.01                     | 0.43              |
| 6:M:159:LYS:HB3   | 6:M:178:TYR:CZ   | 2.53                     | 0.43              |
| 4:R:89:ALA:O      | 4:R:93:ARG:HG3   | 2.19                     | 0.43              |
| 11:V:88:MET:HE3   | 11:V:90:VAL:HG22 | 2.00                     | 0.43              |
| 14:Y:183:LEU:HD22 | 14:Y:198:PHE:HD2 | 1.84                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:C:155:ASP:HB3   | 4:D:63:SER:HB2   | 2.00                     | 0.43              |
| 4:D:89:ALA:O      | 4:D:93:ARG:HG3   | 2.19                     | 0.43              |
| 6:F:107:THR:OG1   | 6:F:138:GLY:HA3  | 2.19                     | 0.43              |
| 6:F:159:LYS:HB3   | 6:F:178:TYR:CZ   | 2.54                     | 0.43              |
| 7:G:63:GLU:O      | 7:G:64:LYS:HB2   | 2.19                     | 0.43              |
| 11:K:50:MET:O     | 11:K:51:VAL:HB   | 2.18                     | 0.43              |
| 5:L:224:ASN:HD21  | 5:L:228:ARG:HD2  | 1.84                     | 0.43              |
| 7:N:97:TYR:CE2    | 7:N:105:ILE:HA   | 2.54                     | 0.43              |
| 11:V:134:HIS:CE1  | 11:V:176:ALA:HB1 | 2.54                     | 0.43              |
| 1:A:103:THR:HG22  | 1:A:105:GLU:H    | 1.84                     | 0.43              |
| 2:B:154:PHE:CD1   | 2:B:164:GLN:HA   | 2.54                     | 0.43              |
| 11:K:134:HIS:CE1  | 11:K:176:ALA:HB1 | 2.54                     | 0.43              |
| 5:L:49:VAL:HG11   | 5:L:195:VAL:HG22 | 2.00                     | 0.43              |
| 5:L:224:ASN:HD21  | 5:L:228:ARG:CD   | 2.31                     | 0.43              |
| 6:M:82:ASP:CG     | 6:M:128:ARG:HH22 | 2.27                     | 0.43              |
| 3:Q:137:TYR:CZ    | 3:Q:217:LYS:HA   | 2.54                     | 0.43              |
| 13:X:161:LEU:HD13 | 13:X:163:PHE:C   | 2.44                     | 0.43              |
| 13:1:47:PHE:HE2   | 13:1:52:ILE:HG13 | 1.84                     | 0.43              |
| 6:M:107:THR:OG1   | 6:M:138:GLY:HA3  | 2.19                     | 0.42              |
| 7:N:100:GLN:HE21  | 9:T:86:ARG:NH1   | 2.17                     | 0.42              |
| 13:1:123:ARG:HD3  | 13:1:158:TYR:CD2 | 2.53                     | 0.42              |
| 2:B:110:GLU:HA    | 2:B:154:PHE:CE2  | 2.53                     | 0.42              |
| 3:C:98:VAL:HA     | 11:K:139:ARG:HG3 | 2.01                     | 0.42              |
| 3:C:137:TYR:CZ    | 3:C:217:LYS:HA   | 2.54                     | 0.42              |
| 4:D:40:ILE:HD11   | 4:D:182:MET:CG   | 2.47                     | 0.42              |
| 8:H:66:ARG:NE     | 8:H:103:TYR:OH   | 2.52                     | 0.42              |
| 4:R:35:SER:HB3    | 4:R:66:ARG:NH1   | 2.34                     | 0.42              |
| 9:T:138:LEU:HD23  | 14:Y:205:SER:O   | 2.19                     | 0.42              |
| 1:A:78:ALA:HA     | 1:A:81:ARG:NH1   | 2.35                     | 0.42              |
| 4:D:102:ASN:HA    | 12:W:105:ASN:ND2 | 2.34                     | 0.42              |
| 11:K:193:PRO:HG3  | 13:1:172:ALA:HA  | 2.01                     | 0.42              |
| 8:S:53:LEU:HB2    | 8:S:60:VAL:HG13  | 2.00                     | 0.42              |
| 10:U:35:PHE:HZ    | 10:U:168:SER:HB3 | 1.84                     | 0.42              |
| 13:1:161:LEU:HD13 | 13:1:163:PHE:C   | 2.44                     | 0.42              |
| 5:E:49:VAL:HG11   | 5:E:195:VAL:HG22 | 2.00                     | 0.42              |
| 5:E:119:ALA:O     | 5:E:123:GLN:HG3  | 2.19                     | 0.42              |
| 6:F:82:ASP:CG     | 6:F:128:ARG:HH22 | 2.27                     | 0.42              |
| 14:Y:245:VAL:HG12 | 14:Y:263:ASP:HA  | 2.00                     | 0.42              |
| 13:1:233:LYS:HB3  | 13:1:234:PRO:HD3 | 2.01                     | 0.42              |
| 7:G:97:TYR:CE2    | 7:G:105:ILE:HA   | 2.54                     | 0.42              |
| 5:L:18:PRO:HA     | 6:M:24:TYR:CD1   | 2.53                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:N:90:LEU:HD21   | 7:N:114:LEU:HD22 | 2.01                     | 0.42              |
| 2:P:91:LYS:HG2    | 2:P:119:LEU:CD1  | 2.50                     | 0.42              |
| 9:T:168:GLN:HG3   | 9:T:196:PHE:HD2  | 1.85                     | 0.42              |
| 14:2:245:VAL:HG12 | 14:2:263:ASP:HA  | 2.00                     | 0.42              |
| 6:F:76:TYR:HB2    | 6:F:132:VAL:HG13 | 2.01                     | 0.42              |
| 3:Q:103:LEU:HD12  | 3:Q:104:PRO:HD2  | 2.00                     | 0.42              |
| 8:S:66:ARG:NE     | 8:S:103:TYR:OH   | 2.52                     | 0.42              |
| 13:X:41:THR:H     | 13:X:56:ASP:CG   | 2.28                     | 0.42              |
| 13:X:174:ILE:CG2  | 13:X:175:ALA:N   | 2.82                     | 0.42              |
| 4:D:73:HIS:NE2    | 4:D:106:ASN:HB3  | 2.34                     | 0.42              |
| 2:P:154:PHE:CD1   | 2:P:164:GLN:HA   | 2.54                     | 0.42              |
| 7:N:123:GLN:HG3   | 1:O:125:ARG:HB3  | 2.01                     | 0.42              |
| 3:Q:214:ILE:O     | 3:Q:221:PHE:HA   | 2.20                     | 0.42              |
| 4:R:187:CYS:SG    | 4:R:220:ILE:HD11 | 2.59                     | 0.42              |
| 10:U:42:ALA:HA    | 10:U:50:ILE:O    | 2.20                     | 0.42              |
| 14:Y:159:MET:HE2  | 14:Y:169:MET:HG2 | 2.01                     | 0.42              |
| 14:Y:168:SER:HA   | 14:Y:188:GLU:OE1 | 2.20                     | 0.42              |
| 12:Z:28:PHE:CE2   | 12:Z:33:VAL:HG23 | 2.53                     | 0.42              |
| 13:1:205:ASP:OD1  | 13:1:206:LEU:N   | 2.53                     | 0.42              |
| 5:E:163:PHE:HD2   | 5:E:166:THR:HG22 | 1.85                     | 0.42              |
| 6:F:76:TYR:HB3    | 6:F:83:TYR:CD1   | 2.55                     | 0.42              |
| 9:I:13:VAL:HG11   | 9:I:105:ALA:HB1  | 2.01                     | 0.42              |
| 9:I:168:GLN:HG3   | 9:I:196:PHE:HD2  | 1.85                     | 0.42              |
| 5:L:163:PHE:HD2   | 5:L:166:THR:HG22 | 1.85                     | 0.42              |
| 6:M:49:GLU:HB2    | 6:M:195:LEU:HD23 | 2.01                     | 0.42              |
| 6:M:76:TYR:HB3    | 6:M:83:TYR:CD1   | 2.55                     | 0.42              |
| 4:R:104:GLY:HA3   | 12:Z:101:ASN:ND2 | 2.35                     | 0.42              |
| 8:S:201:LYS:HB3   | 13:1:249:PRO:O   | 2.19                     | 0.42              |
| 9:I:35:MET:HG2    | 9:I:45:LEU:CD2   | 2.50                     | 0.42              |
| 10:J:56:ARG:NH1   | 10:J:215:VAL:O   | 2.53                     | 0.42              |
| 5:L:119:ALA:O     | 5:L:123:GLN:HG3  | 2.19                     | 0.42              |
| 7:N:63:GLU:O      | 7:N:64:LYS:HB2   | 2.19                     | 0.42              |
| 3:Q:27:GLU:O      | 3:Q:31:GLN:HG2   | 2.20                     | 0.42              |
| 2:B:91:LYS:HG2    | 2:B:119:LEU:CD1  | 2.50                     | 0.41              |
| 6:F:49:GLU:HB2    | 6:F:195:LEU:HD23 | 2.01                     | 0.41              |
| 9:I:108:ASP:OD2   | 9:I:111:GLU:N    | 2.45                     | 0.41              |
| 7:N:2:SER:O       | 7:N:4:ARG:N      | 2.53                     | 0.41              |
| 9:T:35:MET:HG2    | 9:T:45:LEU:CD2   | 2.50                     | 0.41              |
| 1:A:91:CYS:HA     | 1:A:102:VAL:HG21 | 2.02                     | 0.41              |
| 8:H:142:CYS:O     | 8:H:143:THR:C    | 2.61                     | 0.41              |
| 9:I:101:ASN:HB3   | 9:I:132:HIS:ND1  | 2.36                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:P:167:ALA:CB    | 2:P:181:LEU:HD21  | 2.51                     | 0.41              |
| 9:T:91:TYR:CD2    | 9:T:98:TYR:CE2    | 3.08                     | 0.41              |
| 11:V:192:GLN:HE21 | 11:V:196:ARG:HG3  | 1.83                     | 0.41              |
| 14:2:159:MET:HE2  | 14:2:169:MET:HG2  | 2.01                     | 0.41              |
| 8:H:50:TYR:CD2    | 8:H:190:ILE:HD11  | 2.55                     | 0.41              |
| 9:I:139:THR:O     | 9:I:142:ILE:N     | 2.50                     | 0.41              |
| 11:K:139:ARG:HA   | 11:K:139:ARG:HD3  | 1.77                     | 0.41              |
| 6:M:143:ARG:NH2   | 7:N:59:VAL:HG12   | 2.35                     | 0.41              |
| 3:Q:107:ARG:HE    | 11:V:122:LEU:HD23 | 1.85                     | 0.41              |
| 11:V:59:LEU:HD23  | 11:V:66:VAL:HG12  | 2.02                     | 0.41              |
| 1:A:186:LEU:HA    | 1:A:189:LYS:HB2   | 2.02                     | 0.41              |
| 3:C:27:GLU:O      | 3:C:31:GLN:HG2    | 2.20                     | 0.41              |
| 6:M:213:CYS:HB2   | 6:M:218:PHE:HD1   | 1.85                     | 0.41              |
| 7:N:45:LEU:N      | 7:N:214:ALA:O     | 2.48                     | 0.41              |
| 3:Q:212:ILE:HD11  | 3:Q:224:TYR:HD2   | 1.86                     | 0.41              |
| 4:R:162:TRP:HB3   | 4:R:182:MET:SD    | 2.60                     | 0.41              |
| 10:U:56:ARG:NH1   | 10:U:215:VAL:O    | 2.53                     | 0.41              |
| 13:X:205:ASP:OD1  | 13:X:206:LEU:N    | 2.53                     | 0.41              |
| 13:1:151:SER:O    | 13:1:158:TYR:HA   | 2.20                     | 0.41              |
| 9:I:173:LEU:HD22  | 9:T:172:ILE:HG22  | 2.01                     | 0.41              |
| 11:K:188:ALA:HA   | 11:K:192:GLN:HB2  | 2.03                     | 0.41              |
| 12:W:127:GLU:HB2  | 12:W:130:GLN:NE2  | 2.35                     | 0.41              |
| 13:X:158:TYR:CD1  | 13:X:158:TYR:O    | 2.74                     | 0.41              |
| 12:Z:132:TYR:HA   | 12:Z:140:ILE:O    | 2.21                     | 0.41              |
| 2:B:10:ARG:C      | 2:B:11:GLY:O      | 2.63                     | 0.41              |
| 8:S:50:TYR:CD2    | 8:S:190:ILE:HD11  | 2.55                     | 0.41              |
| 9:T:5:ILE:HD11    | 9:T:143:LEU:HD11  | 2.02                     | 0.41              |
| 9:T:29:LYS:HD3    | 9:T:32:HIS:HB2    | 2.03                     | 0.41              |
| 2:B:66:LYS:HE2    | 2:B:82:ILE:HD11   | 2.03                     | 0.41              |
| 2:B:167:ALA:CB    | 2:B:181:LEU:HD21  | 2.51                     | 0.41              |
| 7:G:45:LEU:N      | 7:G:214:ALA:O     | 2.48                     | 0.41              |
| 7:G:99:LEU:HD12   | 8:H:65:GLN:HB3    | 2.03                     | 0.41              |
| 8:S:36:THR:HG21   | 9:T:125:ALA:HB1   | 2.01                     | 0.41              |
| 9:T:3:TYR:OH      | 9:T:139:THR:HG21  | 2.21                     | 0.41              |
| 11:V:193:PRO:HG3  | 13:X:172:ALA:HA   | 2.02                     | 0.41              |
| 2:B:10:ARG:HH11   | 2:B:10:ARG:CB     | 2.30                     | 0.41              |
| 3:C:214:ILE:O     | 3:C:221:PHE:HA    | 2.20                     | 0.41              |
| 6:F:213:CYS:HB2   | 6:F:218:PHE:HD1   | 1.85                     | 0.41              |
| 9:I:102:LEU:HD12  | 9:I:118:MET:SD    | 2.60                     | 0.41              |
| 6:M:76:TYR:HB2    | 6:M:132:VAL:HG13  | 2.01                     | 0.41              |
| 2:P:202:LEU:HA    | 2:P:205:VAL:HG22  | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:T:102:LEU:HD12  | 9:T:118:MET:SD    | 2.60                     | 0.41              |
| 9:T:108:ASP:OD2   | 9:T:111:GLU:N     | 2.45                     | 0.41              |
| 11:V:137:LEU:HD22 | 11:V:155:MET:HE1  | 2.03                     | 0.41              |
| 14:2:168:SER:HA   | 14:2:188:GLU:OE1  | 2.19                     | 0.41              |
| 2:B:184:VAL:HG21  | 2:B:201:ILE:HD11  | 2.03                     | 0.41              |
| 2:B:202:LEU:HA    | 2:B:205:VAL:HG22  | 2.03                     | 0.41              |
| 8:H:27:ARG:NH1    | 8:H:180:VAL:O     | 2.54                     | 0.41              |
| 8:H:36:THR:HG21   | 9:I:125:ALA:HB1   | 2.03                     | 0.41              |
| 8:H:48:ARG:NH2    | 8:H:192:LYS:O     | 2.48                     | 0.41              |
| 9:I:1:MET:SD      | 9:I:133:GLY:HA2   | 2.61                     | 0.41              |
| 9:I:185:ARG:H     | 9:I:185:ARG:HG3   | 1.59                     | 0.41              |
| 10:J:35:PHE:HZ    | 10:J:168:SER:HB3  | 1.84                     | 0.41              |
| 10:J:236:VAL:HG13 | 10:J:237:PRO:HD2  | 2.03                     | 0.41              |
| 11:K:224:ARG:CZ   | 13:1:174:ILE:HG21 | 2.51                     | 0.41              |
| 1:O:146:GLN:CD    | 1:O:159:ASN:HD21  | 2.27                     | 0.41              |
| 1:O:186:LEU:HA    | 1:O:189:LYS:HB2   | 2.02                     | 0.41              |
| 9:T:101:ASN:HB3   | 9:T:132:HIS:ND1   | 2.36                     | 0.41              |
| 13:X:123:ARG:HH21 | 13:X:123:ARG:HG2  | 1.86                     | 0.41              |
| 13:1:41:THR:H     | 13:1:56:ASP:CG    | 2.28                     | 0.41              |
| 7:G:90:LEU:HD21   | 7:G:114:LEU:HD22  | 2.01                     | 0.41              |
| 7:G:109:GLN:OE1   | 9:I:71:ASN:ND2    | 2.44                     | 0.41              |
| 8:H:6:TYR:CE2     | 9:I:121:LEU:HD12  | 2.55                     | 0.41              |
| 8:H:48:ARG:HD3    | 8:H:112:LEU:HD12  | 2.02                     | 0.41              |
| 5:L:2:SER:OG      | 5:L:3:ARG:N       | 2.53                     | 0.41              |
| 7:N:95:GLN:HB3    | 8:S:69:PHE:CD1    | 2.55                     | 0.41              |
| 4:R:102:ASN:HA    | 12:Z:105:ASN:ND2  | 2.35                     | 0.41              |
| 8:S:109:ILE:HB    | 8:S:122:CYS:SG    | 2.62                     | 0.41              |
| 12:W:54:LEU:HB3   | 12:W:62:TYR:HD1   | 1.86                     | 0.41              |
| 3:C:212:ILE:HD11  | 3:C:224:TYR:HD2   | 1.86                     | 0.40              |
| 6:F:74:LEU:HD23   | 6:F:87:VAL:HG22   | 2.03                     | 0.40              |
| 9:I:117:TYR:CE1   | 9:I:132:HIS:CE1   | 3.09                     | 0.40              |
| 5:L:107:TYR:CD2   | 13:1:114:ARG:HD2  | 2.56                     | 0.40              |
| 1:O:12:PRO:HA     | 2:P:26:TYR:CE1    | 2.57                     | 0.40              |
| 8:S:27:ARG:NH1    | 8:S:180:VAL:O     | 2.54                     | 0.40              |
| 5:E:103:TYR:HB2   | 12:W:81:TYR:CD1   | 2.56                     | 0.40              |
| 9:I:168:GLN:HG3   | 9:I:196:PHE:CD2   | 2.56                     | 0.40              |
| 5:L:120:ASP:OD2   | 6:M:88:HIS:HE1    | 2.04                     | 0.40              |
| 6:M:74:LEU:HD23   | 6:M:87:VAL:HG22   | 2.03                     | 0.40              |
| 6:M:140:ASN:HB2   | 6:M:145:TYR:HE2   | 1.86                     | 0.40              |
| 6:M:160:ALA:O     | 7:N:55:LEU:HD13   | 2.21                     | 0.40              |
| 2:P:202:LEU:HG    | 2:P:206:MET:HE2   | 2.04                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:86:LEU:O      | 6:F:90:ALA:N      | 2.41                     | 0.40              |
| 6:F:118:MET:HE2   | 6:F:151:PRO:HA    | 2.03                     | 0.40              |
| 11:K:90:VAL:HG13  | 11:K:116:VAL:HG21 | 2.03                     | 0.40              |
| 11:K:194:LEU:HD21 | 13:1:175:ALA:O    | 2.21                     | 0.40              |
| 1:O:94:HIS:CD2    | 1:O:102:VAL:HG22  | 2.56                     | 0.40              |
| 8:S:48:ARG:HD3    | 8:S:112:LEU:HD12  | 2.02                     | 0.40              |
| 11:V:90:VAL:HG13  | 11:V:116:VAL:HG21 | 2.03                     | 0.40              |
| 14:2:183:LEU:HD22 | 14:2:198:PHE:HD2  | 1.84                     | 0.40              |
| 2:B:202:LEU:HG    | 2:B:206:MET:HE2   | 2.04                     | 0.40              |
| 10:J:42:ALA:HA    | 10:J:50:ILE:O     | 2.20                     | 0.40              |
| 10:J:74:LEU:HB3   | 10:J:100:LEU:HD11 | 2.04                     | 0.40              |
| 6:M:101:TYR:HE1   | 8:S:90:MET:HG2    | 1.86                     | 0.40              |
| 1:O:91:CYS:HA     | 1:O:102:VAL:HG21  | 2.02                     | 0.40              |
| 2:P:182:GLN:HG2   | 3:Q:56:LEU:HD22   | 2.03                     | 0.40              |
| 9:T:171:PHE:HE2   | 9:T:173:LEU:HB2   | 1.86                     | 0.40              |
| 11:V:91:ASN:CG    | 11:V:92:ASN:H     | 2.29                     | 0.40              |
| 14:2:89:ASP:HB2   | 14:2:243:GLY:O    | 2.22                     | 0.40              |
| 9:I:3:TYR:OH      | 9:I:139:THR:HG21  | 2.21                     | 0.40              |
| 10:J:213:ARG:HA   | 13:1:65:VAL:HB    | 2.03                     | 0.40              |
| 1:O:98:VAL:HG12   | 1:O:100:ASP:H     | 1.87                     | 0.40              |
| 2:P:161:THR:HG21  | 3:Q:60:GLN:HE21   | 1.86                     | 0.40              |
| 9:T:1:MET:SD      | 9:T:133:GLY:HA2   | 2.61                     | 0.40              |
| 11:V:188:ALA:HA   | 11:V:192:GLN:HB2  | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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     | 230/248 (93%) | 221 (96%) | 9 (4%)  | 0        | 100         | 100 |
| 1   | O     | 230/248 (93%) | 220 (96%) | 10 (4%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 2   | B     | 232/241 (96%)   | 221 (95%)  | 10 (4%)  | 1 (0%)   | 30          | 60  |
| 2   | P     | 232/241 (96%)   | 225 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 3   | C     | 233/263 (89%)   | 225 (97%)  | 8 (3%)   | 0        | 100         | 100 |
| 3   | Q     | 233/263 (89%)   | 225 (97%)  | 8 (3%)   | 0        | 100         | 100 |
| 4   | D     | 238/255 (93%)   | 229 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 4   | R     | 238/255 (93%)   | 229 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 5   | E     | 242/246 (98%)   | 231 (96%)  | 11 (4%)  | 0        | 100         | 100 |
| 5   | L     | 241/246 (98%)   | 231 (96%)  | 10 (4%)  | 0        | 100         | 100 |
| 6   | F     | 229/234 (98%)   | 221 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 6   | M     | 227/234 (97%)   | 220 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 7   | G     | 244/261 (94%)   | 232 (95%)  | 12 (5%)  | 0        | 100         | 100 |
| 7   | N     | 244/261 (94%)   | 231 (95%)  | 12 (5%)  | 1 (0%)   | 30          | 60  |
| 8   | H     | 202/205 (98%)   | 193 (96%)  | 8 (4%)   | 1 (0%)   | 24          | 55  |
| 8   | S     | 202/205 (98%)   | 192 (95%)  | 9 (4%)   | 1 (0%)   | 24          | 55  |
| 9   | I     | 196/201 (98%)   | 189 (96%)  | 7 (4%)   | 0        | 100         | 100 |
| 9   | T     | 195/201 (97%)   | 189 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 10  | J     | 211/241 (88%)   | 206 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 10  | U     | 211/241 (88%)   | 205 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 11  | K     | 214/264 (81%)   | 207 (97%)  | 6 (3%)   | 1 (0%)   | 24          | 55  |
| 11  | V     | 214/264 (81%)   | 208 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 12  | W     | 197/219 (90%)   | 187 (95%)  | 10 (5%)  | 0        | 100         | 100 |
| 12  | Z     | 197/219 (90%)   | 189 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 13  | 1     | 217/273 (80%)   | 205 (94%)  | 11 (5%)  | 1 (0%)   | 24          | 55  |
| 13  | X     | 217/273 (80%)   | 205 (94%)  | 10 (5%)  | 2 (1%)   | 14          | 43  |
| 14  | 2     | 199/276 (72%)   | 191 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 14  | Y     | 199/276 (72%)   | 192 (96%)  | 7 (4%)   | 0        | 100         | 100 |
| All | All   | 6164/6854 (90%) | 5919 (96%) | 237 (4%) | 8 (0%)   | 49          | 75  |

All (8) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | N     | 3   | ARG  |
| 13  | X     | 239 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 11  | GLY  |
| 8   | H     | 115 | LYS  |
| 8   | S     | 115 | LYS  |
| 11  | K     | 51  | VAL  |
| 13  | X     | 249 | PRO  |
| 13  | 1     | 249 | PRO  |

### 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 PDB entries followed by that with respect to all EM entries.

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     | 196/211 (93%) | 195 (100%) | 1 (0%)   | 81          | 83  |
| 1   | O     | 196/211 (93%) | 195 (100%) | 1 (0%)   | 81          | 83  |
| 2   | B     | 196/203 (97%) | 196 (100%) | 0        | 100         | 100 |
| 2   | P     | 196/203 (97%) | 196 (100%) | 0        | 100         | 100 |
| 3   | C     | 201/225 (89%) | 201 (100%) | 0        | 100         | 100 |
| 3   | Q     | 201/225 (89%) | 201 (100%) | 0        | 100         | 100 |
| 4   | D     | 198/212 (93%) | 197 (100%) | 1 (0%)   | 81          | 83  |
| 4   | R     | 198/212 (93%) | 198 (100%) | 0        | 100         | 100 |
| 5   | E     | 208/210 (99%) | 208 (100%) | 0        | 100         | 100 |
| 5   | L     | 207/210 (99%) | 207 (100%) | 0        | 100         | 100 |
| 6   | F     | 189/191 (99%) | 188 (100%) | 1 (0%)   | 81          | 83  |
| 6   | M     | 188/191 (98%) | 188 (100%) | 0        | 100         | 100 |
| 7   | G     | 207/221 (94%) | 206 (100%) | 1 (0%)   | 81          | 83  |
| 7   | N     | 207/221 (94%) | 206 (100%) | 1 (0%)   | 81          | 83  |
| 8   | H     | 174/175 (99%) | 174 (100%) | 0        | 100         | 100 |
| 8   | S     | 174/175 (99%) | 174 (100%) | 0        | 100         | 100 |
| 9   | I     | 169/171 (99%) | 168 (99%)  | 1 (1%)   | 78          | 81  |
| 9   | T     | 168/171 (98%) | 167 (99%)  | 1 (1%)   | 78          | 81  |
| 10  | J     | 177/198 (89%) | 176 (99%)  | 1 (1%)   | 78          | 81  |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 10  | U     | 177/198 (89%)   | 177 (100%)  | 0        | 100         | 100 |
| 11  | K     | 178/215 (83%)   | 176 (99%)   | 2 (1%)   | 65          | 76  |
| 11  | V     | 177/215 (82%)   | 176 (99%)   | 1 (1%)   | 78          | 81  |
| 12  | W     | 153/167 (92%)   | 153 (100%)  | 0        | 100         | 100 |
| 12  | Z     | 153/167 (92%)   | 153 (100%)  | 0        | 100         | 100 |
| 13  | 1     | 170/216 (79%)   | 169 (99%)   | 1 (1%)   | 78          | 81  |
| 13  | X     | 170/216 (79%)   | 169 (99%)   | 1 (1%)   | 78          | 81  |
| 14  | 2     | 166/222 (75%)   | 166 (100%)  | 0        | 100         | 100 |
| 14  | Y     | 166/222 (75%)   | 165 (99%)   | 1 (1%)   | 78          | 81  |
| All | All   | 5160/5674 (91%) | 5145 (100%) | 15 (0%)  | 84          | 86  |

All (15) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 38  | LYS  |
| 4   | D     | 220 | ILE  |
| 6   | F     | 184 | LEU  |
| 7   | G     | 3   | ARG  |
| 9   | I     | 185 | ARG  |
| 10  | J     | 222 | LYS  |
| 11  | K     | 50  | MET  |
| 11  | K     | 59  | LEU  |
| 7   | N     | 1   | MET  |
| 1   | O     | 38  | LYS  |
| 9   | T     | 185 | ARG  |
| 11  | V     | 59  | LEU  |
| 13  | X     | 237 | ARG  |
| 14  | Y     | 112 | TYR  |
| 13  | 1     | 236 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 92  | GLN  |
| 1   | A     | 94  | HIS  |
| 1   | A     | 116 | GLN  |
| 1   | A     | 122 | ASN  |
| 2   | B     | 73  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 99  | HIS  |
| 2   | B     | 155 | HIS  |
| 2   | B     | 227 | HIS  |
| 3   | C     | 20  | HIS  |
| 3   | C     | 68  | ASN  |
| 3   | C     | 121 | GLN  |
| 3   | C     | 143 | HIS  |
| 4   | D     | 73  | HIS  |
| 4   | D     | 121 | HIS  |
| 4   | D     | 144 | ASN  |
| 5   | E     | 90  | GLN  |
| 5   | E     | 100 | ASN  |
| 5   | E     | 123 | GLN  |
| 5   | E     | 193 | GLN  |
| 6   | F     | 88  | HIS  |
| 6   | F     | 102 | GLN  |
| 6   | F     | 109 | GLN  |
| 6   | F     | 140 | ASN  |
| 7   | G     | 100 | GLN  |
| 7   | G     | 235 | GLN  |
| 7   | G     | 240 | HIS  |
| 8   | H     | 33  | GLN  |
| 9   | I     | 8   | GLN  |
| 9   | I     | 27  | GLN  |
| 10  | J     | 174 | GLN  |
| 10  | J     | 180 | GLN  |
| 11  | K     | 110 | GLN  |
| 11  | K     | 114 | GLN  |
| 11  | K     | 126 | HIS  |
| 11  | K     | 192 | GLN  |
| 5   | L     | 100 | ASN  |
| 5   | L     | 123 | GLN  |
| 5   | L     | 224 | ASN  |
| 6   | M     | 21  | GLN  |
| 6   | M     | 88  | HIS  |
| 6   | M     | 109 | GLN  |
| 6   | M     | 166 | ASN  |
| 6   | M     | 169 | ASN  |
| 6   | M     | 189 | HIS  |
| 7   | N     | 100 | GLN  |
| 7   | N     | 102 | GLN  |
| 7   | N     | 240 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 92  | GLN  |
| 1   | O     | 94  | HIS  |
| 1   | O     | 116 | GLN  |
| 2   | P     | 73  | HIS  |
| 2   | P     | 99  | HIS  |
| 2   | P     | 155 | HIS  |
| 2   | P     | 227 | HIS  |
| 3   | Q     | 20  | HIS  |
| 3   | Q     | 68  | ASN  |
| 3   | Q     | 69  | HIS  |
| 3   | Q     | 121 | GLN  |
| 3   | Q     | 143 | HIS  |
| 4   | R     | 106 | ASN  |
| 4   | R     | 111 | HIS  |
| 4   | R     | 144 | ASN  |
| 8   | S     | 33  | GLN  |
| 9   | T     | 8   | GLN  |
| 9   | T     | 27  | GLN  |
| 9   | T     | 32  | HIS  |
| 10  | U     | 174 | GLN  |
| 11  | V     | 114 | GLN  |
| 11  | V     | 192 | GLN  |
| 12  | W     | 58  | HIS  |
| 12  | W     | 205 | HIS  |
| 13  | X     | 74  | HIS  |
| 14  | Y     | 96  | ASN  |
| 14  | Y     | 234 | HIS  |
| 12  | Z     | 205 | HIS  |
| 13  | 1     | 153 | HIS  |
| 14  | 2     | 234 | HIS  |

### 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

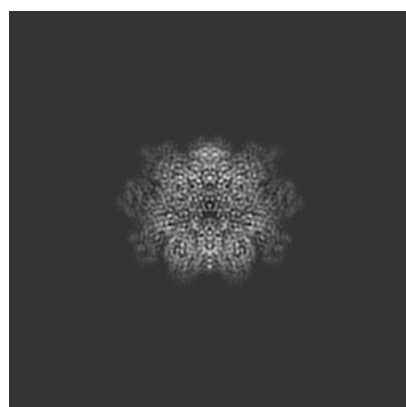
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30825. These allow visual inspection of the internal detail of the map and identification of artifacts.

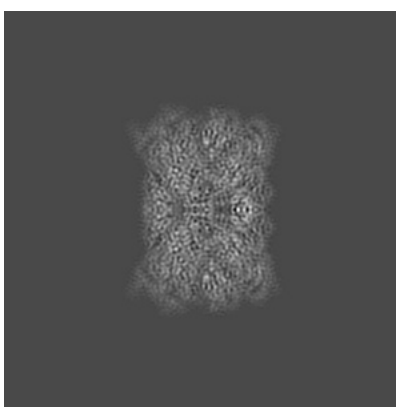
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

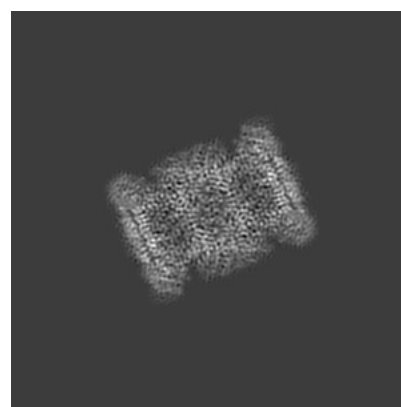
#### 6.1.1 Primary map



X



Y

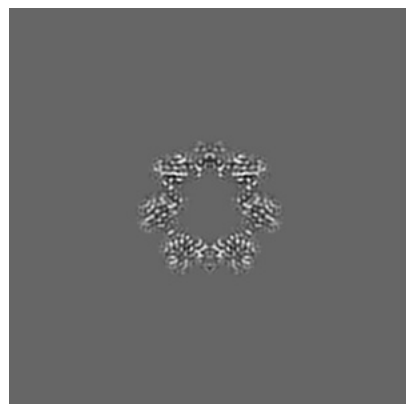


Z

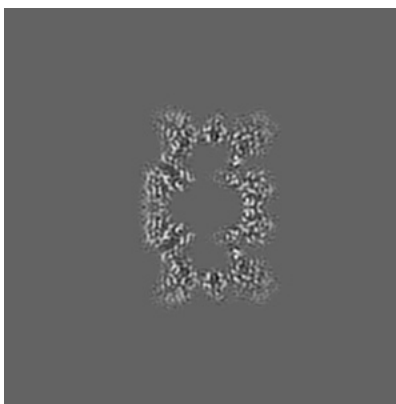
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

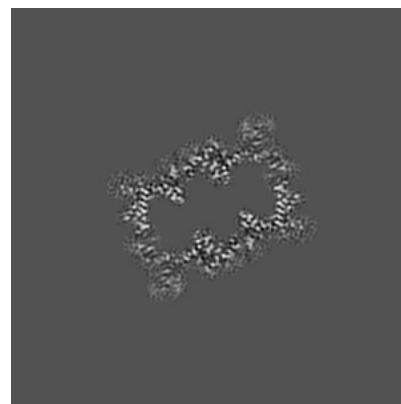
#### 6.2.1 Primary map



X Index: 128



Y Index: 128



Z Index: 128

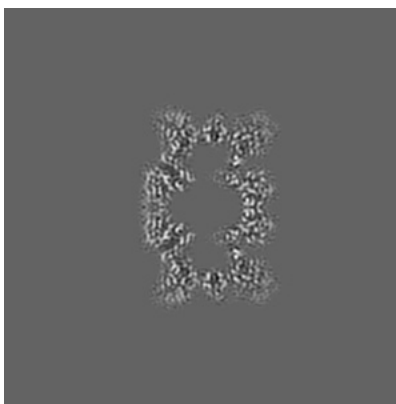
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

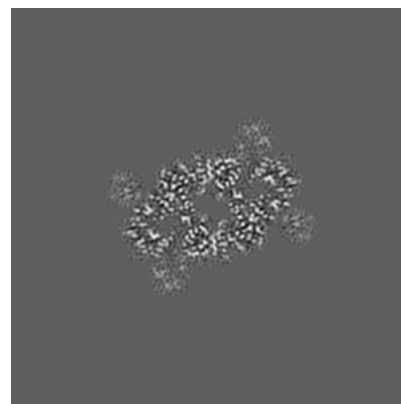
### 6.3.1 Primary map



X Index: 131



Y Index: 128

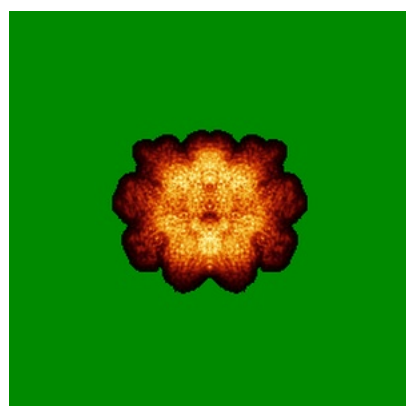


Z Index: 146

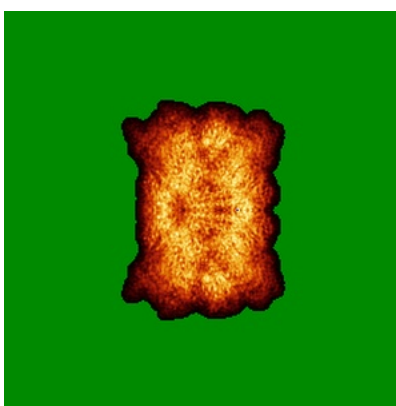
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

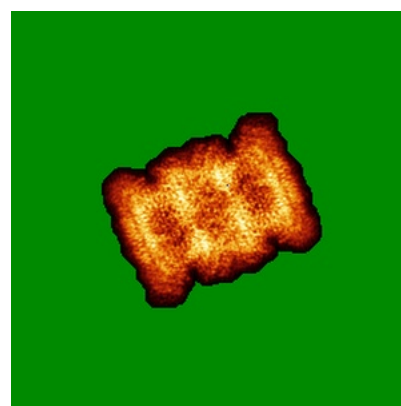
### 6.4.1 Primary map



X



Y



Z

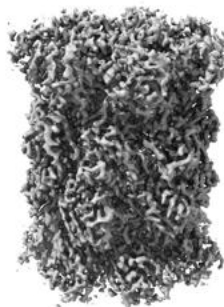
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

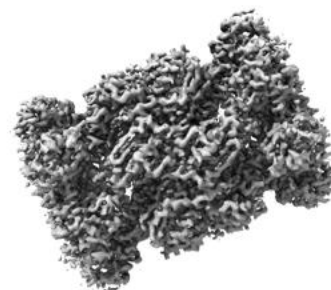
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

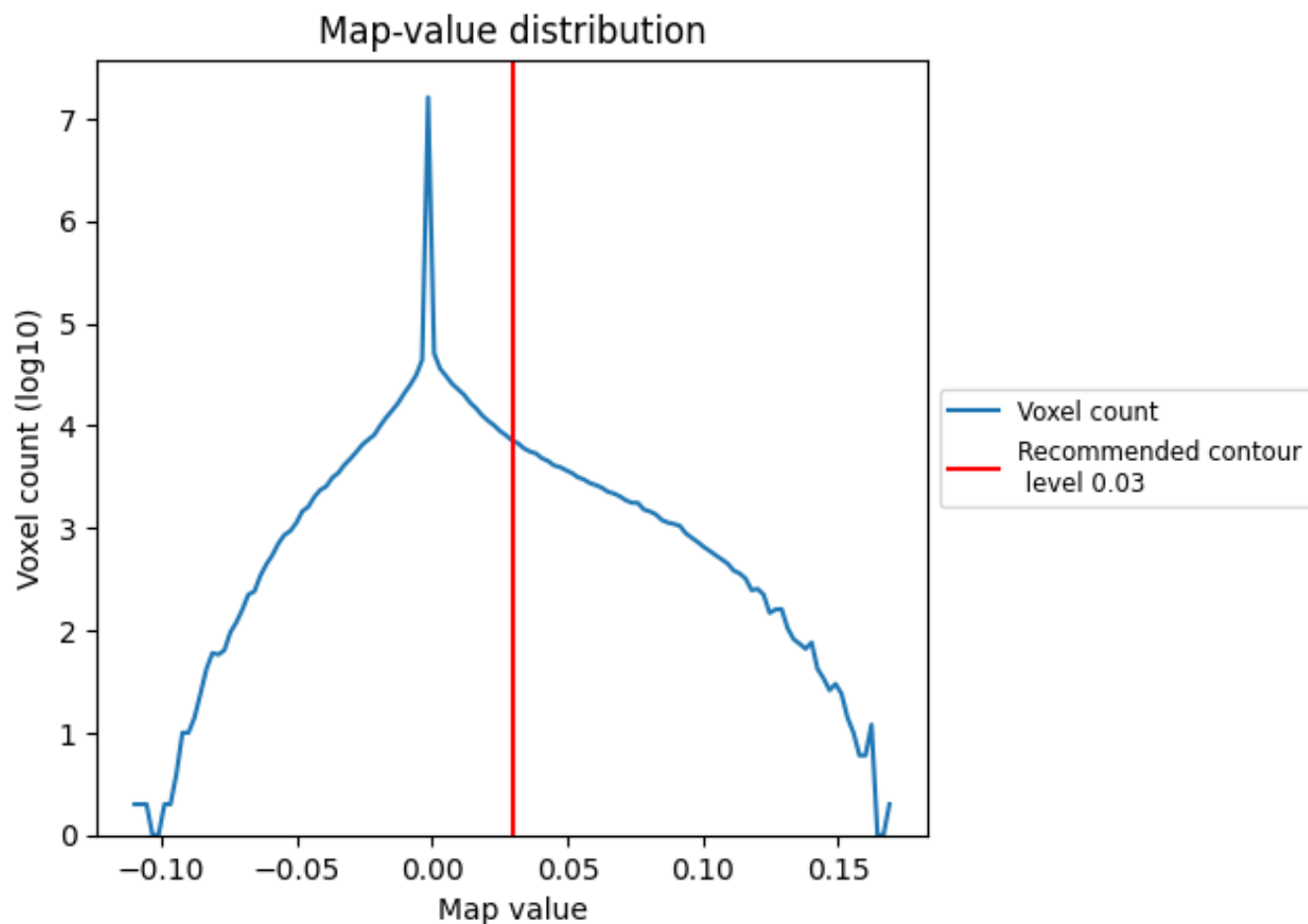
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

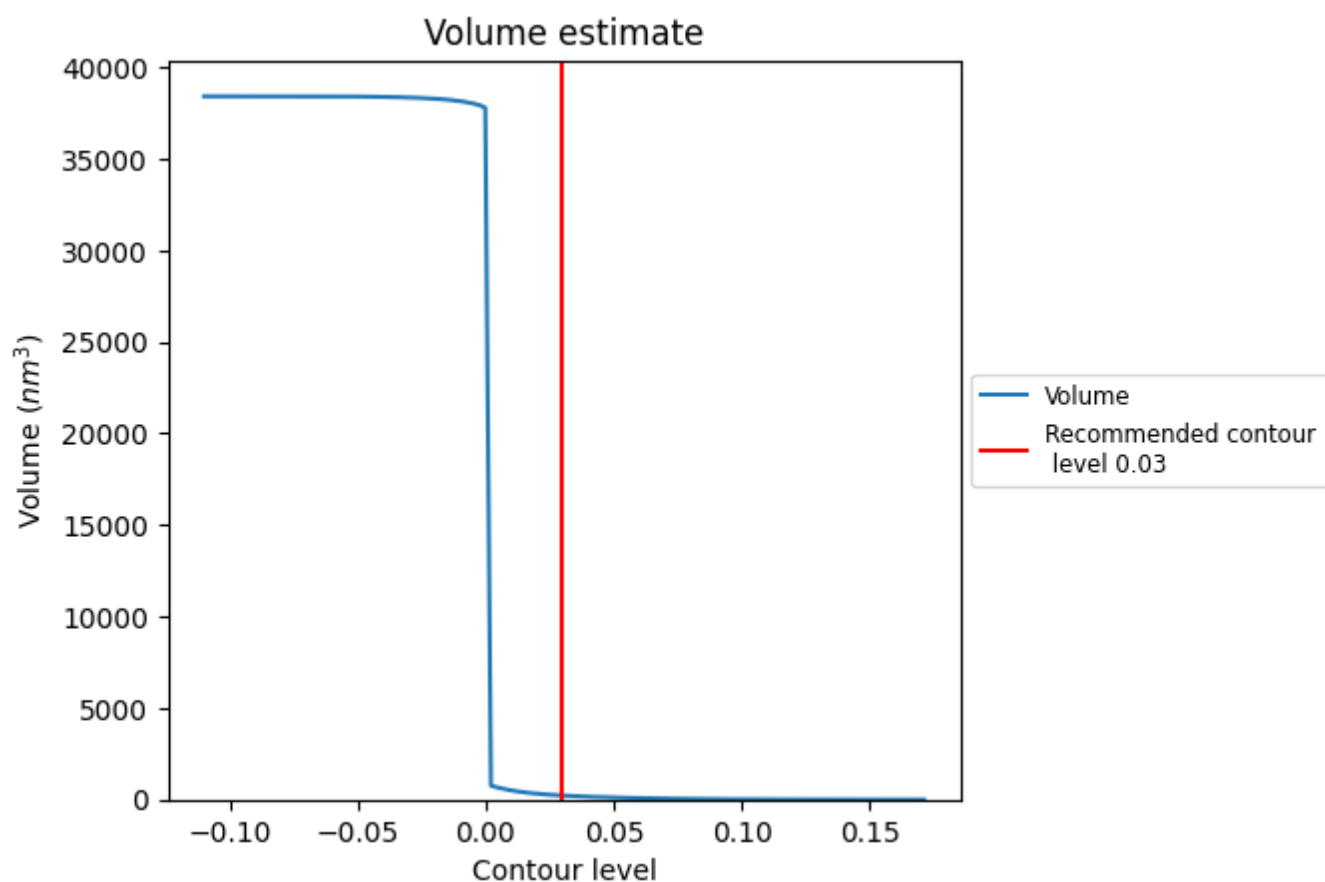
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

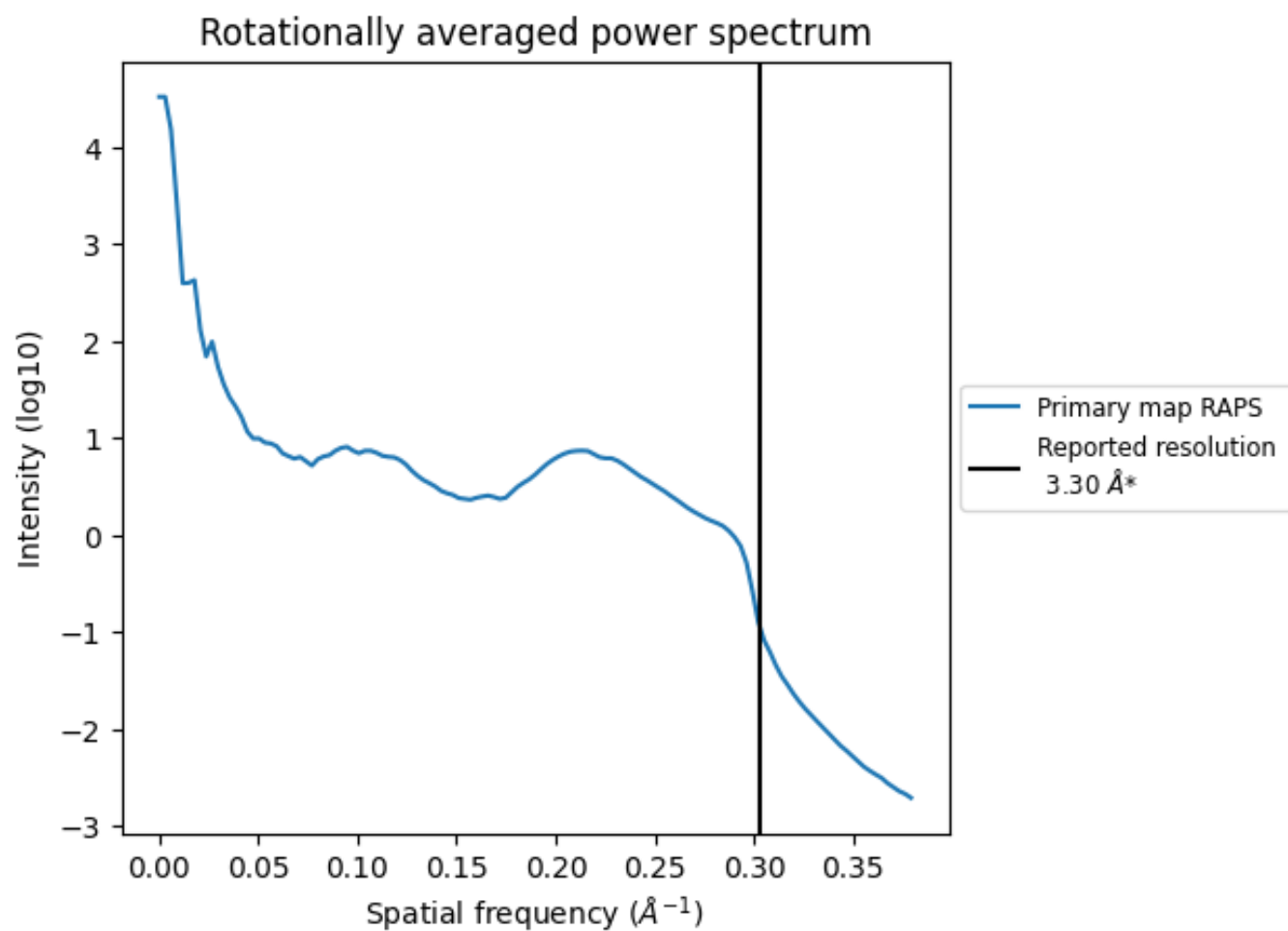
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 221 nm<sup>3</sup>; this corresponds to an approximate mass of 199 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

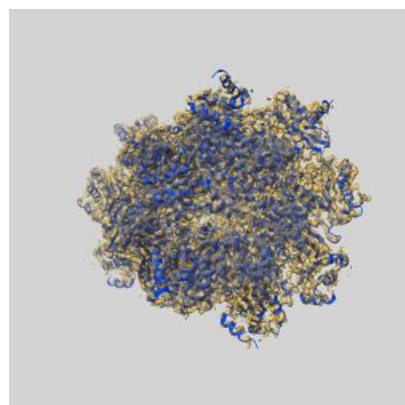
## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

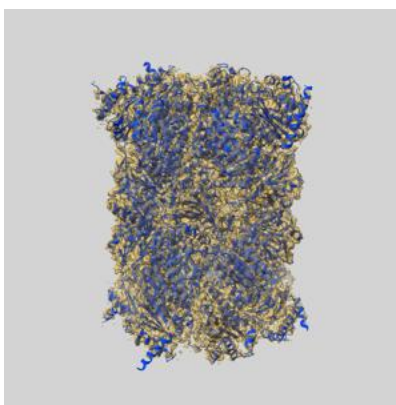
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30825 and PDB model 7DR7. Per-residue inclusion information can be found in section [3](#) on page [7](#).

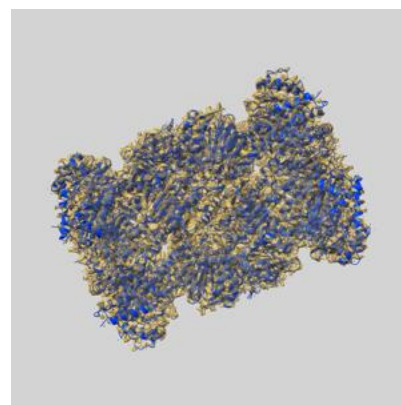
### 9.1 Map-model overlay [i](#)



X



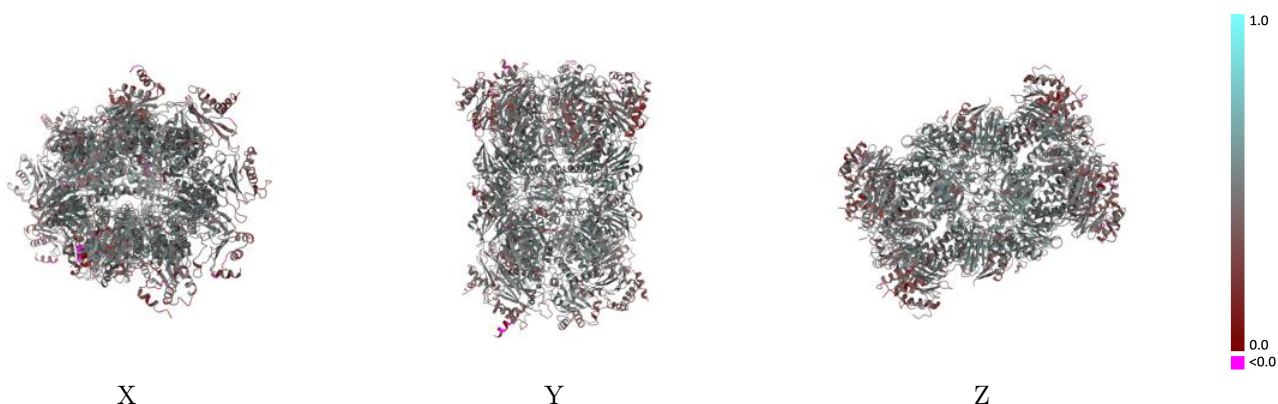
Y



Z

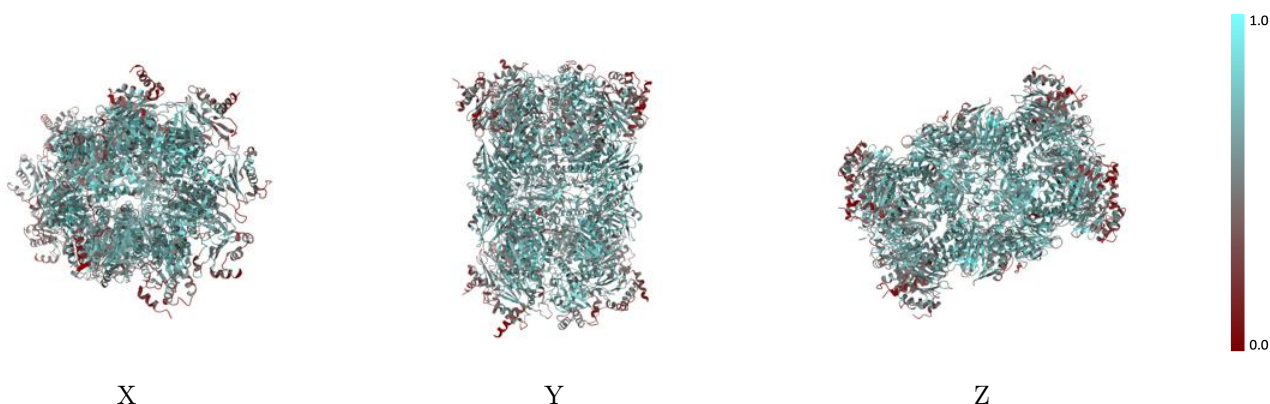
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



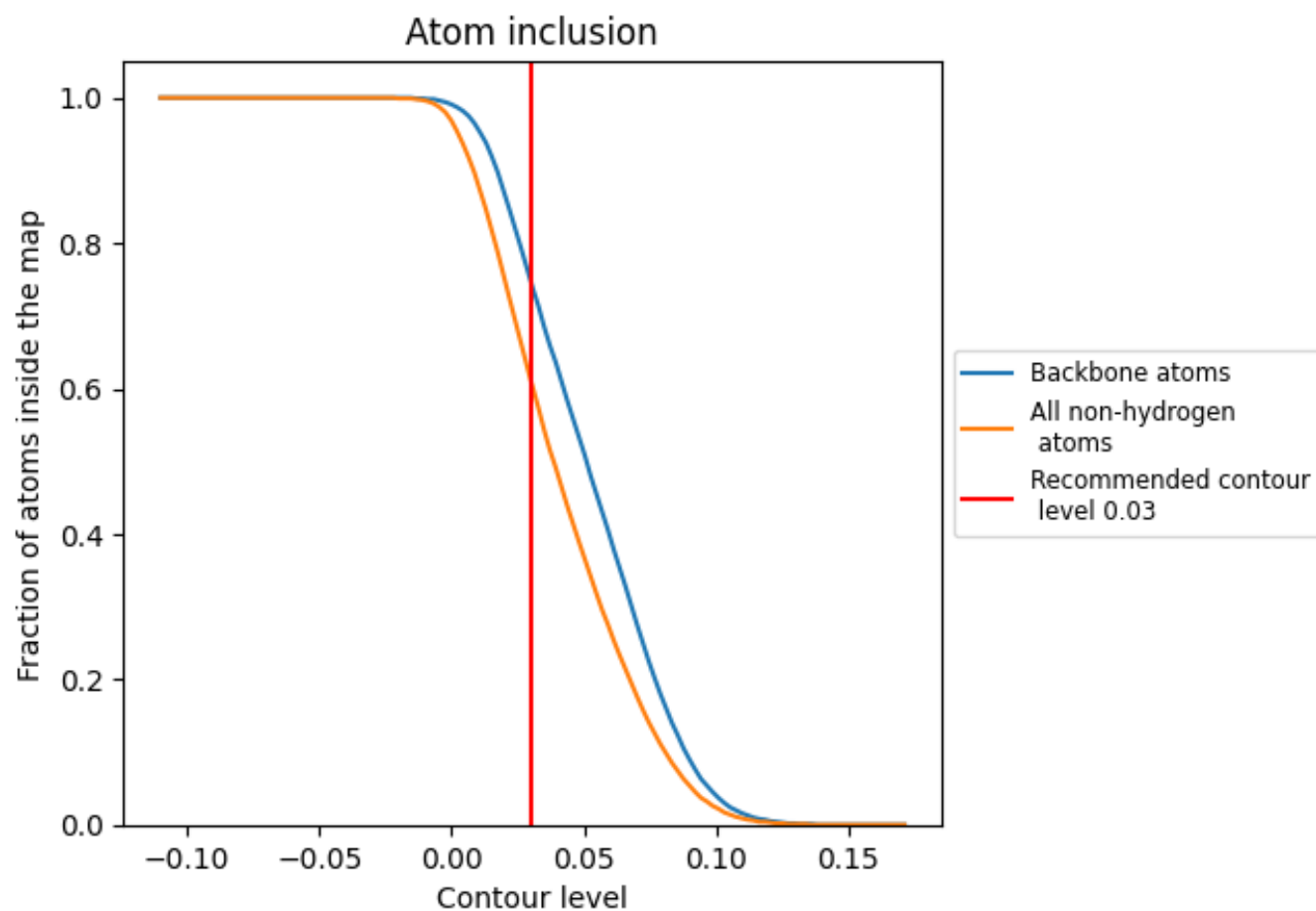
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.6100   |  0.4480   |
| 1     |  0.6370   |  0.4720   |
| 2     |  0.6770   |  0.4750   |
| A     |  0.5310   |  0.4120   |
| B     |  0.5290   |  0.4200   |
| C     |  0.5770   |  0.4330   |
| D     |  0.5760   |  0.4170   |
| E     |  0.5420   |  0.4130   |
| F     |  0.5930   |  0.4470   |
| G     |  0.5640   |  0.4250   |
| H     |  0.6980   |  0.4910   |
| I     |  0.6750   |  0.4760   |
| J     |  0.6190   |  0.4600   |
| K     |  0.6770   |  0.4630   |
| L     |  0.5440  |  0.4170  |
| M     |  0.5910 |  0.4390 |
| N     |  0.5660 |  0.4270 |
| O     |  0.5350 |  0.4080 |
| P     |  0.5230 |  0.4150 |
| Q     |  0.5700 |  0.4300 |
| R     |  0.5710 |  0.4160 |
| S     |  0.6930 |  0.4870 |
| T     |  0.6770 |  0.4830 |
| U     |  0.6280 |  0.4660 |
| V     |  0.6810 |  0.4630 |
| W     |  0.7170 |  0.5010 |
| X     |  0.6460 |  0.4820 |
| Y     |  0.6850 |  0.4840 |
| Z     |  0.6990 |  0.4890 |

