



## Full wwPDB EM Validation Report ⓘ

May 23, 2026 – 05:59 PM EDT

PDB ID : 9CGC / pdb\_00009cgc  
EMDB ID : EMD-45579  
Title : Yeast 26S proteasome non-substrate-engaged (S1 state)  
Authors : Arkinson, C.; Gee, C.L.; Martin, A.  
Deposited on : 2024-06-28  
Resolution : 3.61 Å(reported)  
Based on initial model : 6j2q

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:

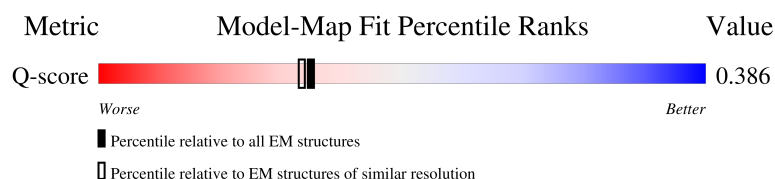
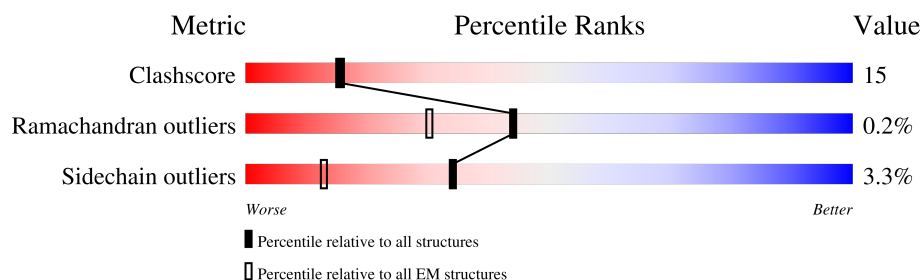
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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

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

The reported resolution of this entry is 3.61 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                       | 11801 ( 3.11 - 4.10 )                                    |

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   | 1     | 215    |                  |
| 1   | b     | 215    |                  |
| 2   | 2     | 261    |                  |
| 2   | i     | 261    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | 3     | 205    |                  |
| 3   | h     | 205    |                  |
| 4   | 4     | 198    |                  |
| 4   | g     | 198    |                  |
| 5   | 5     | 287    |                  |
| 5   | f     | 287    |                  |
| 6   | 6     | 241    |                  |
| 6   | e     | 241    |                  |
| 7   | 7     | 266    |                  |
| 7   | a     | 266    |                  |
| 8   | A     | 252    |                  |
| 9   | B     | 250    |                  |
| 10  | C     | 258    |                  |
| 11  | D     | 254    |                  |
| 12  | E     | 260    |                  |
| 13  | F     | 234    |                  |
| 14  | G     | 288    |                  |
| 15  | I     | 437    |                  |
| 16  | K     | 428    |                  |
| 17  | L     | 437    |                  |
| 18  | O     | 393    |                  |
| 19  | P     | 445    |                  |
| 20  | R     | 429    |                  |
| 21  | S     | 523    |                  |
| 22  | V     | 306    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 23  | W     | 268    |                  |
| 24  | Y     | 89     |                  |
| 25  | J     | 405    |                  |
| 26  | H     | 467    |                  |
| 27  | M     | 434    |                  |
| 28  | Q     | 434    |                  |
| 29  | U     | 338    |                  |
| 30  | N     | 945    |                  |
| 31  | T     | 274    |                  |
| 32  | o     | 993    |                  |

## 2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 92952 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 beta type-1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | 1     | 205      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1576  | 996 | 261 | 312 | 7 |         |       |
| 1   | b     | 205      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1576  | 996 | 261 | 312 | 7 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | 2     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1684  | 1061 | 293 | 323 | 7 |         |       |
| 2   | i     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1684  | 1061 | 293 | 323 | 7 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | 3     | 204      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 1010 | 258 | 305 | 8 |         |       |
| 3   | h     | 204      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 1010 | 258 | 305 | 8 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | 4     | 198      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1585  | 1005 | 269 | 305 | 6 |         |       |
| 4   | g     | 198      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1585  | 1005 | 269 | 305 | 6 |         |       |

- Molecule 5 is a protein called Proteasome subunit beta type-5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | 5     | 212      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1644  | 1045 | 280 | 312 | 7 |         |       |
| 5   | f     | 212      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1644  | 1045 | 280 | 312 | 7 |         |       |

- Molecule 6 is a protein called Proteasome subunit beta type-6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | 6     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1757  | 1115 | 303 | 335 | 4 |         |       |
| 6   | e     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1757  | 1115 | 303 | 335 | 4 |         |       |

- Molecule 7 is a protein called Proteasome subunit beta type-7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | 7     | 233      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1824  | 1154 | 312 | 351 | 7 |         |       |
| 7   | a     | 233      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1824  | 1154 | 312 | 351 | 7 |         |       |

- Molecule 8 is a protein called Proteasome subunit alpha type-1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8   | A     | 243      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1921  | 1221 | 322 | 370 | 8 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9   | B     | 250      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1915  | 1219 | 315 | 377 | 4 |         |       |

- Molecule 10 is a protein called Proteasome subunit alpha type-3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10  | C     | 244      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1904  | 1201 | 321 | 379 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 11  | D     | 241      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1890  | 1181 | 331 | 374 | 4 |         |       |

- Molecule 12 is a protein called Proteasome subunit alpha type-5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12  | E     | 242      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1861  | 1162 | 314 | 378 | 7 |         |       |

- Molecule 13 is a protein called Proteasome subunit alpha type-6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | F     | 233      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1795  | 1129 | 312 | 350 | 4 |         |       |

- Molecule 14 is a protein called Probable proteasome subunit alpha type-7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | G     | 243      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1888  | 1201 | 328 | 355 | 4 |         |       |

- Molecule 15 is a protein called 26S proteasome regulatory subunit 4 homolog.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 15  | I     | 392      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3078  | 1937 | 516 | 608 | 17 |         |       |

- Molecule 16 is a protein called 26S proteasome regulatory subunit 6B homolog.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 16  | K     | 383      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3035  | 1908 | 532 | 585 | 10 |         |       |

- Molecule 17 is a protein called 26S proteasome subunit RPT4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 17  | L     | 359      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2820  | 1783 | 490 | 535 | 12 |         |       |

- Molecule 18 is a protein called 26S proteasome regulatory subunit RPN9.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 18  | O     | 386      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3169  | 2040 | 517 | 604 | 8 |         |       |

- Molecule 19 is a protein called 26S proteasome regulatory subunit RPN5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 19  | P     | 436      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3575  | 2279 | 597 | 690 | 9 |         |       |

- Molecule 20 is a protein called 26S proteasome regulatory subunit RPN7.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 20  | R     | 397      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3195  | 2043 | 524 | 618 | 10 |         |       |

- Molecule 21 is a protein called 26S proteasome regulatory subunit RPN3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 21  | S     | 461      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3770  | 2412 | 629 | 714 | 15 |         |       |

- Molecule 22 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 22  | V     | 288      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2267  | 1421 | 388 | 444 | 14 |         |       |

- Molecule 23 is a protein called 26S proteasome regulatory subunit RPN10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | W     | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1484  | 933 | 262 | 287 | 2 |         |       |

- Molecule 24 is a protein called 26S proteasome complex subunit SEM1.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 24  | Y     | 33       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 281   | 176 | 38 | 67 |         |       |

- Molecule 25 is a protein called 26S proteasome regulatory subunit 8 homolog.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 25  | J     | 370      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2913  | 1836 | 524 | 536 | 17 |         |       |

- Molecule 26 is a protein called 26S proteasome regulatory subunit 7 homolog.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 26  | H     | 385      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3016  | 1896 | 540 | 563 | 17 |         |       |

- Molecule 27 is a protein called 26S proteasome regulatory subunit 6A.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 27  | M     | 363      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2827  | 1771 | 493 | 550 | 13 |         |       |

- Molecule 28 is a protein called 26S proteasome regulatory subunit RPN6.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 28  | Q     | 411      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3347  | 2137 | 552 | 643 | 15 |         |       |

- Molecule 29 is a protein called 26S proteasome regulatory subunit RPN8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 29  | U     | 292      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2333  | 1476 | 401 | 449 | 7 |         |       |

- Molecule 30 is a protein called 26S proteasome regulatory subunit RPN2.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 30  | N     | 869      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6725  | 4275 | 1130 | 1292 | 28 |         |       |

- Molecule 31 is a protein called 26S proteasome regulatory subunit RPN12.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 31  | T     | 257      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2106  | 1357 | 335 | 410 | 4 |         |       |

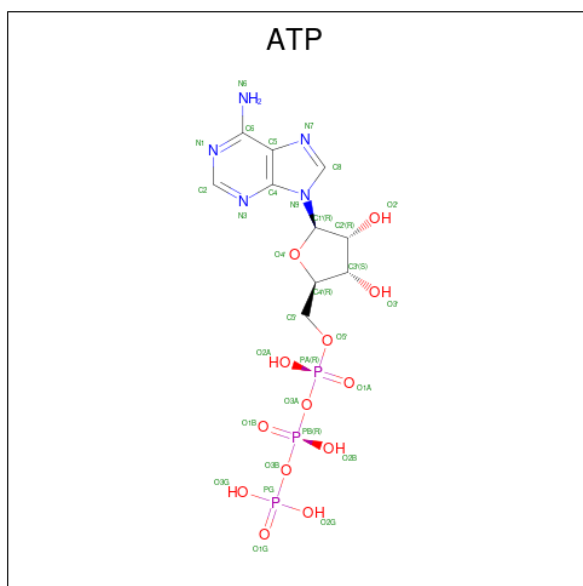
- Molecule 32 is a protein called 26S proteasome regulatory subunit RPN1.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 32  | o     | 819      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6347  | 4039 | 1040 | 1239 | 29 |         |       |

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 33  | I     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 33  | K     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 33  | L     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 33  | H     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 33  | M     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 34 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 34  | K     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 34  | L     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 34  | J     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |

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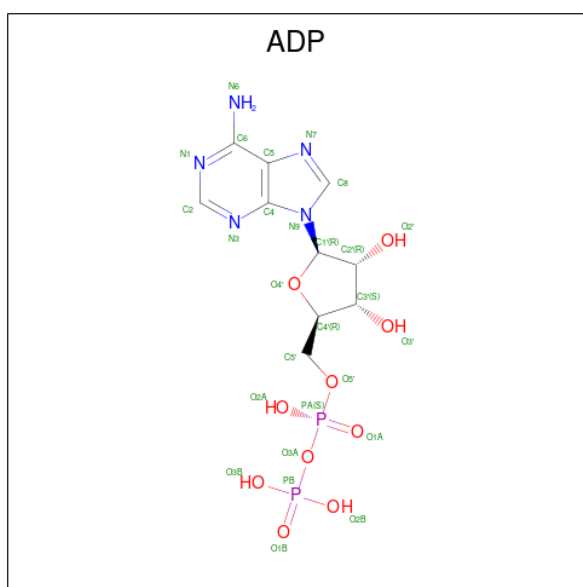
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| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 34  | H     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 34  | M     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |

- Molecule 35 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 35  | V     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

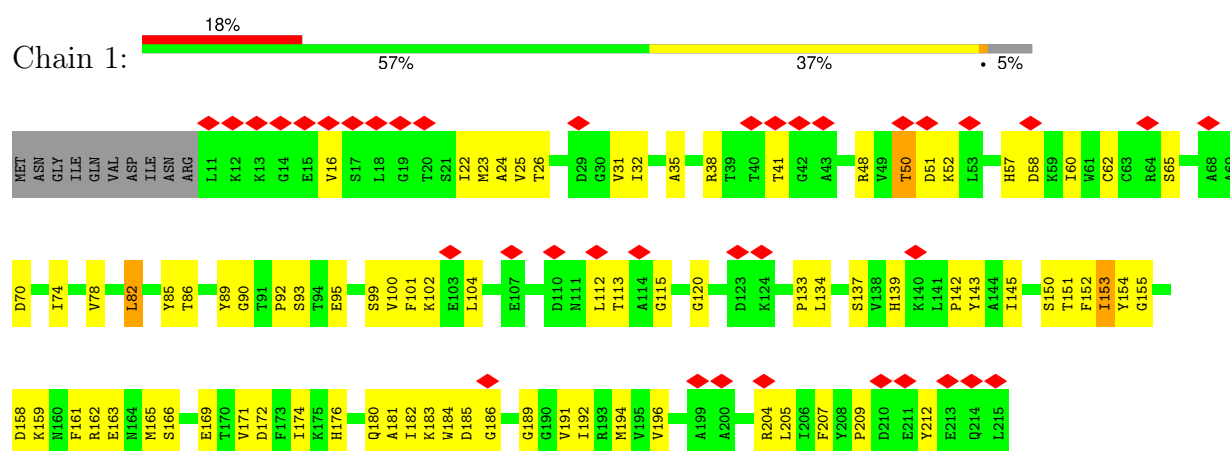


| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 36  | J     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |

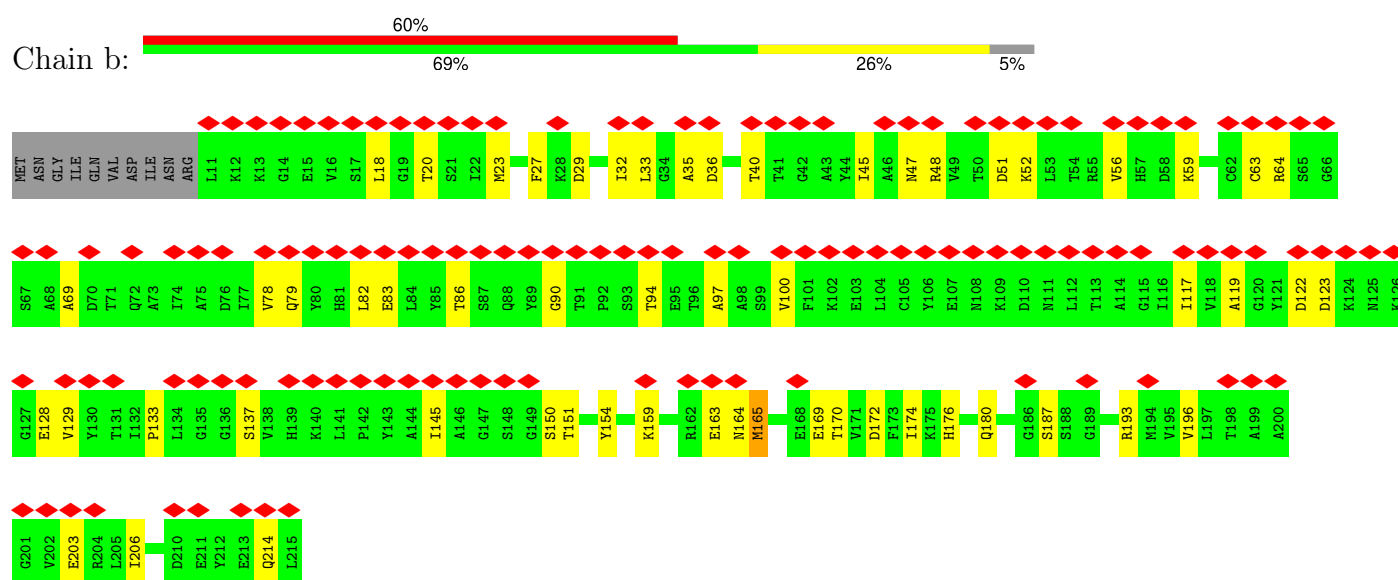
### 3 Residue-property plots

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 beta type-1



#### • Molecule 1: Proteasome subunit beta type-1

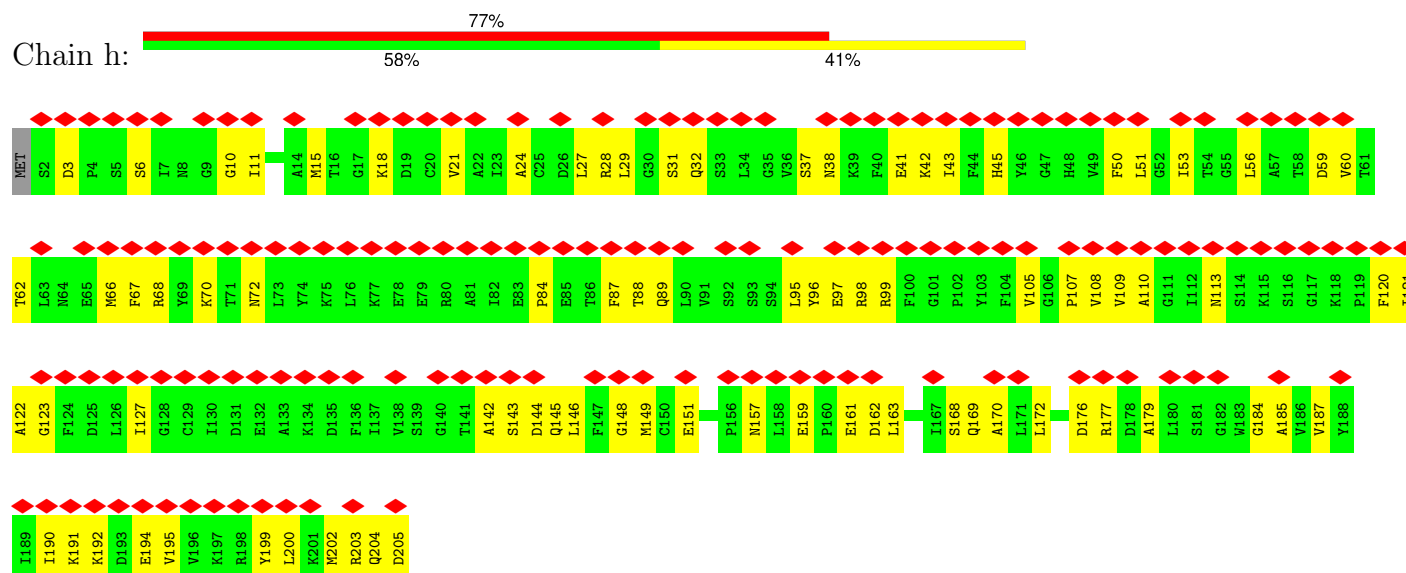


#### • Molecule 2: Proteasome subunit beta type-2

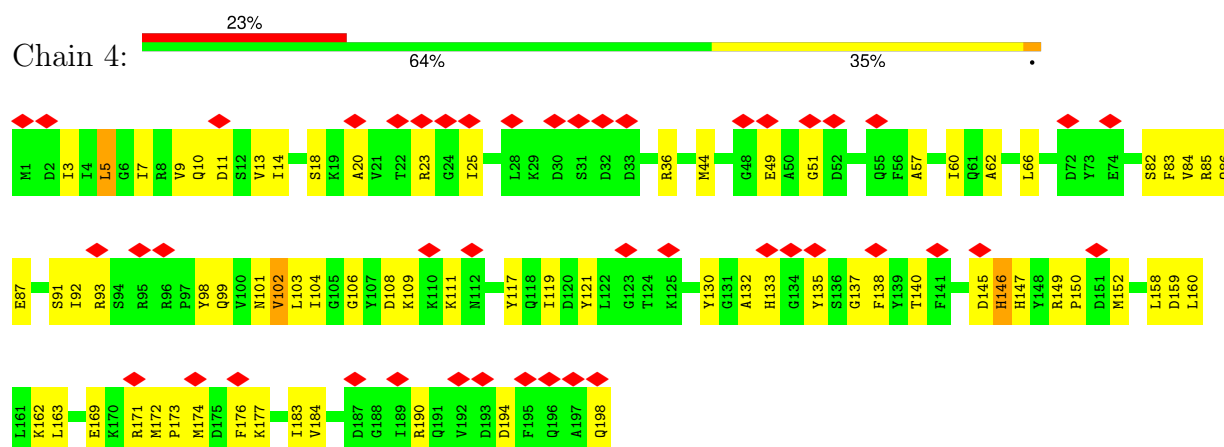




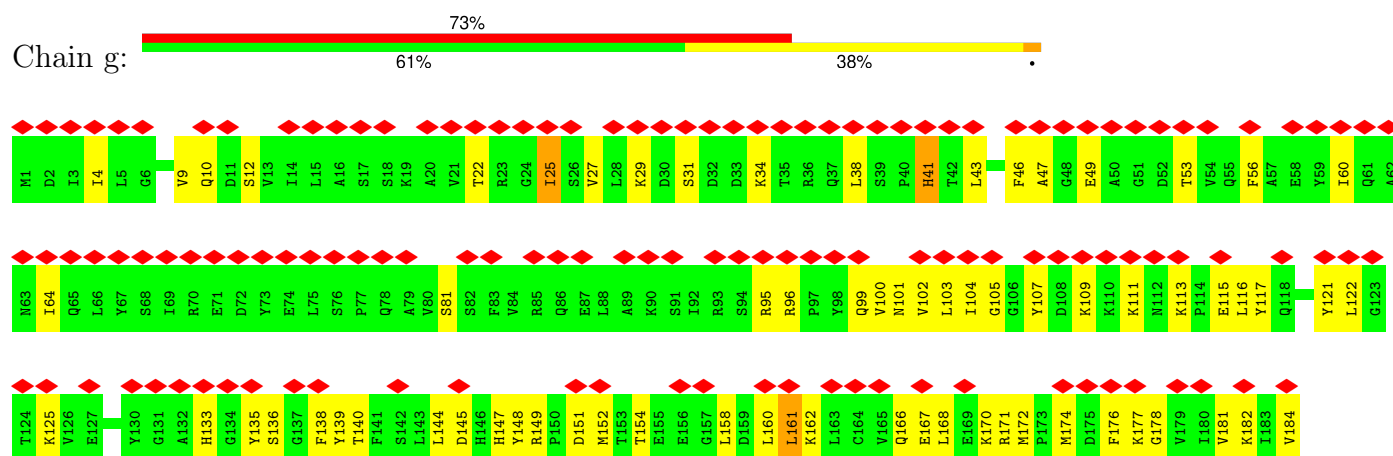
- Molecule 3: Proteasome subunit beta type-3

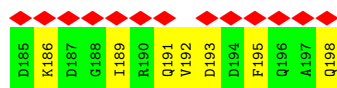


- Molecule 4: Proteasome subunit beta type-4

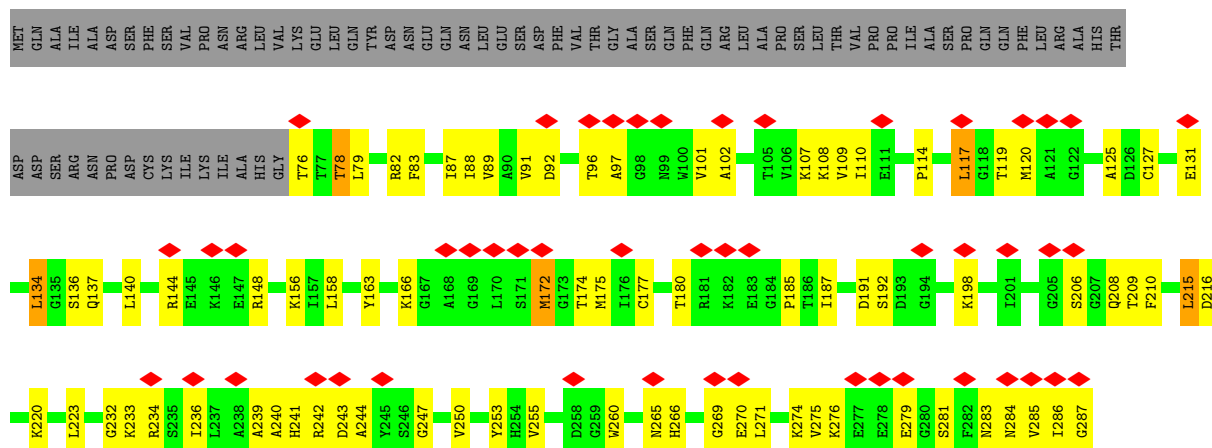
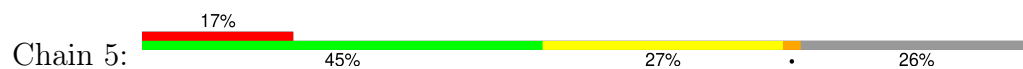


- Molecule 4: Proteasome subunit beta type-4

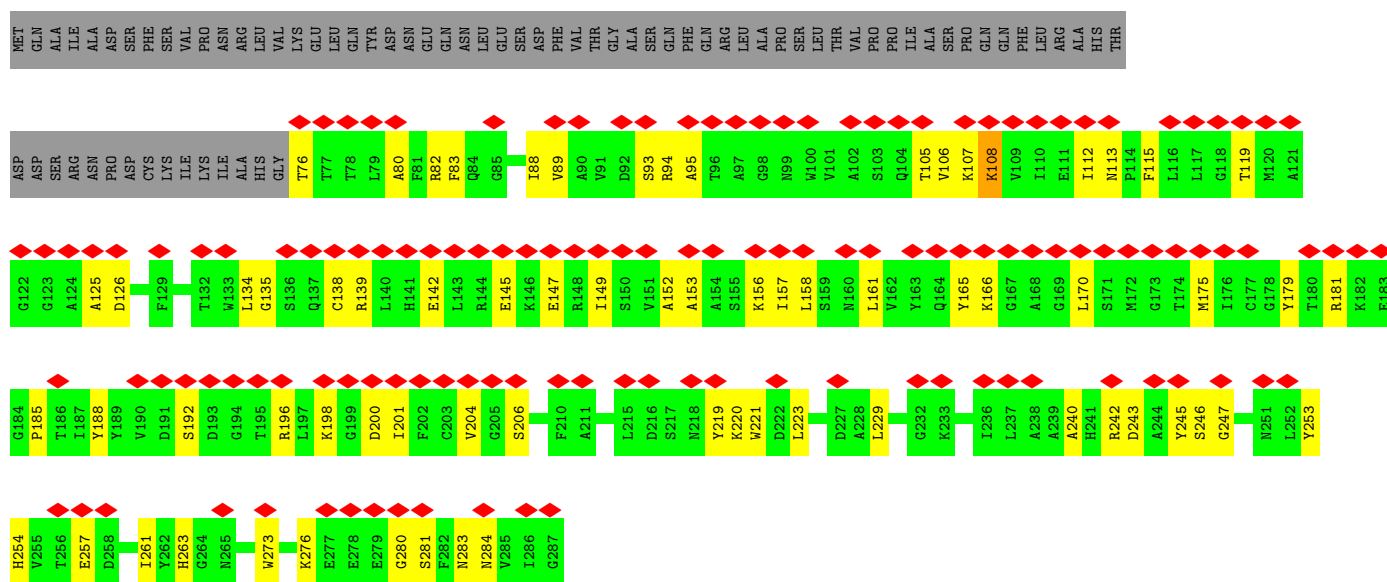




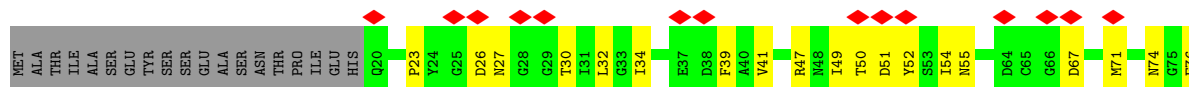
• Molecule 5: Proteasome subunit beta type-5

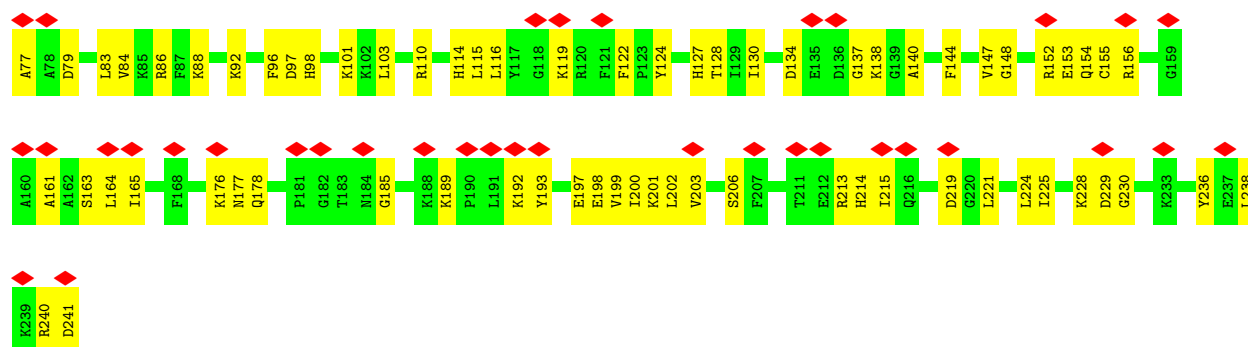


• Molecule 5: Proteasome subunit beta type-5

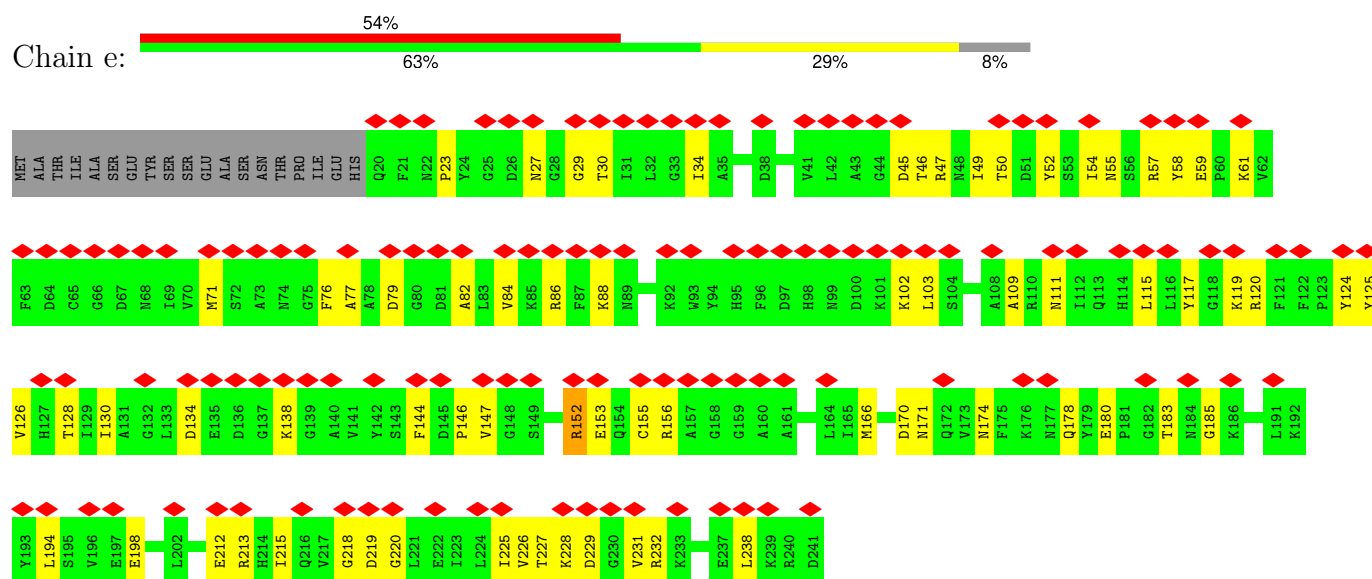


• Molecule 6: Proteasome subunit beta type-6

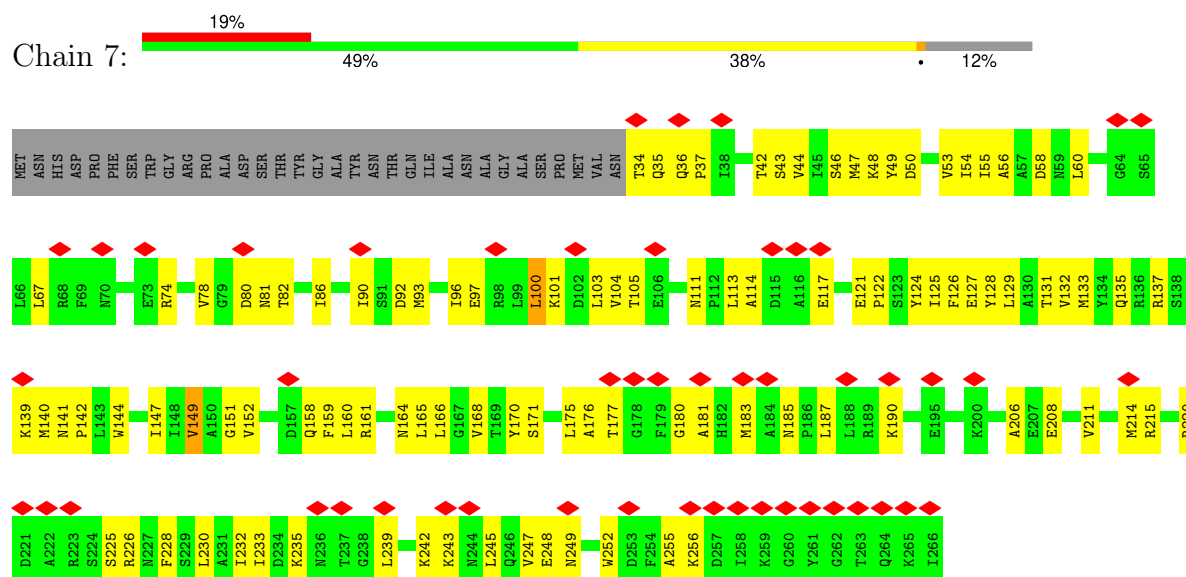




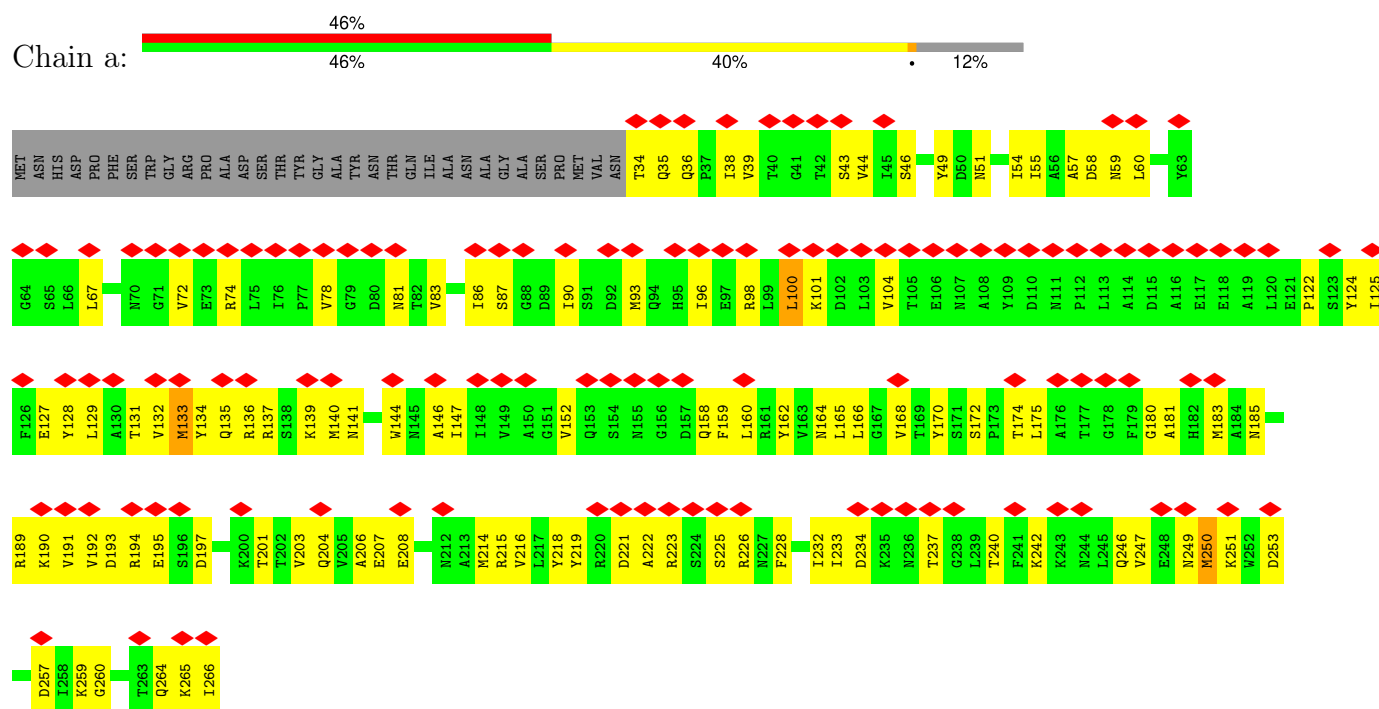
• Molecule 6: Proteasome subunit beta type-6



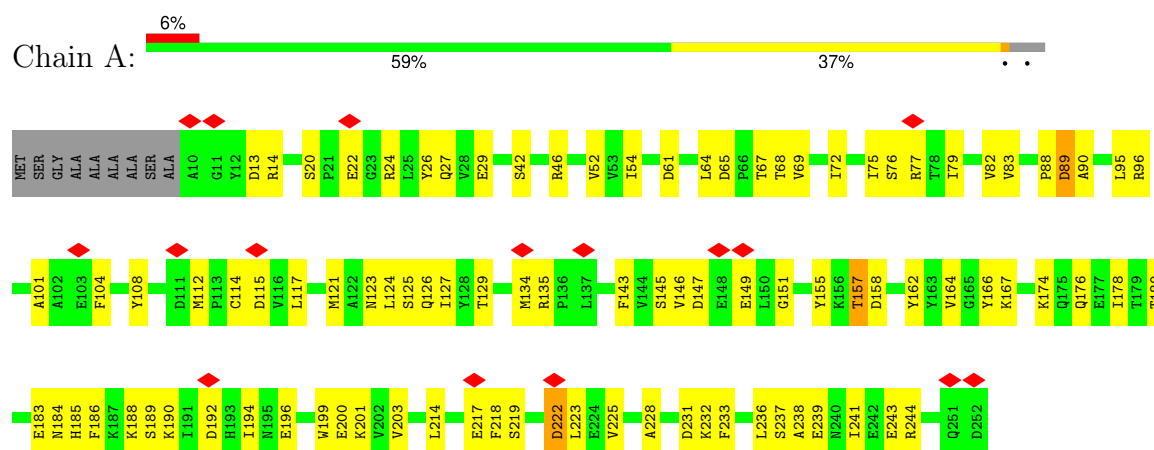
• Molecule 7: Proteasome subunit beta type-7



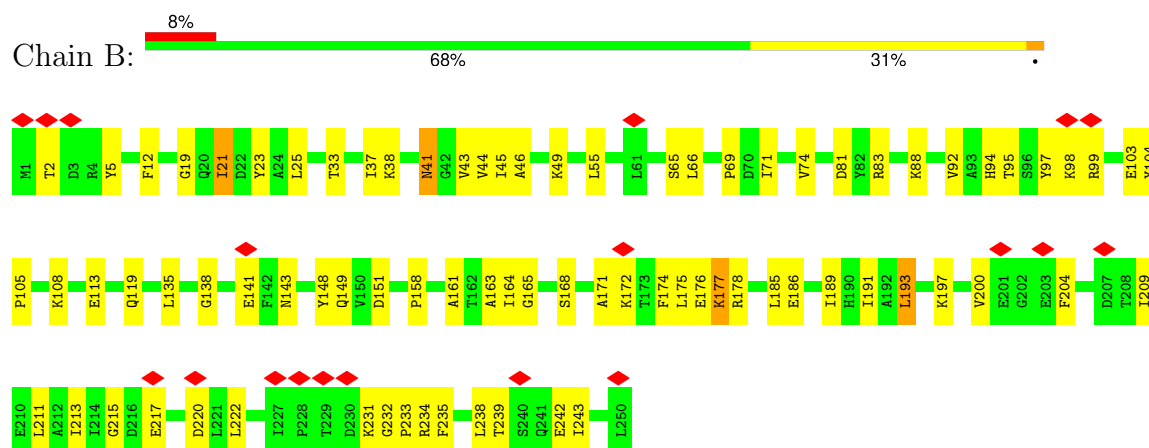
• Molecule 7: Proteasome subunit beta type-7



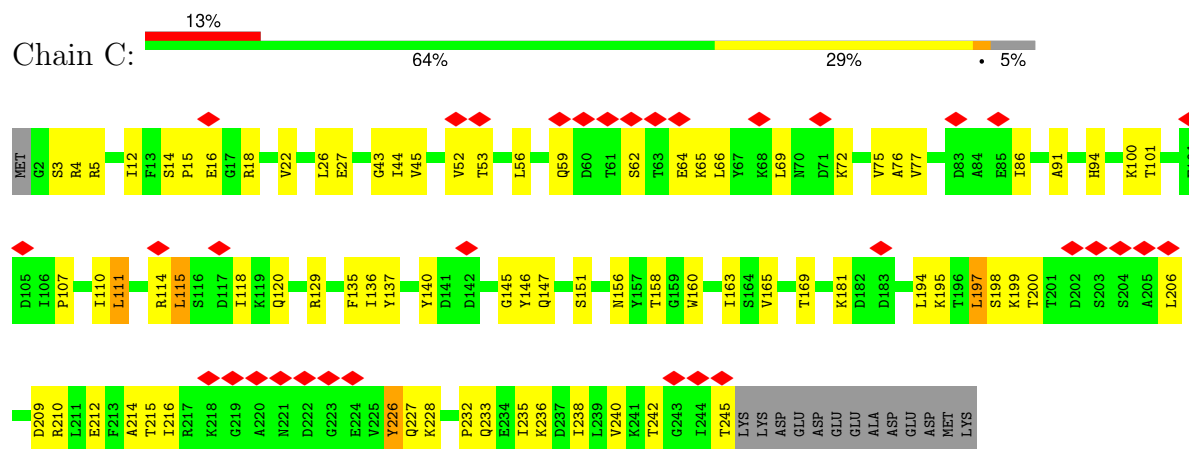
• Molecule 8: Proteasome subunit alpha type-1



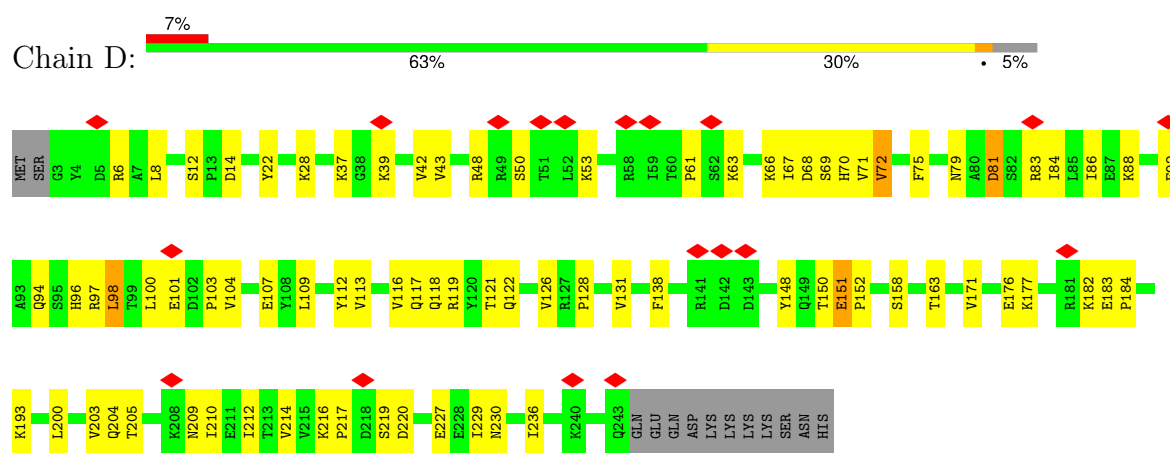
• Molecule 9: Proteasome subunit alpha type-2



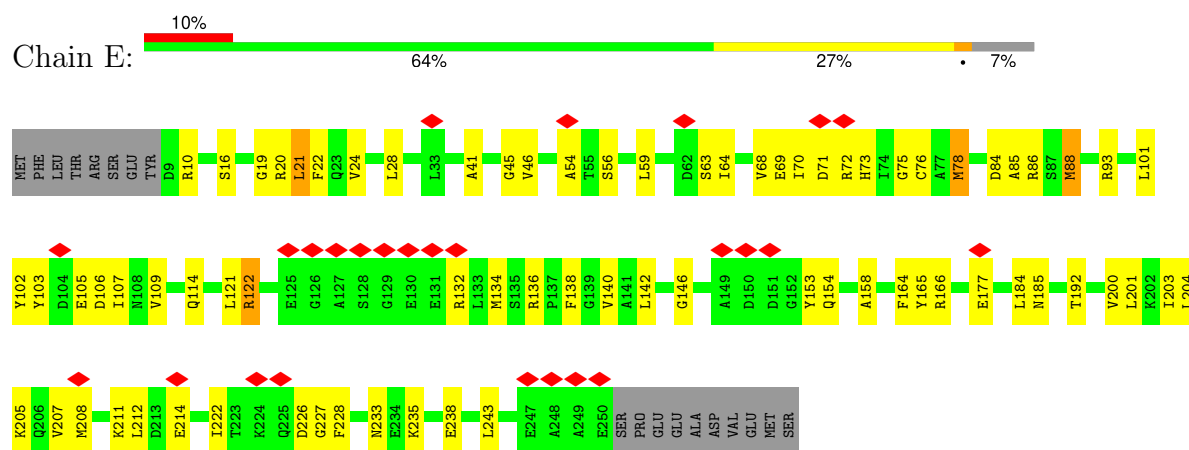
- Molecule 10: Proteasome subunit alpha type-3



- Molecule 11: Proteasome subunit alpha type-4

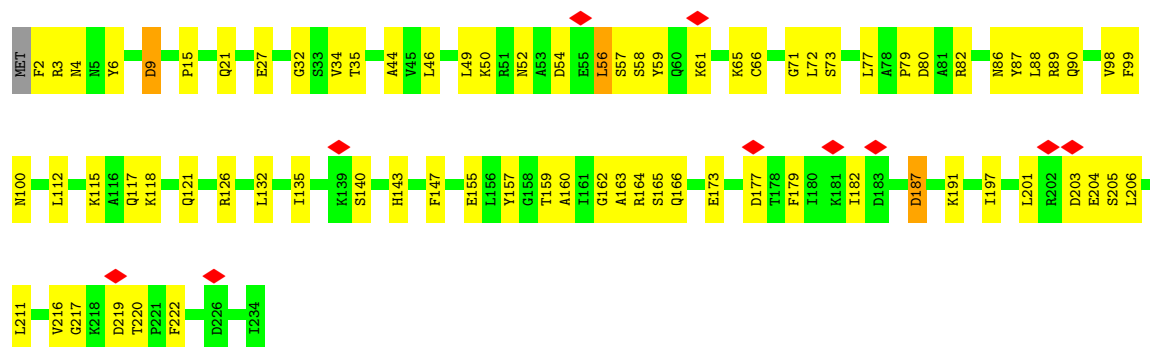


- Molecule 12: Proteasome subunit alpha type-5

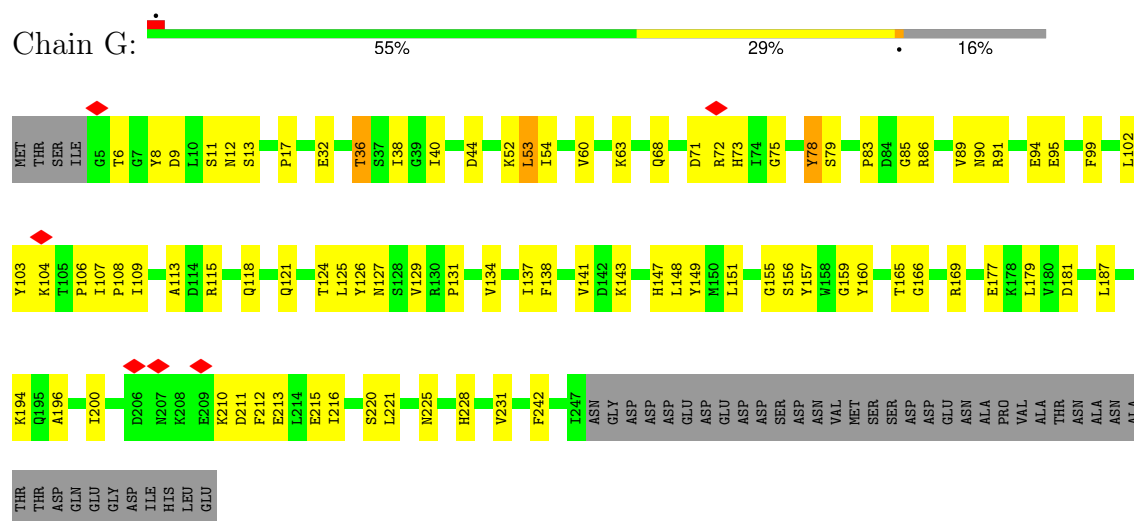


- Molecule 13: Proteasome subunit alpha type-6

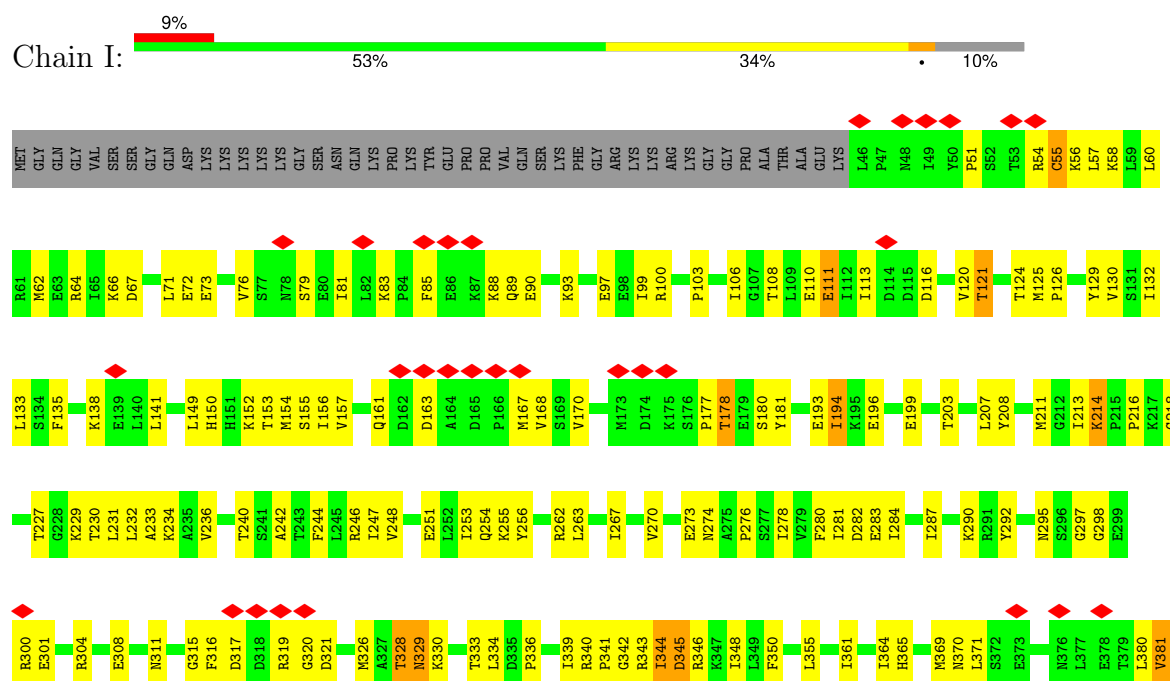




- Molecule 14: Probable proteasome subunit alpha type-7



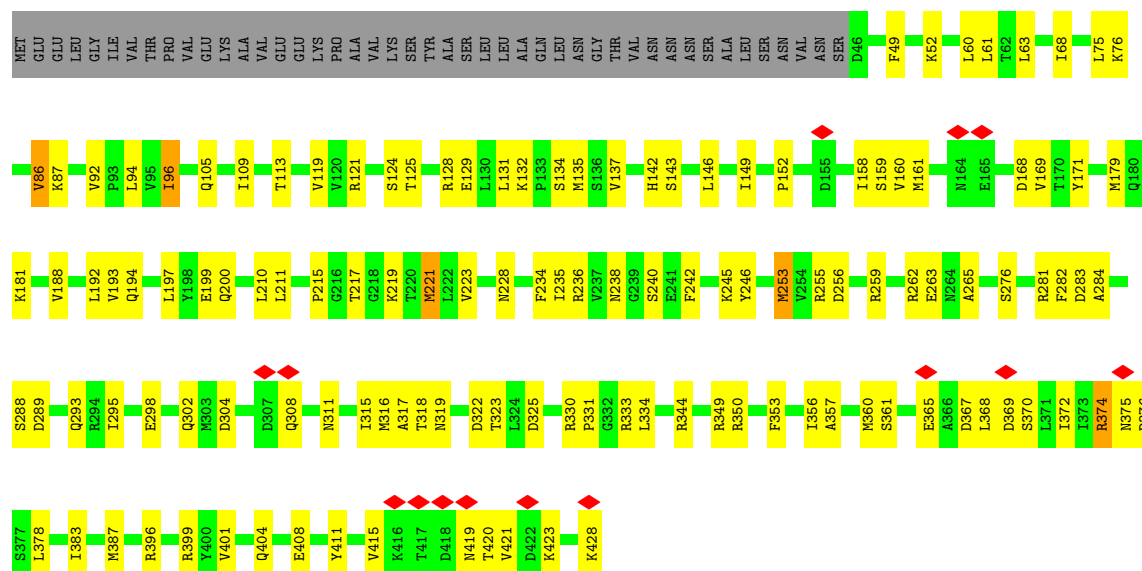
- Molecule 15: 26S proteasome regulatory subunit 4 homolog





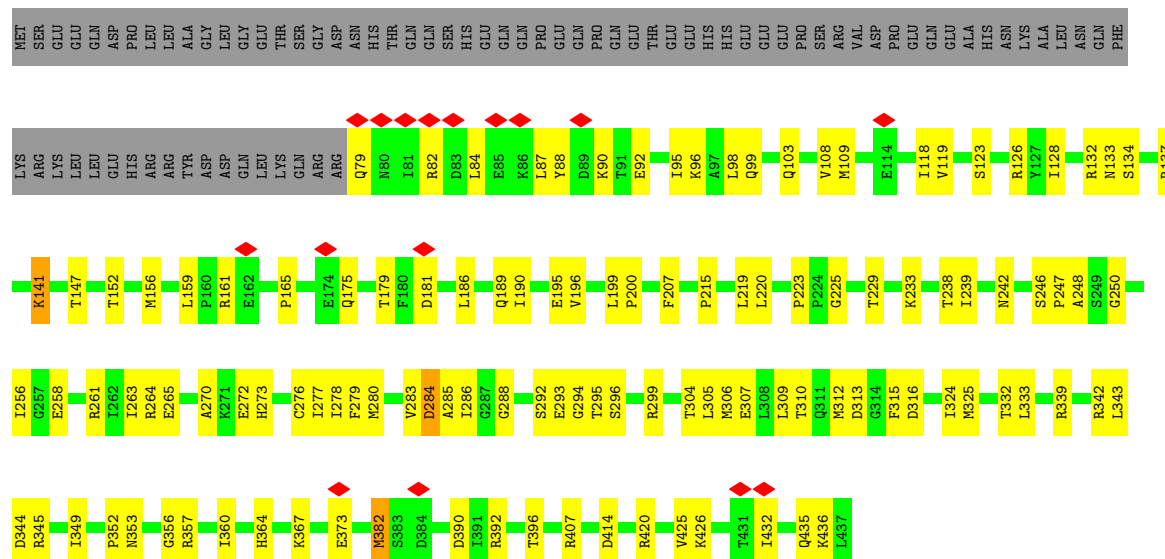
- Molecule 16: 26S proteasome regulatory subunit 6B homolog

Chain K: 59% 29% 11%



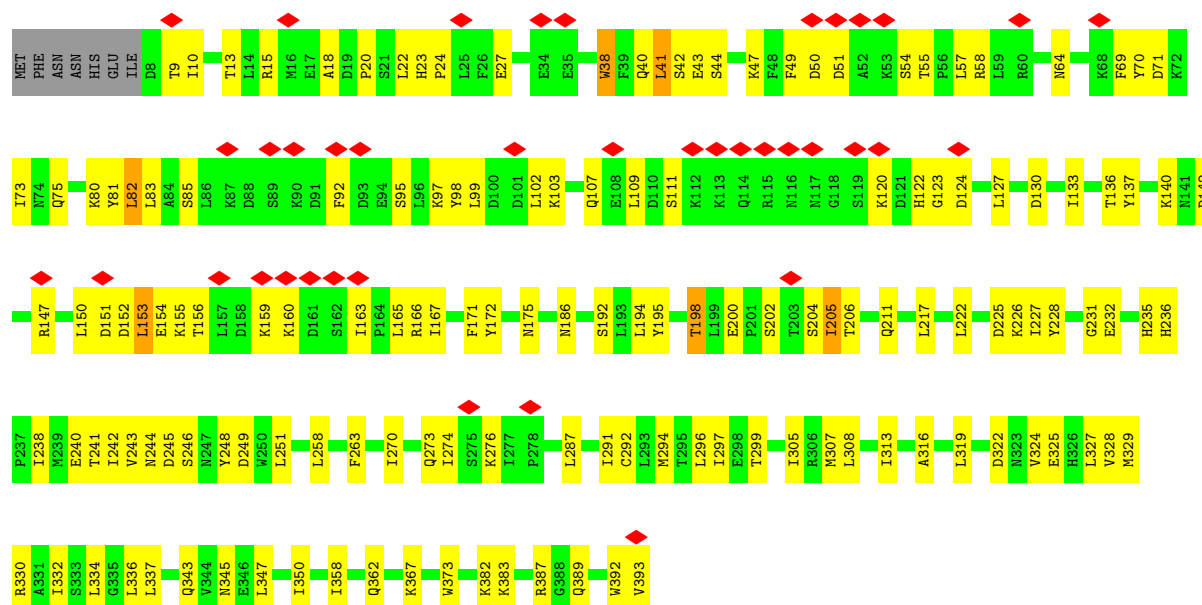
- Molecule 17: 26S proteasome subunit RPT4

Chain L: 55% 27% 18%

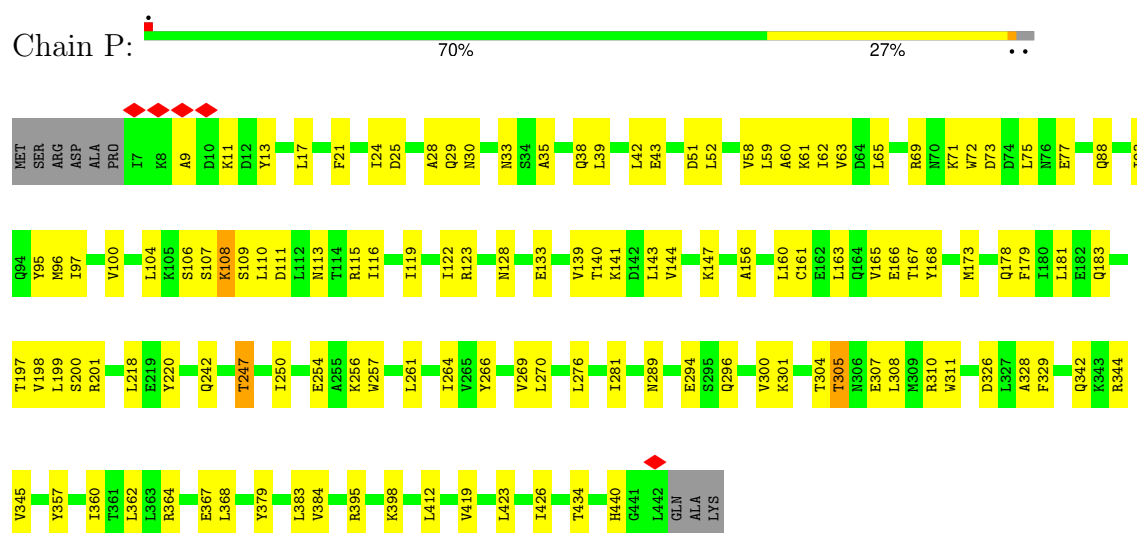


- Molecule 18: 26S proteasome regulatory subunit RPN9

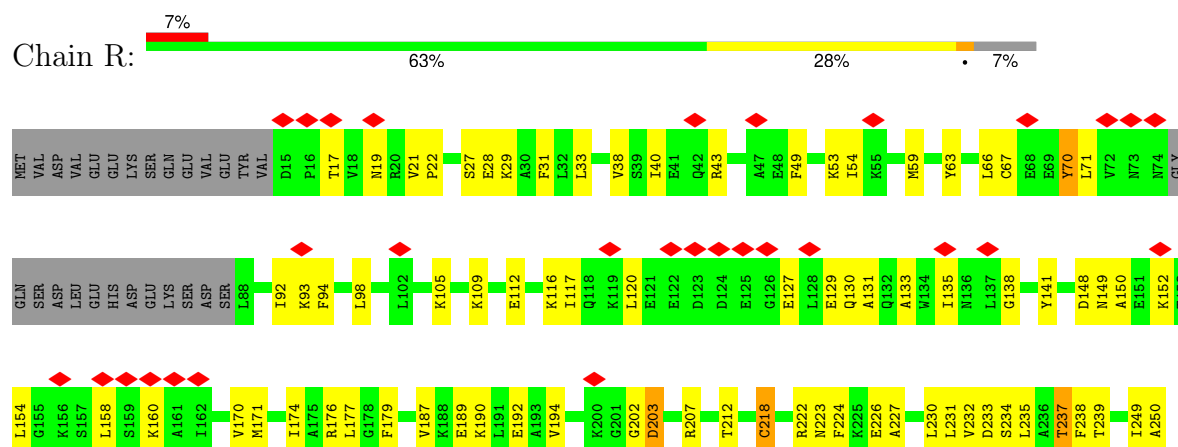
Chain O: 10% 60% 36%

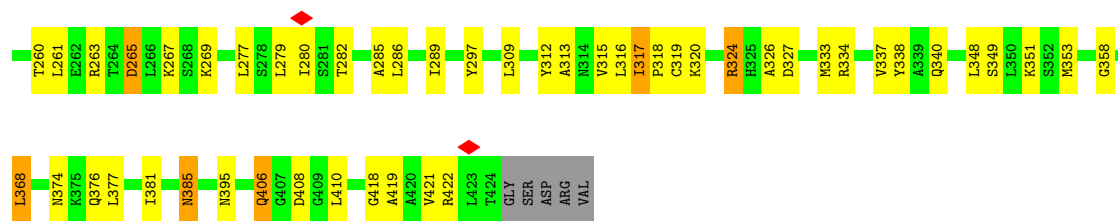


• Molecule 19: 26S proteasome regulatory subunit RPN5



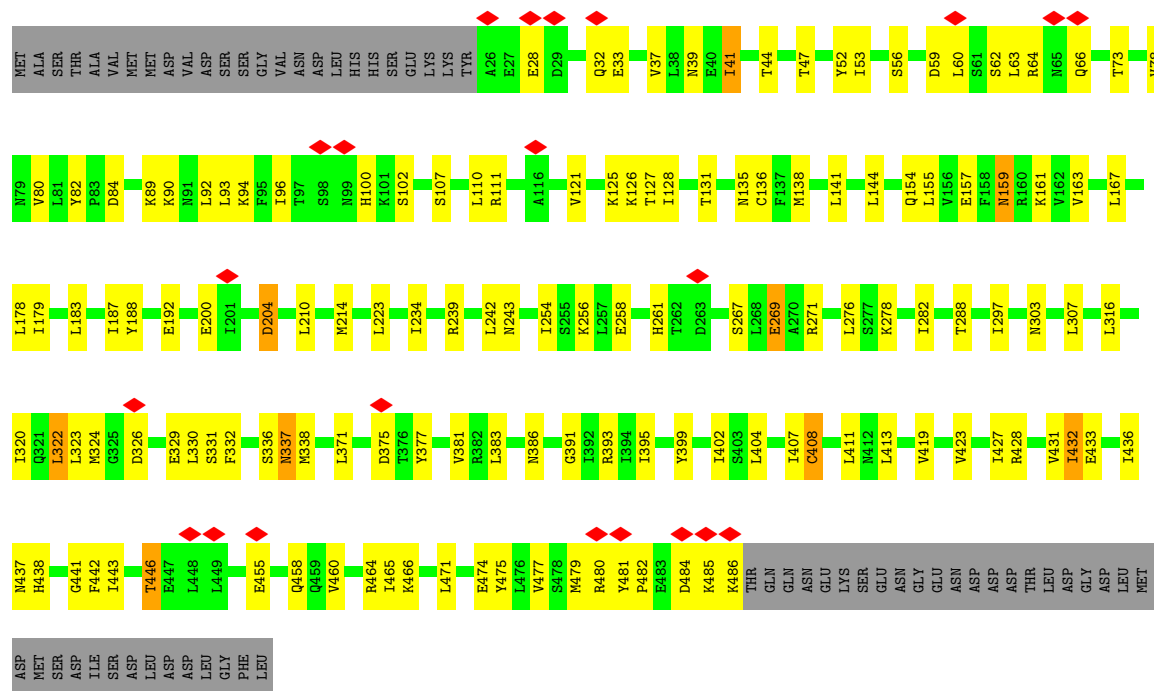
• Molecule 20: 26S proteasome regulatory subunit RPN7





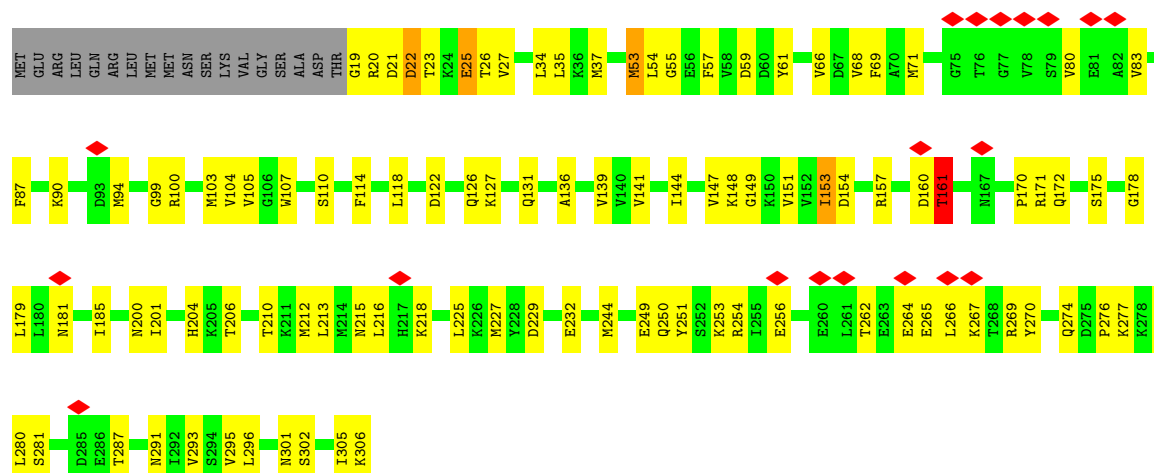
• Molecule 21: 26S proteasome regulatory subunit RPN3

Chain S: 61% 25% 12%

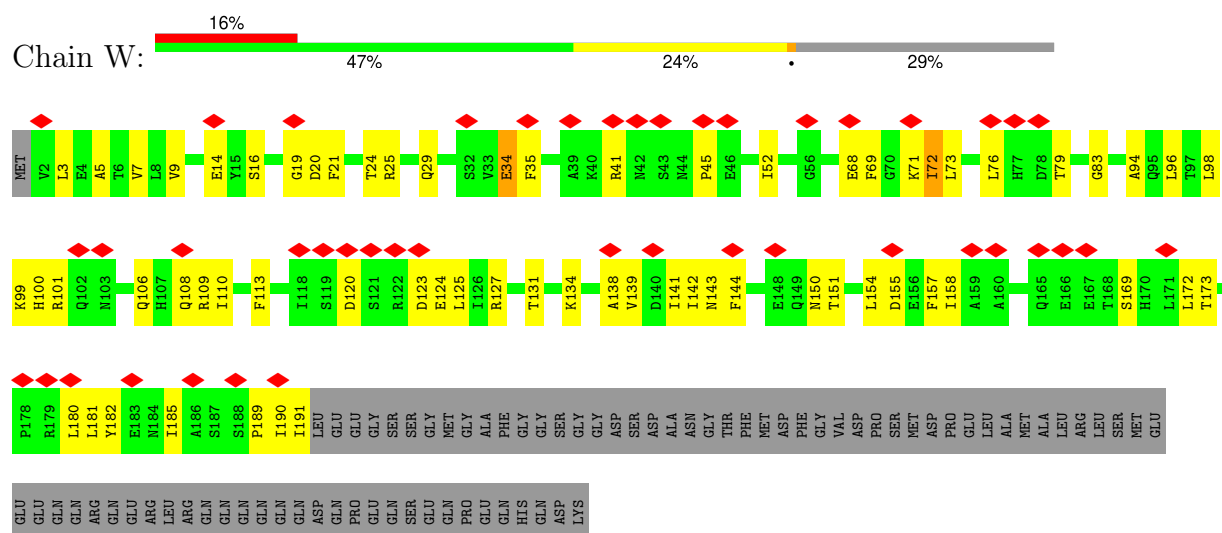


• Molecule 22: Ubiquitin carboxyl-terminal hydrolase RPN11

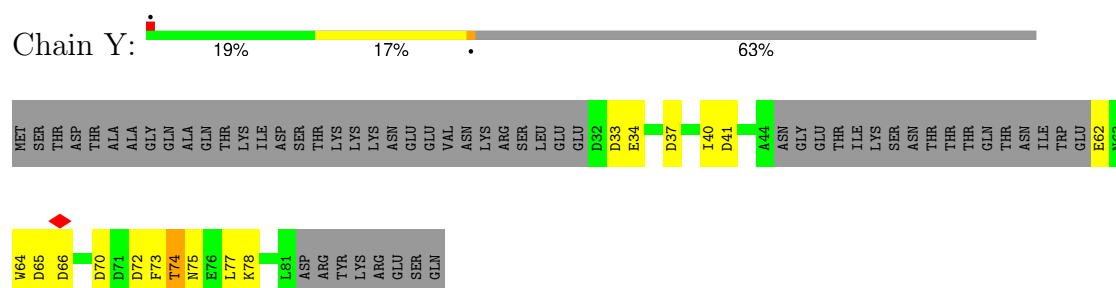
Chain V: 6% 60% 32% 6%



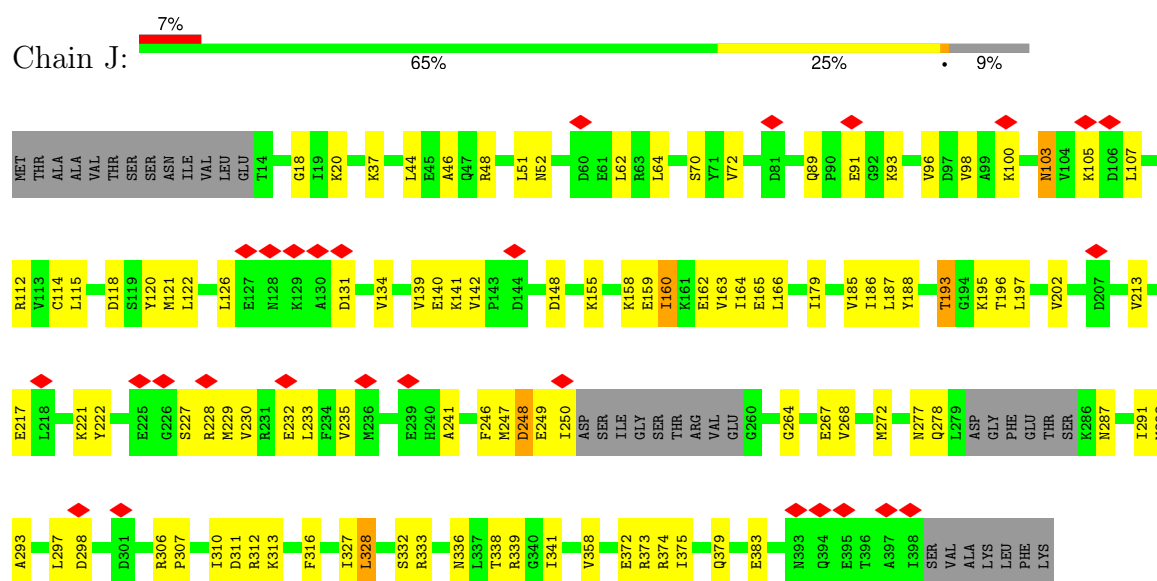
- Molecule 23: 26S proteasome regulatory subunit RPN10



- Molecule 24: 26S proteasome complex subunit SEM1

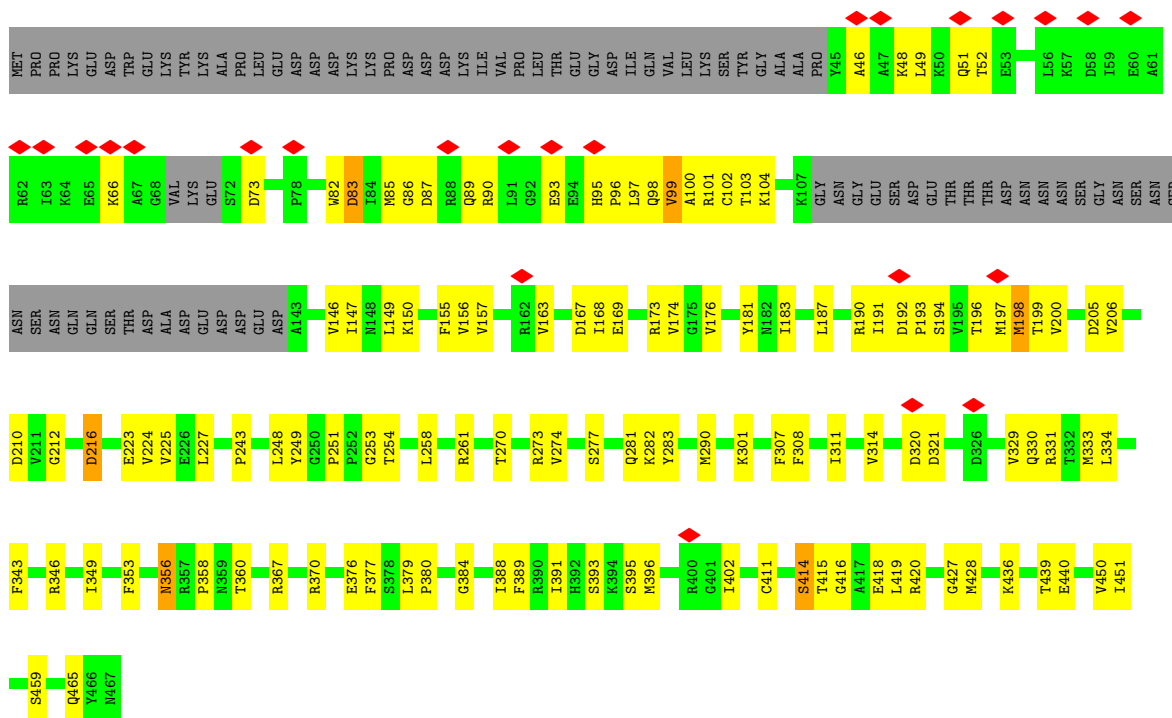


- Molecule 25: 26S proteasome regulatory subunit 8 homolog

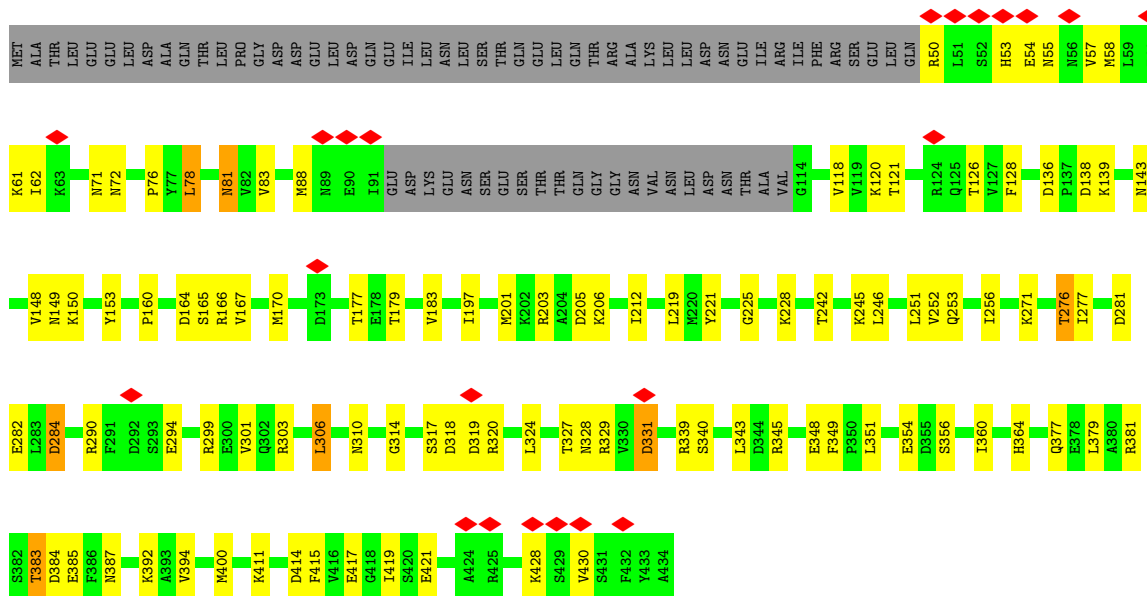


- Molecule 26: 26S proteasome regulatory subunit 7 homolog

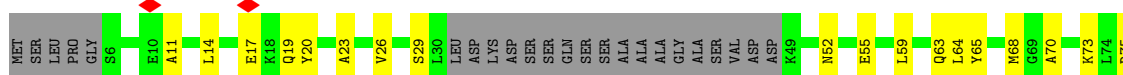


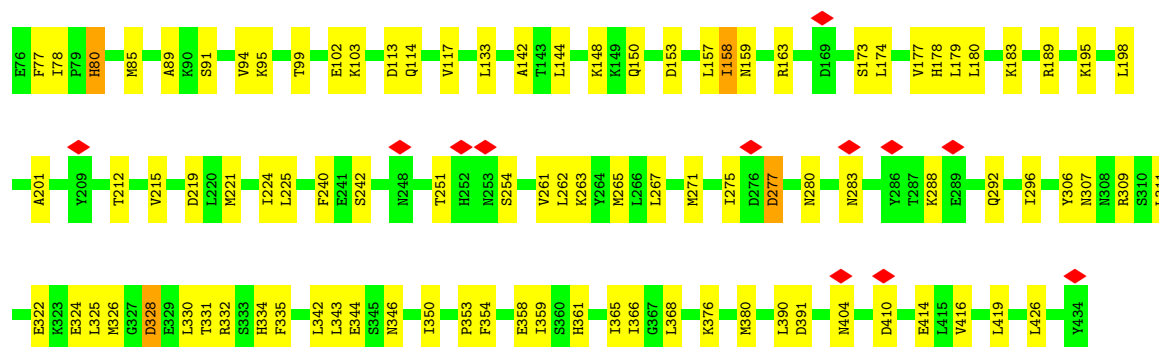


- Molecule 27: 26S proteasome regulatory subunit 6A

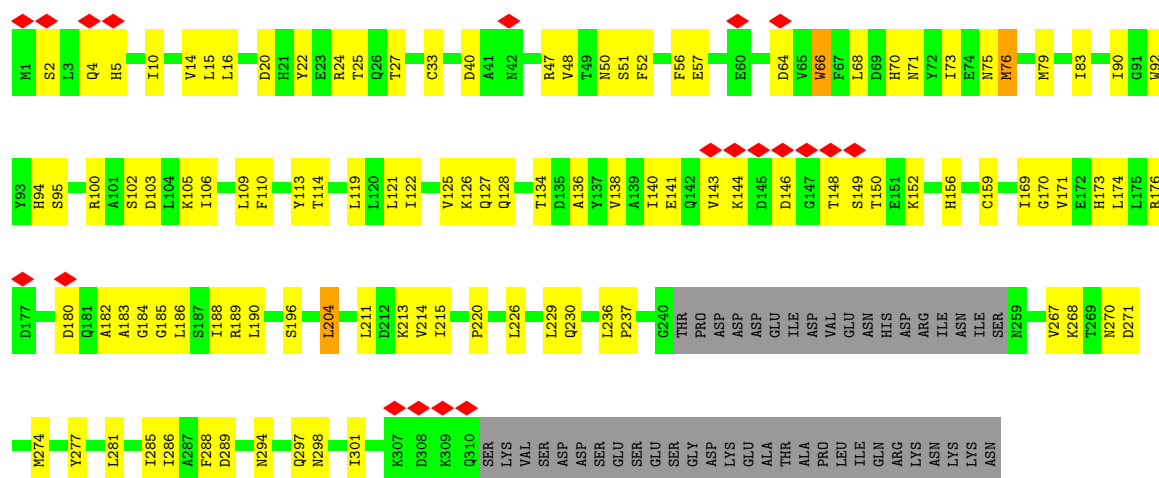


- Molecule 28: 26S proteasome regulatory subunit RPN6

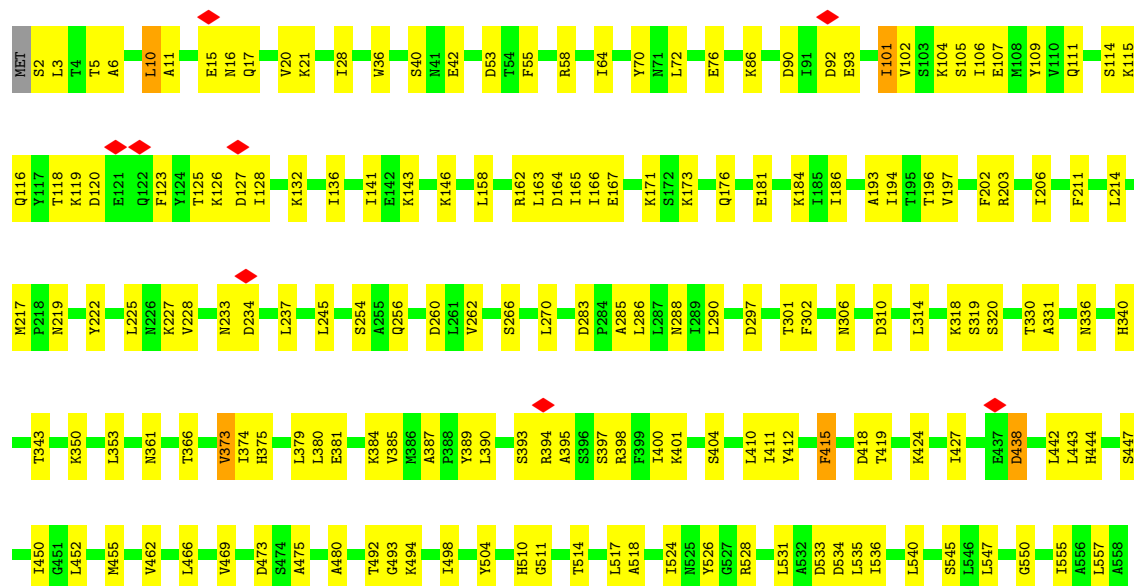


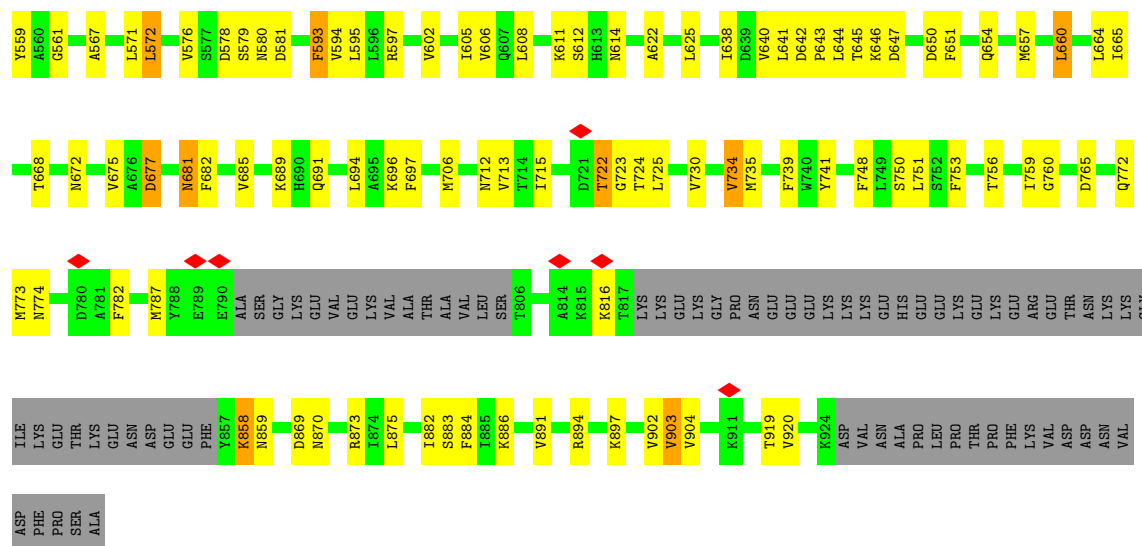


• Molecule 29: 26S proteasome regulatory subunit RPN8

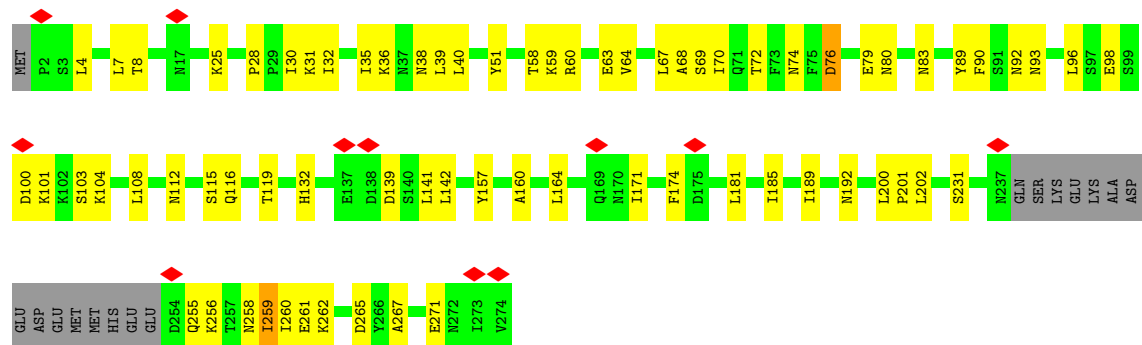


• Molecule 30: 26S proteasome regulatory subunit RPN2

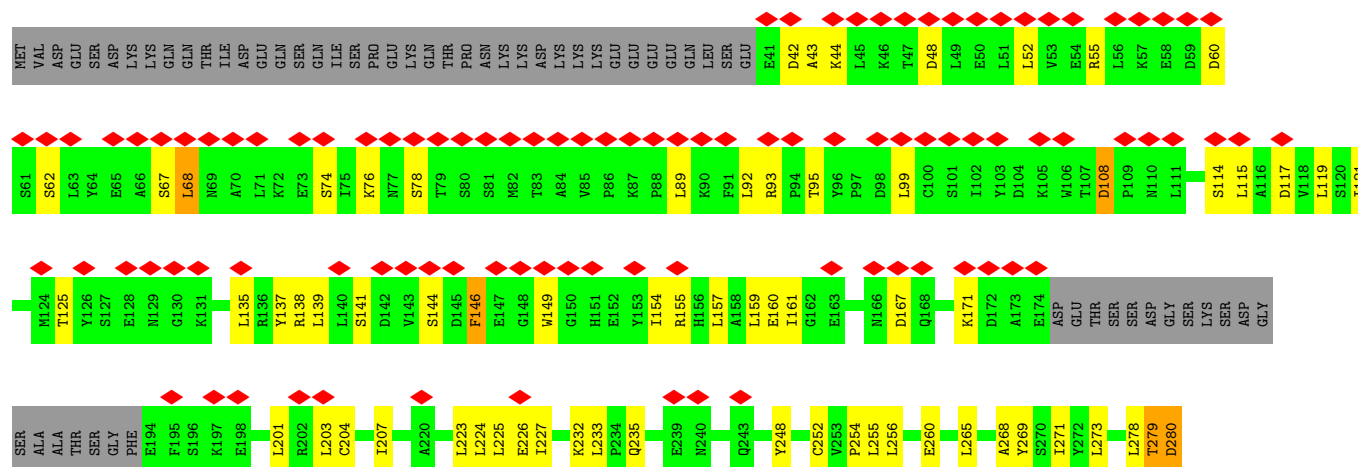




• Molecule 31: 26S proteasome regulatory subunit RPN12



• Molecule 32: 26S proteasome regulatory subunit RPN1





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 110527                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TALOS ARCTICA                       | Depositor |
| Voltage (kV)                         | 200                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 2000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 1.926                                   | Depositor |
| Minimum map value                    | -0.797                                  | Depositor |
| Average map value                    | 0.002                                   | Depositor |
| Map value standard deviation         | 0.072                                   | Depositor |
| Recommended contour level            | 0.33                                    | Depositor |
| Map size (Å)                         | 379.1, 379.1, 379.1                     | wwPDB     |
| Map dimensions                       | 340, 340, 340                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.115, 1.115, 1.115                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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   | 1     | 0.11         | 0/1605      | 0.30        | 0/2171        |
| 1   | b     | 0.11         | 0/1605      | 0.28        | 0/2171        |
| 2   | 2     | 0.11         | 0/1715      | 0.31        | 0/2326        |
| 2   | i     | 0.09         | 0/1715      | 0.27        | 0/2326        |
| 3   | 3     | 0.11         | 0/1611      | 0.29        | 0/2174        |
| 3   | h     | 0.11         | 0/1611      | 0.28        | 0/2174        |
| 4   | 4     | 0.11         | 0/1613      | 0.34        | 0/2173        |
| 4   | g     | 0.11         | 0/1613      | 0.32        | 0/2173        |
| 5   | 5     | 0.10         | 0/1681      | 0.30        | 0/2274        |
| 5   | f     | 0.09         | 0/1681      | 0.29        | 0/2274        |
| 6   | 6     | 0.10         | 0/1795      | 0.29        | 0/2420        |
| 6   | e     | 0.09         | 0/1795      | 0.24        | 0/2420        |
| 7   | 7     | 0.12         | 0/1855      | 0.36        | 0/2514        |
| 7   | a     | 0.12         | 0/1855      | 0.36        | 0/2514        |
| 8   | A     | 0.13         | 0/1959      | 0.33        | 0/2652        |
| 9   | B     | 0.13         | 0/1952      | 0.37        | 1/2642 (0.0%) |
| 10  | C     | 0.11         | 0/1934      | 0.31        | 0/2618        |
| 11  | D     | 0.12         | 0/1919      | 0.31        | 0/2598        |
| 12  | E     | 0.11         | 0/1886      | 0.29        | 0/2541        |
| 13  | F     | 0.16         | 0/1823      | 0.34        | 0/2463        |
| 14  | G     | 0.14         | 0/1928      | 0.37        | 0/2603        |
| 15  | I     | 0.14         | 0/3120      | 0.42        | 1/4204 (0.0%) |
| 16  | K     | 0.14         | 0/3078      | 0.35        | 0/4154        |
| 17  | L     | 0.14         | 0/2862      | 0.35        | 0/3851        |
| 18  | O     | 0.11         | 0/3230      | 0.33        | 0/4357        |
| 19  | P     | 0.11         | 0/3629      | 0.31        | 0/4894        |
| 20  | R     | 0.12         | 0/3249      | 0.33        | 0/4385        |
| 21  | S     | 0.11         | 0/3839      | 0.31        | 0/5186        |
| 22  | V     | 0.15         | 0/2302      | 0.39        | 0/3105        |
| 23  | W     | 0.11         | 0/1507      | 0.29        | 0/2045        |
| 24  | Y     | 0.15         | 0/287       | 0.40        | 0/391         |
| 25  | J     | 0.13         | 0/2950      | 0.35        | 0/3960        |

| Mol | Chain | Bond lengths |         | Bond angles |                 |
|-----|-------|--------------|---------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5         |
| 26  | H     | 0.14         | 0/3063  | 0.37        | 0/4120          |
| 27  | M     | 0.13         | 0/2863  | 0.36        | 0/3855          |
| 28  | Q     | 0.12         | 0/3402  | 0.31        | 0/4577          |
| 29  | U     | 0.14         | 0/2364  | 0.37        | 0/3190          |
| 30  | N     | 0.12         | 0/6835  | 0.32        | 1/9243 (0.0%)   |
| 31  | T     | 0.12         | 0/2147  | 0.32        | 0/2900          |
| 32  | o     | 0.12         | 0/6462  | 0.32        | 0/8771          |
| All | All   | 0.12         | 0/94340 | 0.33        | 3/127409 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 16  | K     | 0                   | 1                   |
| 32  | o     | 0                   | 1                   |
| All | All   | 0                   | 2                   |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 15  | I     | 381 | VAL  | N-CA-C  | -6.17 | 107.27      | 113.20   |
| 30  | N     | 86  | LYS  | CB-CA-C | -5.48 | 109.78      | 117.23   |
| 9   | B     | 2   | THR  | CB-CA-C | -5.32 | 109.46      | 115.79   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 16  | K     | 92  | VAL  | Peptide |
| 32  | o     | 953 | THR  | Peptide |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 1     | 1576  | 0        | 1552     | 62      | 0            |
| 1   | b     | 1576  | 0        | 1552     | 51      | 0            |
| 2   | 2     | 1684  | 0        | 1685     | 62      | 0            |
| 2   | i     | 1684  | 0        | 1685     | 54      | 0            |
| 3   | 3     | 1581  | 0        | 1571     | 62      | 0            |
| 3   | h     | 1581  | 0        | 1571     | 62      | 0            |
| 4   | 4     | 1585  | 0        | 1590     | 58      | 0            |
| 4   | g     | 1585  | 0        | 1590     | 61      | 0            |
| 5   | 5     | 1644  | 0        | 1592     | 66      | 0            |
| 5   | f     | 1644  | 0        | 1592     | 55      | 0            |
| 6   | 6     | 1757  | 0        | 1708     | 66      | 0            |
| 6   | e     | 1757  | 0        | 1708     | 55      | 0            |
| 7   | 7     | 1824  | 0        | 1829     | 79      | 0            |
| 7   | a     | 1824  | 0        | 1829     | 81      | 0            |
| 8   | A     | 1921  | 0        | 1910     | 73      | 0            |
| 9   | B     | 1915  | 0        | 1929     | 59      | 0            |
| 10  | C     | 1904  | 0        | 1901     | 57      | 0            |
| 11  | D     | 1890  | 0        | 1900     | 59      | 0            |
| 12  | E     | 1861  | 0        | 1836     | 60      | 0            |
| 13  | F     | 1795  | 0        | 1797     | 61      | 0            |
| 14  | G     | 1888  | 0        | 1880     | 71      | 0            |
| 15  | I     | 3078  | 0        | 3147     | 131     | 0            |
| 16  | K     | 3035  | 0        | 3099     | 102     | 0            |
| 17  | L     | 2820  | 0        | 2895     | 99      | 0            |
| 18  | O     | 3169  | 0        | 3196     | 105     | 0            |
| 19  | P     | 3575  | 0        | 3662     | 99      | 0            |
| 20  | R     | 3195  | 0        | 3214     | 94      | 0            |
| 21  | S     | 3770  | 0        | 3819     | 101     | 0            |
| 22  | V     | 2267  | 0        | 2266     | 77      | 0            |
| 23  | W     | 1484  | 0        | 1494     | 47      | 0            |
| 24  | Y     | 281   | 0        | 224      | 15      | 0            |
| 25  | J     | 2913  | 0        | 3050     | 89      | 0            |
| 26  | H     | 3016  | 0        | 3086     | 111     | 0            |
| 27  | M     | 2827  | 0        | 2887     | 89      | 0            |
| 28  | Q     | 3347  | 0        | 3380     | 75      | 0            |
| 29  | U     | 2333  | 0        | 2396     | 83      | 0            |
| 30  | N     | 6725  | 0        | 6796     | 189     | 0            |
| 31  | T     | 2106  | 0        | 2099     | 50      | 0            |
| 32  | o     | 6347  | 0        | 6319     | 192     | 0            |
| 33  | H     | 1     | 0        | 0        | 0       | 0            |
| 33  | I     | 1     | 0        | 0        | 0       | 0            |
| 33  | K     | 1     | 0        | 0        | 0       | 0            |
| 33  | L     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 33  | M     | 1     | 0        | 0        | 0       | 0            |
| 34  | H     | 31    | 0        | 12       | 3       | 0            |
| 34  | J     | 31    | 0        | 12       | 3       | 0            |
| 34  | K     | 31    | 0        | 12       | 6       | 0            |
| 34  | L     | 31    | 0        | 12       | 0       | 0            |
| 34  | M     | 31    | 0        | 12       | 4       | 0            |
| 35  | V     | 1     | 0        | 0        | 0       | 0            |
| 36  | J     | 27    | 0        | 12       | 4       | 0            |
| All | All   | 92952 | 0        | 93308    | 2720    | 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 15.

All (2720) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:K:61:LEU:HD21  | 25:J:37:LYS:HB3   | 1.49                     | 0.94              |
| 28:Q:419:LEU:HD23 | 29:U:285:ILE:HD12 | 1.48                     | 0.93              |
| 29:U:126:LYS:HB2  | 29:U:128:GLN:HE22 | 1.36                     | 0.90              |
| 15:I:67:ASP:HB3   | 32:o:614:VAL:HG11 | 1.58                     | 0.85              |
| 12:E:166:ARG:HG2  | 13:F:58:SER:HB3   | 1.59                     | 0.82              |
| 19:P:97:ILE:HD11  | 19:P:122:ILE:HG23 | 1.61                     | 0.81              |
| 25:J:230:VAL:HG11 | 25:J:268:VAL:HG13 | 1.62                     | 0.81              |
| 13:F:179:PHE:HA   | 13:F:182:ILE:HD12 | 1.62                     | 0.80              |
| 3:h:187:VAL:HG23  | 3:h:200:LEU:HD21  | 1.64                     | 0.79              |
| 32:o:470:ALA:O    | 32:o:474:LEU:HB2  | 1.82                     | 0.79              |
| 32:o:737:ALA:HA   | 32:o:775:MET:HE1  | 1.64                     | 0.79              |
| 6:6:47:ARG:HB2    | 6:6:219:ASP:HB2   | 1.65                     | 0.79              |
| 16:K:282:PHE:HE2  | 16:K:293:GLN:HB2  | 1.48                     | 0.78              |
| 28:Q:277:ASP:N    | 28:Q:277:ASP:OD1  | 2.16                     | 0.78              |
| 21:S:465:ILE:HD11 | 29:U:277:TYR:HA   | 1.66                     | 0.78              |
| 22:V:216:LEU:HD13 | 29:U:171:VAL:HG11 | 1.66                     | 0.77              |
| 21:S:482:PRO:HB3  | 29:U:298:ASN:HB2  | 1.67                     | 0.77              |
| 4:g:174:MET:HE3   | 4:g:174:MET:H     | 1.49                     | 0.76              |
| 19:P:59:LEU:HD13  | 19:P:62:ILE:HD11  | 1.68                     | 0.76              |
| 32:o:894:MET:HB3  | 32:o:900:LEU:HD11 | 1.67                     | 0.76              |
| 18:O:242:ILE:HG21 | 18:O:248:TYR:HB2  | 1.66                     | 0.76              |
| 30:N:657:MET:HE1  | 30:N:685:VAL:HG21 | 1.67                     | 0.75              |
| 11:D:122:GLN:NE2  | 12:E:134:MET:SD   | 2.60                     | 0.75              |
| 4:4:162:LYS:NZ    | 4:4:194:ASP:O     | 2.20                     | 0.75              |
| 16:K:245:LYS:NZ   | 17:L:258:GLU:OE2  | 2.19                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:V:212:MET:SD   | 29:U:15:LEU:HD21  | 2.27                     | 0.74              |
| 30:N:254:SER:HB3  | 30:N:286:LEU:HD21 | 1.67                     | 0.74              |
| 16:K:378:LEU:HD21 | 16:K:415:VAL:HG21 | 1.69                     | 0.74              |
| 13:F:173:GLU:OE2  | 27:M:381:ARG:NH1  | 2.20                     | 0.74              |
| 14:G:107:ILE:HD12 | 14:G:108:PRO:HD2  | 1.67                     | 0.74              |
| 17:L:87:LEU:HA    | 17:L:90:LYS:HD2   | 1.69                     | 0.74              |
| 21:S:431:VAL:HG13 | 21:S:432:ILE:HG12 | 1.69                     | 0.74              |
| 7:a:226:ARG:HG3   | 7:a:247:VAL:HG23  | 1.69                     | 0.74              |
| 4:4:62:ALA:HB2    | 11:D:98:LEU:HD11  | 1.70                     | 0.74              |
| 25:J:52:ASN:HD21  | 30:N:612:SER:HA   | 1.51                     | 0.74              |
| 10:C:206:LEU:HA   | 10:C:210:ARG:HH12 | 1.51                     | 0.74              |
| 32:o:597:SER:HB2  | 32:o:623:ARG:HH22 | 1.53                     | 0.74              |
| 10:C:107:PRO:HG2  | 10:C:110:ILE:HG12 | 1.68                     | 0.73              |
| 17:L:88:TYR:OH    | 27:M:61:LYS:HB2   | 1.88                     | 0.73              |
| 3:3:15:MET:HB2    | 3:3:22:ALA:HB3    | 1.70                     | 0.73              |
| 2:2:196:LEU:HB3   | 6:e:215:ILE:HB    | 1.68                     | 0.73              |
| 20:R:218:CYS:SG   | 20:R:223:ASN:ND2  | 2.62                     | 0.73              |
| 4:4:103:LEU:HD13  | 4:4:133:HIS:HE1   | 1.52                     | 0.73              |
| 31:T:90:PHE:HB3   | 31:T:132:HIS:HD2  | 1.54                     | 0.73              |
| 22:V:178:GLY:HA2  | 22:V:200:ASN:HD21 | 1.54                     | 0.73              |
| 22:V:19:GLY:HA2   | 30:N:361:ASN:HD21 | 1.52                     | 0.73              |
| 29:U:144:LYS:HD3  | 29:U:148:THR:HB   | 1.70                     | 0.72              |
| 18:O:160:LYS:HB2  | 18:O:163:ILE:HG22 | 1.71                     | 0.72              |
| 18:O:200:GLU:HG2  | 18:O:202:SER:H    | 1.55                     | 0.72              |
| 21:S:258:GLU:OE1  | 21:S:258:GLU:N    | 2.21                     | 0.72              |
| 32:o:384:SER:HB3  | 32:o:406:TRP:HZ2  | 1.54                     | 0.72              |
| 13:F:49:LEU:HB2   | 13:F:197:ILE:HD11 | 1.70                     | 0.72              |
| 21:S:155:LEU:O    | 21:S:159:ASN:ND2  | 2.23                     | 0.72              |
| 5:f:80:ALA:HB3    | 5:f:175:MET:HE2   | 1.71                     | 0.72              |
| 27:M:242:THR:HB   | 27:M:276:THR:HG22 | 1.71                     | 0.72              |
| 30:N:518:ALA:HB1  | 30:N:550:GLY:HA3  | 1.71                     | 0.72              |
| 15:I:100:ARG:NH2  | 26:H:73:ASP:O     | 2.22                     | 0.72              |
| 8:A:184:ASN:OD1   | 8:A:185:HIS:N     | 2.23                     | 0.72              |
| 30:N:557:LEU:HD21 | 30:N:734:VAL:HG21 | 1.71                     | 0.71              |
| 5:5:242:ARG:HH22  | 5:5:284:ASN:HD21  | 1.38                     | 0.71              |
| 26:H:48:LYS:O     | 26:H:52:THR:OG1   | 2.09                     | 0.71              |
| 22:V:179:LEU:HB3  | 30:N:694:LEU:HD21 | 1.73                     | 0.71              |
| 25:J:195:LYS:NZ   | 36:J:502:ADP:O1B  | 2.23                     | 0.71              |
| 32:o:474:LEU:HD13 | 32:o:493:LEU:HG   | 1.72                     | 0.71              |
| 15:I:66:LYS:NZ    | 26:H:52:THR:O     | 2.23                     | 0.71              |
| 26:H:258:LEU:HD22 | 34:H:501:ATP:H2'  | 1.71                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:Q:65:TYR:HA    | 28:Q:68:MET:HE2   | 1.72                     | 0.71              |
| 16:K:135:MET:HE2  | 16:K:135:MET:HA   | 1.73                     | 0.71              |
| 7:a:164:ASN:HD21  | 7:a:168:VAL:HB    | 1.55                     | 0.71              |
| 26:H:331:ARG:HD3  | 27:M:252:VAL:HG21 | 1.74                     | 0.70              |
| 32:o:268:ALA:HA   | 32:o:271:ILE:HD12 | 1.73                     | 0.70              |
| 20:R:261:LEU:HB3  | 20:R:265:ASP:HB2  | 1.71                     | 0.70              |
| 11:D:204:GLN:O    | 11:D:205:THR:OG1  | 2.10                     | 0.70              |
| 4:4:172:MET:HA    | 4:4:172:MET:HE3   | 1.71                     | 0.70              |
| 9:B:189:ILE:HD12  | 9:B:213:ILE:HD11  | 1.74                     | 0.70              |
| 15:I:253:ILE:HD11 | 15:I:287:ILE:HA   | 1.74                     | 0.70              |
| 28:Q:309:ARG:O    | 28:Q:346:ASN:ND2  | 2.24                     | 0.70              |
| 10:C:69:LEU:HD11  | 10:C:75:VAL:HB    | 1.74                     | 0.70              |
| 15:I:120:VAL:HG21 | 15:I:149:LEU:HD21 | 1.71                     | 0.70              |
| 32:o:777:PRO:HB3  | 32:o:811:SER:HA   | 1.74                     | 0.70              |
| 13:F:82:ARG:HH21  | 13:F:86:ASN:HD21  | 1.38                     | 0.70              |
| 19:P:59:LEU:HD12  | 19:P:96:MET:HG3   | 1.74                     | 0.69              |
| 7:a:83:VAL:HG12   | 7:a:233:ILE:HD11  | 1.73                     | 0.69              |
| 2:i:235:PRO:O     | 2:i:238:THR:OG1   | 2.10                     | 0.69              |
| 9:B:103:GLU:OE1   | 9:B:103:GLU:N     | 2.25                     | 0.69              |
| 21:S:90:LYS:HG2   | 21:S:94:LYS:HE3   | 1.74                     | 0.69              |
| 11:D:148:TYR:HE1  | 11:D:158:SER:HB2  | 1.57                     | 0.69              |
| 18:O:50:ASP:OD1   | 18:O:80:LYS:NZ    | 2.25                     | 0.69              |
| 3:3:164:PHE:HB2   | 3:3:189:ILE:HD11  | 1.75                     | 0.69              |
| 3:3:96:TYR:HA     | 3:3:99:ARG:HH12   | 1.57                     | 0.69              |
| 5:5:82:ARG:HD2    | 5:5:185:PRO:HB2   | 1.75                     | 0.69              |
| 16:K:105:GLN:NE2  | 22:V:267:LYS:O    | 2.26                     | 0.69              |
| 17:L:284:ASP:OD2  | 27:M:290:ARG:NH1  | 2.26                     | 0.69              |
| 21:S:93:LEU:HD23  | 21:S:96:ILE:HD11  | 1.75                     | 0.69              |
| 2:2:197:GLY:H     | 6:e:52:TYR:HE1    | 1.41                     | 0.69              |
| 13:F:72:LEU:HD11  | 13:F:88:LEU:HD23  | 1.74                     | 0.69              |
| 19:P:119:ILE:HG21 | 19:P:143:LEU:HB2  | 1.75                     | 0.69              |
| 19:P:160:LEU:HG   | 19:P:183:GLN:HG3  | 1.73                     | 0.69              |
| 6:6:185:GLY:HA3   | 2:i:240:ALA:HB2   | 1.75                     | 0.68              |
| 27:M:294:GLU:OE1  | 27:M:294:GLU:N    | 2.25                     | 0.68              |
| 30:N:194:ILE:HA   | 30:N:203:ARG:HH12 | 1.56                     | 0.68              |
| 1:1:158:ASP:HB3   | 1:b:180:GLN:HE22  | 1.58                     | 0.68              |
| 13:F:100:ASN:O    | 13:F:100:ASN:ND2  | 2.27                     | 0.68              |
| 11:D:48:ARG:HB2   | 11:D:209:ASN:HB2  | 1.74                     | 0.68              |
| 2:2:243:LYS:HB3   | 3:3:199:TYR:HD2   | 1.58                     | 0.68              |
| 4:4:3:ILE:HD13    | 4:4:176:PHE:HB3   | 1.76                     | 0.68              |
| 1:b:165:MET:SD    | 1:b:170:THR:OG1   | 2.50                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:A:95:LEU:HD22   | 14:G:118:GLN:HG3  | 1.75                     | 0.68              |
| 12:E:85:ALA:HB2   | 12:E:140:VAL:HG21 | 1.76                     | 0.68              |
| 29:U:148:THR:HG22 | 29:U:149:SER:H    | 1.59                     | 0.68              |
| 1:b:196:VAL:HB    | 1:b:203:GLU:HB2   | 1.76                     | 0.68              |
| 26:H:147:ILE:HD12 | 26:H:157:VAL:HB   | 1.76                     | 0.68              |
| 32:o:452:LEU:HD11 | 32:o:474:LEU:HD23 | 1.75                     | 0.68              |
| 7:a:137:ARG:NH1   | 6:e:23:PRO:O      | 2.26                     | 0.68              |
| 30:N:301:THR:HG22 | 30:N:920:VAL:HG23 | 1.76                     | 0.68              |
| 16:K:94:LEU:HB2   | 17:L:128:ILE:HB   | 1.76                     | 0.68              |
| 19:P:165:VAL:HA   | 19:P:168:TYR:HD2  | 1.59                     | 0.67              |
| 5:f:220:LYS:HB2   | 5:f:223:LEU:HG    | 1.75                     | 0.67              |
| 16:K:219:LYS:NZ   | 34:K:501:ATP:O1G  | 2.27                     | 0.67              |
| 17:L:179:THR:HG23 | 17:L:181:ASP:H    | 1.58                     | 0.67              |
| 6:e:171:ASN:OD1   | 6:e:178:GLN:NE2   | 2.26                     | 0.67              |
| 2:2:39:ASN:ND2    | 2:2:208:GLU:OE2   | 2.28                     | 0.67              |
| 32:o:812:ILE:HD11 | 32:o:847:ILE:HG23 | 1.76                     | 0.67              |
| 11:D:163:THR:HG21 | 11:D:171:VAL:HB   | 1.76                     | 0.67              |
| 1:1:32:ILE:HD12   | 1:1:196:VAL:HG22  | 1.76                     | 0.67              |
| 19:P:384:VAL:HG11 | 28:Q:353:PRO:HB3  | 1.75                     | 0.67              |
| 2:i:105:VAL:HG21  | 2:i:138:HIS:HB2   | 1.76                     | 0.67              |
| 30:N:578:ASP:OD1  | 30:N:579:SER:N    | 2.28                     | 0.67              |
| 19:P:119:ILE:HD12 | 19:P:139:VAL:HG13 | 1.76                     | 0.67              |
| 4:4:172:MET:HE3   | 4:4:173:PRO:HD2   | 1.77                     | 0.67              |
| 15:I:231:LEU:HD22 | 34:J:501:ATP:H2'  | 1.77                     | 0.67              |
| 19:P:266:TYR:OH   | 19:P:296:GLN:NE2  | 2.27                     | 0.67              |
| 19:P:357:TYR:HD2  | 19:P:360:ILE:HB   | 1.60                     | 0.67              |
| 22:V:215:ASN:HA   | 22:V:218:LYS:HD3  | 1.77                     | 0.67              |
| 25:J:185:VAL:HG13 | 25:J:312:ARG:HB2  | 1.77                     | 0.67              |
| 2:2:105:VAL:HG11  | 2:2:138:HIS:HB2   | 1.77                     | 0.66              |
| 16:K:420:THR:OG1  | 16:K:421:VAL:N    | 2.28                     | 0.66              |
| 22:V:26:THR:HG22  | 22:V:200:ASN:HB2  | 1.77                     | 0.66              |
| 31:T:60:ARG:O     | 31:T:64:VAL:HG23  | 1.95                     | 0.66              |
| 32:o:843:ASP:OD1  | 32:o:843:ASP:N    | 2.28                     | 0.66              |
| 7:7:126:PHE:HB2   | 7:7:149:VAL:HG11  | 1.76                     | 0.66              |
| 7:a:43:SER:OG     | 7:a:180:GLY:N     | 2.27                     | 0.66              |
| 7:a:34:THR:N      | 7:a:140:MET:O     | 2.28                     | 0.66              |
| 1:1:60:ILE:HD13   | 1:1:120:GLY:HA3   | 1.76                     | 0.66              |
| 4:4:152:MET:HE1   | 4:4:160:LEU:HD12  | 1.77                     | 0.66              |
| 10:C:4:ARG:HG2    | 11:D:6:ARG:HH22   | 1.61                     | 0.66              |
| 17:L:88:TYR:HE1   | 27:M:58:MET:HE2   | 1.60                     | 0.66              |
| 4:g:158:LEU:O     | 4:g:162:LYS:HG2   | 1.95                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:164:MET:HA    | 2:2:167:LEU:HG    | 1.78                     | 0.66              |
| 20:R:138:GLY:HA3  | 20:R:154:LEU:HD21 | 1.77                     | 0.66              |
| 7:a:38:ILE:HG22   | 7:a:39:VAL:HG23   | 1.78                     | 0.66              |
| 6:e:49:ILE:HG22   | 6:e:54:ILE:HA     | 1.76                     | 0.66              |
| 6:e:120:ARG:HD2   | 5:f:170:LEU:HD21  | 1.77                     | 0.66              |
| 8:A:243:GLU:OE1   | 8:A:244:ARG:NH1   | 2.29                     | 0.66              |
| 16:K:194:GLN:OE1  | 25:J:373:ARG:NH2  | 2.29                     | 0.66              |
| 18:O:163:ILE:HD12 | 18:O:167:ILE:HB   | 1.77                     | 0.66              |
| 22:V:59:ASP:OD1   | 22:V:61:TYR:N     | 2.28                     | 0.66              |
| 32:o:463:HIS:ND1  | 32:o:468:GLU:OE2  | 2.29                     | 0.66              |
| 6:6:49:ILE:HG22   | 6:6:54:ILE:HA     | 1.76                     | 0.66              |
| 30:N:2:SER:OG     | 30:N:3:LEU:N      | 2.29                     | 0.66              |
| 32:o:736:LEU:HD13 | 32:o:772:ILE:HD11 | 1.78                     | 0.66              |
| 20:R:238:PHE:O    | 25:J:339:ARG:NH1  | 2.29                     | 0.65              |
| 7:7:60:LEU:HD11   | 7:7:67:LEU:HB3    | 1.78                     | 0.65              |
| 13:F:6:TYR:OH     | 14:G:9:ASP:OD2    | 2.09                     | 0.65              |
| 22:V:148:LYS:HG2  | 29:U:169:ILE:HD12 | 1.79                     | 0.65              |
| 10:C:91:ALA:HB2   | 10:C:115:LEU:HD21 | 1.77                     | 0.65              |
| 7:a:166:LEU:HB3   | 6:e:76:PHE:HZ     | 1.62                     | 0.65              |
| 8:A:135:ARG:HB3   | 14:G:13:SER:HB2   | 1.77                     | 0.65              |
| 22:V:100:ARG:NH2  | 29:U:20:ASP:OD2   | 2.29                     | 0.65              |
| 4:4:169:GLU:O     | 4:g:177:LYS:NZ    | 2.29                     | 0.65              |
| 22:V:126:GLN:NE2  | 22:V:136:ALA:O    | 2.30                     | 0.65              |
| 22:V:225:LEU:O    | 22:V:301:ASN:ND2  | 2.28                     | 0.65              |
| 23:W:98:LEU:HD13  | 23:W:108:GLN:HB3  | 1.78                     | 0.65              |
| 29:U:14:VAL:HG21  | 29:U:48:VAL:HG12  | 1.78                     | 0.65              |
| 30:N:283:ASP:HB3  | 30:N:286:LEU:HD12 | 1.78                     | 0.65              |
| 3:3:23:ILE:HG23   | 3:3:188:TYR:HB2   | 1.77                     | 0.65              |
| 3:3:201:LYS:HG2   | 5:f:273:TRP:HZ2   | 1.61                     | 0.65              |
| 16:K:256:ASP:OD1  | 16:K:259:ARG:NH2  | 2.29                     | 0.65              |
| 18:O:171:PHE:O    | 18:O:175:ASN:ND2  | 2.30                     | 0.65              |
| 26:H:206:VAL:HG21 | 26:H:261:ARG:HB3  | 1.79                     | 0.65              |
| 7:7:161:ARG:HE    | 7:7:171:SER:HB2   | 1.61                     | 0.65              |
| 17:L:339:ARG:HH21 | 17:L:342:ARG:HG3  | 1.61                     | 0.65              |
| 20:R:319:CYS:SG   | 20:R:320:LYS:N    | 2.69                     | 0.65              |
| 10:C:137:TYR:HE1  | 10:C:151:SER:HB3  | 1.63                     | 0.64              |
| 11:D:83:ARG:HA    | 11:D:86:ILE:HD12  | 1.78                     | 0.64              |
| 20:R:408:ASP:OD1  | 21:S:464:ARG:NE   | 2.30                     | 0.64              |
| 32:o:514:ALA:HB2  | 32:o:545:SER:HB3  | 1.79                     | 0.64              |
| 4:4:102:VAL:HG12  | 4:4:119:ILE:HB    | 1.78                     | 0.64              |
| 10:C:53:THR:HG21  | 10:C:210:ARG:HB3  | 1.79                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:b:48:ARG:NH2    | 2:i:153:TYR:OH    | 2.30                     | 0.64              |
| 32:o:161:ILE:HD11 | 32:o:203:LEU:HD23 | 1.80                     | 0.64              |
| 20:R:406:GLN:HB3  | 28:Q:416:VAL:HG11 | 1.79                     | 0.64              |
| 1:b:52:LYS:HA     | 1:b:64:ARG:HH21   | 1.62                     | 0.64              |
| 30:N:691:GLN:HB2  | 30:N:696:LYS:HE2  | 1.80                     | 0.64              |
| 15:I:51:PRO:HD2   | 15:I:58:LYS:HB2   | 1.79                     | 0.64              |
| 32:o:788:PRO:HG3  | 32:o:822:THR:HG21 | 1.80                     | 0.64              |
| 4:4:171:ARG:HE    | 4:g:27:VAL:HB     | 1.62                     | 0.64              |
| 6:6:116:LEU:HD13  | 6:6:148:GLY:HA2   | 1.79                     | 0.64              |
| 11:D:69:SER:OG    | 11:D:219:SER:OG   | 2.15                     | 0.64              |
| 7:a:86:ILE:HD12   | 7:a:147:ILE:HG12  | 1.78                     | 0.64              |
| 26:H:330:GLN:O    | 26:H:334:LEU:HG   | 1.98                     | 0.64              |
| 28:Q:306:TYR:HA   | 28:Q:342:LEU:HD21 | 1.79                     | 0.64              |
| 32:o:108:ASP:N    | 32:o:108:ASP:OD1  | 2.31                     | 0.64              |
| 8:A:46:ARG:NH2    | 8:A:192:ASP:OD1   | 2.31                     | 0.64              |
| 18:O:319:LEU:HD12 | 18:O:327:LEU:HD12 | 1.80                     | 0.64              |
| 22:V:21:ASP:O     | 22:V:172:GLN:NE2  | 2.31                     | 0.64              |
| 22:V:53:MET:HG3   | 22:V:68:VAL:HG12  | 1.80                     | 0.64              |
| 28:Q:325:LEU:HD13 | 28:Q:335:PHE:HE2  | 1.63                     | 0.64              |
| 30:N:125:THR:HB   | 30:N:128:ILE:HG12 | 1.80                     | 0.64              |
| 1:1:48:ARG:NH2    | 2:2:153:TYR:OH    | 2.31                     | 0.63              |
| 9:B:239:THR:OG1   | 9:B:242:GLU:OE1   | 2.16                     | 0.63              |
| 28:Q:366:ILE:HG23 | 28:Q:368:LEU:H    | 1.62                     | 0.63              |
| 9:B:5:TYR:OH      | 14:G:127:ASN:ND2  | 2.30                     | 0.63              |
| 10:C:160:TRP:CD2  | 10:C:163:ILE:HD13 | 2.33                     | 0.63              |
| 2:2:42:VAL:HB     | 2:2:206:VAL:HG13  | 1.79                     | 0.63              |
| 8:A:238:ALA:HA    | 8:A:241:ILE:HD12  | 1.79                     | 0.63              |
| 11:D:203:VAL:HG11 | 11:D:210:ILE:HD11 | 1.79                     | 0.63              |
| 15:I:124:THR:OG1  | 15:I:125:MET:SD   | 2.55                     | 0.63              |
| 16:K:68:ILE:HD11  | 30:N:608:LEU:HG   | 1.80                     | 0.63              |
| 20:R:170:VAL:O    | 20:R:174:ILE:HD12 | 1.97                     | 0.63              |
| 13:F:9:ASP:OD1    | 13:F:9:ASP:N      | 2.30                     | 0.63              |
| 16:K:255:ARG:HG2  | 16:K:302:GLN:HE21 | 1.62                     | 0.63              |
| 19:P:266:TYR:HB3  | 19:P:329:PHE:HE2  | 1.63                     | 0.63              |
| 22:V:280:LEU:HD23 | 29:U:286:ILE:HD11 | 1.80                     | 0.63              |
| 6:6:215:ILE:HB    | 2:i:196:LEU:HB3   | 1.81                     | 0.63              |
| 16:K:215:PRO:HB3  | 16:K:319:ASN:HD22 | 1.62                     | 0.63              |
| 4:g:182:LYS:HG2   | 4:g:191:GLN:HG3   | 1.80                     | 0.63              |
| 17:L:285:ALA:HB1  | 27:M:303:ARG:HD3  | 1.81                     | 0.63              |
| 3:3:67:PHE:O      | 3:3:71:THR:HG23   | 1.99                     | 0.63              |
| 15:I:138:LYS:HA   | 15:I:141:LEU:HD12 | 1.80                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:K:236:ARG:HH11 | 17:L:315:PHE:HB3  | 1.64                     | 0.63              |
| 1:1:162:ARG:HH22  | 1:1:169:GLU:HB3   | 1.64                     | 0.62              |
| 4:4:36:ARG:HB2    | 4:4:44:MET:HB3    | 1.81                     | 0.62              |
| 8:A:147:ASP:O     | 8:A:151:GLY:N     | 2.31                     | 0.62              |
| 27:M:201:MET:HE1  | 27:M:277:ILE:HD11 | 1.80                     | 0.62              |
| 30:N:677:ASP:OD1  | 30:N:677:ASP:N    | 2.26                     | 0.62              |
| 12:E:10:ARG:HH21  | 13:F:3:ARG:HD3    | 1.65                     | 0.62              |
| 19:P:39:LEU:HD13  | 19:P:62:ILE:HG22  | 1.81                     | 0.62              |
| 29:U:2:SER:HB2    | 29:U:4:GLN:HG2    | 1.80                     | 0.62              |
| 29:U:134:THR:OG1  | 29:U:159:CYS:SG   | 2.55                     | 0.62              |
| 30:N:163:LEU:HA   | 30:N:166:ILE:HD12 | 1.80                     | 0.62              |
| 30:N:306:ASN:O    | 30:N:712:ASN:ND2  | 2.32                     | 0.62              |
| 4:4:108:ASP:OD2   | 4:4:111:LYS:NZ    | 2.31                     | 0.62              |
| 10:C:158:THR:OG1  | 10:C:160:TRP:NE1  | 2.32                     | 0.62              |
| 19:P:133:GLU:HB3  | 19:P:168:TYR:HD1  | 1.63                     | 0.62              |
| 20:R:54:ILE:HD13  | 20:R:63:TYR:HD1   | 1.64                     | 0.62              |
| 26:H:248:LEU:HD22 | 26:H:377:PHE:HE2  | 1.63                     | 0.62              |
| 5:5:131:GLU:OE2   | 5:5:174:THR:OG1   | 2.16                     | 0.62              |
| 15:I:89:GLN:HG2   | 15:I:90:GLU:H     | 1.64                     | 0.62              |
| 16:K:200:GLN:NE2  | 25:J:375:ILE:O    | 2.26                     | 0.62              |
| 27:M:71:ASN:OD1   | 27:M:72:ASN:ND2   | 2.32                     | 0.62              |
| 3:h:18:LYS:NZ     | 3:h:157:ASN:O     | 2.28                     | 0.62              |
| 30:N:211:PHE:HB2  | 30:N:228:VAL:HG11 | 1.82                     | 0.62              |
| 30:N:645:THR:HG23 | 30:N:646:LYS:HE2  | 1.80                     | 0.62              |
| 16:K:330:ARG:NH1  | 25:J:140:GLU:O    | 2.33                     | 0.62              |
| 20:R:63:TYR:OH    | 20:R:93:LYS:O     | 2.18                     | 0.62              |
| 29:U:64:ASP:OD2   | 29:U:105:LYS:NZ   | 2.32                     | 0.62              |
| 5:f:179:TYR:O     | 5:f:181:ARG:NH2   | 2.33                     | 0.62              |
| 2:2:56:ALA:O      | 6:e:213:ARG:NH2   | 2.33                     | 0.62              |
| 2:2:58:LYS:NZ     | 6:e:212:GLU:O     | 2.31                     | 0.62              |
| 7:7:35:GLN:NE2    | 7:7:142:PRO:O     | 2.32                     | 0.62              |
| 10:C:62:SER:OG    | 10:C:64:GLU:OE2   | 2.13                     | 0.62              |
| 16:K:360:MET:HE1  | 16:K:387:MET:HB3  | 1.82                     | 0.62              |
| 18:O:18:ALA:HB2   | 18:O:57:LEU:HD21  | 1.82                     | 0.62              |
| 19:P:133:GLU:HB3  | 19:P:168:TYR:CD1  | 2.35                     | 0.62              |
| 6:6:23:PRO:O      | 7:7:137:ARG:NH1   | 2.33                     | 0.62              |
| 11:D:107:GLU:HA   | 11:D:148:TYR:HE2  | 1.65                     | 0.62              |
| 2:i:64:HIS:HB3    | 2:i:85:THR:HG21   | 1.80                     | 0.62              |
| 3:3:118:LYS:NZ    | 3:3:119:PRO:O     | 2.33                     | 0.62              |
| 22:V:293:VAL:HG21 | 29:U:189:ARG:HE   | 1.65                     | 0.62              |
| 31:T:200:LEU:HD12 | 31:T:201:PRO:HD2  | 1.81                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:48:ARG:HH12   | 2:2:55:VAL:HG21   | 1.65                     | 0.61              |
| 9:B:33:THR:HA     | 9:B:165:GLY:HA3   | 1.81                     | 0.61              |
| 12:E:41:ALA:HA    | 12:E:46:VAL:HG22  | 1.81                     | 0.61              |
| 14:G:79:SER:OG    | 14:G:165:THR:OG1  | 2.09                     | 0.61              |
| 19:P:218:LEU:HD21 | 19:P:247:THR:HG21 | 1.82                     | 0.61              |
| 3:h:143:SER:HA    | 3:h:146:LEU:HD12  | 1.81                     | 0.61              |
| 25:J:195:LYS:HG2  | 25:J:316:PHE:HD2  | 1.65                     | 0.61              |
| 26:H:104:LYS:NZ   | 27:M:160:PRO:O    | 2.33                     | 0.61              |
| 27:M:331:ASP:OD1  | 27:M:331:ASP:N    | 2.32                     | 0.61              |
| 20:R:368:LEU:HD22 | 20:R:381:ILE:HD11 | 1.82                     | 0.61              |
| 28:Q:198:LEU:HD13 | 28:Q:225:LEU:HD12 | 1.81                     | 0.61              |
| 28:Q:288:LYS:HA   | 28:Q:292:GLN:HB2  | 1.82                     | 0.61              |
| 14:G:137:ILE:HD11 | 14:G:165:THR:HG23 | 1.82                     | 0.61              |
| 16:K:96:ILE:O     | 16:K:113:THR:OG1  | 2.18                     | 0.61              |
| 16:K:331:PRO:O    | 25:J:141:LYS:NZ   | 2.30                     | 0.61              |
| 17:L:292:SER:OG   | 17:L:293:GLU:OE1  | 2.17                     | 0.61              |
| 21:S:322:LEU:HB3  | 21:S:383:LEU:HD21 | 1.82                     | 0.61              |
| 7:a:232:ILE:HB    | 7:a:240:THR:HB    | 1.81                     | 0.61              |
| 10:C:233:GLN:HA   | 10:C:236:LYS:HE2  | 1.81                     | 0.61              |
| 17:L:223:PRO:HB3  | 17:L:432:ILE:HG21 | 1.82                     | 0.61              |
| 32:o:68:LEU:HD11  | 32:o:114:SER:HB2  | 1.82                     | 0.61              |
| 18:O:130:ASP:HA   | 18:O:133:ILE:HD12 | 1.81                     | 0.61              |
| 22:V:53:MET:HE1   | 22:V:139:VAL:HG21 | 1.82                     | 0.61              |
| 23:W:142:ILE:HG23 | 23:W:172:LEU:HD23 | 1.83                     | 0.61              |
| 21:S:210:LEU:HG   | 21:S:214:MET:HE2  | 1.82                     | 0.61              |
| 6:e:229:ASP:OD1   | 6:e:232:ARG:NH2   | 2.33                     | 0.61              |
| 2:i:115:HIS:HA    | 2:i:118:LYS:HE3   | 1.83                     | 0.61              |
| 30:N:447:SER:HB2  | 30:N:466:LEU:HD11 | 1.82                     | 0.61              |
| 31:T:79:GLU:OE2   | 31:T:112:ASN:ND2  | 2.33                     | 0.61              |
| 5:5:276:LYS:NZ    | 5:5:287:GLY:O     | 2.28                     | 0.61              |
| 7:7:181:ALA:O     | 7:7:185:ASN:ND2   | 2.32                     | 0.61              |
| 15:I:255:LYS:NZ   | 25:J:217:GLU:HB3  | 2.16                     | 0.61              |
| 7:a:87:SER:HB3    | 7:a:146:ALA:HB3   | 1.83                     | 0.61              |
| 2:2:48:ARG:HH22   | 6:e:215:ILE:HG22  | 1.66                     | 0.61              |
| 22:V:212:MET:HG2  | 29:U:127:GLN:HE21 | 1.64                     | 0.61              |
| 26:H:216:ASP:N    | 26:H:216:ASP:OD1  | 2.33                     | 0.61              |
| 30:N:222:TYR:HA   | 30:N:225:LEU:HD12 | 1.81                     | 0.61              |
| 8:A:200:GLU:OE1   | 8:A:201:LYS:NZ    | 2.34                     | 0.61              |
| 16:K:236:ARG:NH1  | 17:L:315:PHE:O    | 2.34                     | 0.61              |
| 7:a:132:VAL:O     | 7:a:136:ARG:HG2   | 2.01                     | 0.61              |
| 32:o:55:ARG:HB2   | 32:o:67:SER:HB3   | 1.82                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:5:87:ILE:HB     | 5:5:255:VAL:HB    | 1.83                     | 0.61              |
| 11:D:122:GLN:OE1  | 12:E:136:ARG:NH1  | 2.34                     | 0.61              |
| 16:K:193:VAL:HG12 | 16:K:194:GLN:HG3  | 1.83                     | 0.61              |
| 4:g:47:ALA:N      | 4:g:101:ASN:O     | 2.32                     | 0.61              |
| 25:J:372:GLU:OE1  | 25:J:374:ARG:NH2  | 2.34                     | 0.61              |
| 2:2:192:ILE:HB    | 2:2:199:GLY:HA2   | 1.81                     | 0.60              |
| 7:7:54:ILE:HG12   | 7:7:232:ILE:HG13  | 1.82                     | 0.60              |
| 13:F:219:ASP:N    | 13:F:219:ASP:OD1  | 2.34                     | 0.60              |
| 17:L:196:VAL:HG13 | 17:L:215:PRO:HG2  | 1.83                     | 0.60              |
| 20:R:54:ILE:HA    | 20:R:59:MET:HG2   | 1.81                     | 0.60              |
| 15:I:369:MET:HB3  | 15:I:371:LEU:HG   | 1.83                     | 0.60              |
| 21:S:204:ASP:N    | 21:S:204:ASP:OD1  | 2.31                     | 0.60              |
| 6:e:71:MET:HE1    | 6:e:84:VAL:HG22   | 1.83                     | 0.60              |
| 6:6:77:ALA:HB3    | 7:7:168:VAL:HG12  | 1.82                     | 0.60              |
| 11:D:70:HIS:NE2   | 11:D:104:VAL:O    | 2.30                     | 0.60              |
| 13:F:35:THR:OG1   | 13:F:73:SER:OG    | 2.17                     | 0.60              |
| 6:e:153:GLU:HG3   | 6:e:156:ARG:HG3   | 1.84                     | 0.60              |
| 26:H:253:GLY:O    | 26:H:415:THR:OG1  | 2.15                     | 0.60              |
| 27:M:299:ARG:O    | 27:M:303:ARG:NH2  | 2.34                     | 0.60              |
| 32:o:280:ASP:O    | 32:o:284:LEU:HD12 | 2.00                     | 0.60              |
| 5:5:79:LEU:HD13   | 5:5:215:LEU:HD21  | 1.83                     | 0.60              |
| 6:6:41:VAL:HG12   | 6:6:225:ILE:HG13  | 1.82                     | 0.60              |
| 15:I:130:VAL:HG13 | 15:I:155:SER:HA   | 1.83                     | 0.60              |
| 7:a:214:MET:HE1   | 7:a:247:VAL:HA    | 1.82                     | 0.60              |
| 26:H:89:GLN:O     | 26:H:95:HIS:NE2   | 2.34                     | 0.60              |
| 3:3:125:ASP:OD1   | 3:3:129:CYS:N     | 2.33                     | 0.60              |
| 15:I:256:TYR:HE1  | 16:K:281:ARG:HH22 | 1.49                     | 0.60              |
| 20:R:334:ARG:NH1  | 24:Y:70:ASP:OD2   | 2.35                     | 0.60              |
| 15:I:60:LEU:O     | 15:I:64:ARG:HG2   | 2.01                     | 0.60              |
| 22:V:151:VAL:H    | 29:U:173:HIS:HD2  | 1.50                     | 0.60              |
| 7:a:125:ILE:O     | 7:a:129:LEU:HG    | 2.01                     | 0.60              |
| 4:g:176:PHE:HD1   | 4:g:178:GLY:H     | 1.50                     | 0.60              |
| 27:M:88:MET:O     | 27:M:88:MET:HE3   | 2.02                     | 0.60              |
| 30:N:606:VAL:HG21 | 30:N:625:LEU:HD21 | 1.83                     | 0.60              |
| 32:o:525:MET:HA   | 32:o:528:LEU:HD12 | 1.83                     | 0.60              |
| 11:D:37:LYS:HB3   | 11:D:42:VAL:HG23  | 1.83                     | 0.60              |
| 11:D:151:GLU:HG3  | 11:D:152:PRO:HD2  | 1.84                     | 0.60              |
| 13:F:32:GLY:O     | 13:F:163:ALA:N    | 2.33                     | 0.60              |
| 23:W:155:ASP:N    | 23:W:155:ASP:OD1  | 2.33                     | 0.60              |
| 7:a:60:LEU:HD11   | 7:a:67:LEU:HB3    | 1.82                     | 0.60              |
| 5:f:82:ARG:NH1    | 5:f:185:PRO:O     | 2.34                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:o:518:LEU:O    | 32:o:553:ARG:NH1  | 2.28                     | 0.60              |
| 5:5:156:LYS:HE2   | 11:D:101:GLU:HB2  | 1.83                     | 0.60              |
| 16:K:378:LEU:HD13 | 16:K:383:ILE:HG22 | 1.82                     | 0.60              |
| 18:O:186:ASN:OD1  | 18:O:226:LYS:N    | 2.35                     | 0.60              |
| 21:S:84:ASP:OD1   | 21:S:89:LYS:NZ    | 2.34                     | 0.60              |
| 21:S:482:PRO:HA   | 21:S:485:LYS:HB2  | 1.84                     | 0.60              |
| 7:a:46:SER:HB2    | 7:a:55:ILE:HG13   | 1.82                     | 0.60              |
| 1:1:58:ASP:N      | 1:1:58:ASP:OD1    | 2.34                     | 0.60              |
| 20:R:21:VAL:O     | 20:R:176:ARG:NH1  | 2.34                     | 0.60              |
| 20:R:358:GLY:HA2  | 24:Y:78:LYS:HE2   | 1.83                     | 0.60              |
| 32:o:135:LEU:HD11 | 32:o:160:GLU:HB3  | 1.84                     | 0.60              |
| 8:A:126:GLN:HE21  | 9:B:81:ASP:HA     | 1.67                     | 0.59              |
| 17:L:284:ASP:OD1  | 17:L:284:ASP:N    | 2.34                     | 0.59              |
| 18:O:107:GLN:O    | 18:O:111:SER:HB3  | 2.02                     | 0.59              |
| 20:R:313:ALA:HA   | 20:R:317:ILE:HD11 | 1.84                     | 0.59              |
| 7:a:60:LEU:HD22   | 7:a:225:SER:HB3   | 1.82                     | 0.59              |
| 7:7:180:GLY:HA2   | 7:7:183:MET:HB2   | 1.84                     | 0.59              |
| 8:A:72:ILE:HG12   | 8:A:82:VAL:HG22   | 1.82                     | 0.59              |
| 15:I:246:ARG:HH12 | 25:J:278:GLN:HB3  | 1.68                     | 0.59              |
| 15:I:329:ASN:OD1  | 15:I:329:ASN:N    | 2.35                     | 0.59              |
| 17:L:270:ALA:HB2  | 17:L:278:ILE:HD11 | 1.83                     | 0.59              |
| 22:V:55:GLY:HA2   | 22:V:66:VAL:HG23  | 1.84                     | 0.59              |
| 3:3:28:ARG:NH2    | 3:3:205:ASP:OXT   | 2.36                     | 0.59              |
| 6:6:165:ILE:HD12  | 6:6:206:SER:HB3   | 1.85                     | 0.59              |
| 11:D:182:LYS:HG3  | 11:D:183:GLU:HG2  | 1.84                     | 0.59              |
| 15:I:113:ILE:HD12 | 15:I:113:ILE:O    | 2.02                     | 0.59              |
| 15:I:240:THR:HG22 | 15:I:242:ALA:H    | 1.67                     | 0.59              |
| 18:O:58:ARG:HB3   | 18:O:85:SER:HA    | 1.82                     | 0.59              |
| 26:H:193:PRO:O    | 26:H:196:THR:OG1  | 2.16                     | 0.59              |
| 2:2:48:ARG:NH2    | 2:2:196:LEU:O     | 2.36                     | 0.59              |
| 7:7:113:LEU:HB3   | 7:7:117:GLU:HB3   | 1.84                     | 0.59              |
| 15:I:55:CYS:HG    | 32:o:248:TYR:HH   | 1.51                     | 0.59              |
| 15:I:282:ASP:OD1  | 15:I:283:GLU:N    | 2.35                     | 0.59              |
| 17:L:84:LEU:HB3   | 27:M:58:MET:HE3   | 1.83                     | 0.59              |
| 18:O:130:ASP:HB2  | 18:O:153:LEU:HD21 | 1.83                     | 0.59              |
| 6:e:34:ILE:HD13   | 6:e:155:CYS:HB3   | 1.85                     | 0.59              |
| 32:o:774:ARG:O    | 32:o:810:ASN:ND2  | 2.35                     | 0.59              |
| 2:2:47:THR:HB     | 2:2:59:ASN:HA     | 1.85                     | 0.59              |
| 9:B:215:GLY:O     | 9:B:234:ARG:NH1   | 2.35                     | 0.59              |
| 17:L:79:GLN:OE1   | 17:L:82:ARG:NH1   | 2.36                     | 0.59              |
| 4:g:46:PHE:HD2    | 4:g:53:THR:HB     | 1.67                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:7:56:ALA:HB2    | 7:7:230:LEU:HD13  | 1.84                     | 0.59              |
| 8:A:176:GLN:O     | 8:A:180:THR:HG23  | 2.02                     | 0.59              |
| 26:H:270:THR:HG21 | 26:H:301:LYS:HD3  | 1.83                     | 0.59              |
| 32:o:868:ASN:OD1  | 32:o:868:ASN:N    | 2.35                     | 0.59              |
| 8:A:68:THR:HG21   | 14:G:159:GLY:HA3  | 1.84                     | 0.59              |
| 12:E:201:LEU:HB3  | 12:E:243:LEU:HD22 | 1.83                     | 0.59              |
| 14:G:71:ASP:OD1   | 14:G:72:ARG:N     | 2.35                     | 0.59              |
| 15:I:103:PRO:HG3  | 25:J:120:TYR:HB2  | 1.85                     | 0.59              |
| 17:L:84:LEU:HD22  | 27:M:58:MET:HE1   | 1.85                     | 0.59              |
| 5:f:166:LYS:O     | 4:g:96:ARG:NH2    | 2.36                     | 0.59              |
| 28:Q:75:ARG:HH21  | 28:Q:113:ASP:HA   | 1.67                     | 0.59              |
| 30:N:398:ARG:HD2  | 30:N:438:ASP:HA   | 1.85                     | 0.59              |
| 14:G:177:GLU:HG3  | 17:L:420:ARG:HH12 | 1.67                     | 0.59              |
| 15:I:129:TYR:HB3  | 26:H:97:LEU:HB2   | 1.83                     | 0.59              |
| 15:I:380:LEU:HD22 | 15:I:381:VAL:HG23 | 1.84                     | 0.59              |
| 16:K:142:HIS:ND1  | 16:K:142:HIS:O    | 2.36                     | 0.59              |
| 7:a:54:ILE:HG12   | 7:a:232:ILE:HG12  | 1.83                     | 0.59              |
| 6:e:71:MET:HB3    | 6:e:130:ILE:HG22  | 1.84                     | 0.59              |
| 4:4:3:ILE:HB      | 4:4:18:SER:HB3    | 1.85                     | 0.59              |
| 13:F:46:LEU:HG    | 13:F:135:ILE:HD13 | 1.85                     | 0.59              |
| 14:G:52:LYS:HZ3   | 14:G:213:GLU:HG3  | 1.67                     | 0.59              |
| 15:I:196:GLU:O    | 15:I:208:TYR:OH   | 2.18                     | 0.59              |
| 19:P:161:CYS:HA   | 19:P:183:GLN:HE21 | 1.67                     | 0.59              |
| 31:T:7:LEU:HB3    | 31:T:30:ILE:HG12  | 1.85                     | 0.59              |
| 15:I:135:PHE:HD1  | 26:H:82:TRP:HB2   | 1.68                     | 0.58              |
| 16:K:255:ARG:NH1  | 16:K:298:GLU:OE2  | 2.34                     | 0.58              |
| 20:R:312:TYR:HE1  | 20:R:326:ALA:HB1  | 1.68                     | 0.58              |
| 24:Y:73:PHE:O     | 24:Y:75:ASN:N     | 2.35                     | 0.58              |
| 5:5:241:HIS:CE1   | 3:h:204:GLN:HB3   | 2.38                     | 0.58              |
| 7:7:60:LEU:HD21   | 7:7:67:LEU:HD13   | 1.84                     | 0.58              |
| 15:I:73:GLU:O     | 26:H:66:LYS:NZ    | 2.36                     | 0.58              |
| 16:K:121:ARG:HH22 | 25:J:64:LEU:HD13  | 1.68                     | 0.58              |
| 17:L:186:LEU:HD12 | 17:L:189:GLN:HB2  | 1.84                     | 0.58              |
| 18:O:330:ARG:NH1  | 19:P:307:GLU:OE2  | 2.35                     | 0.58              |
| 6:e:46:THR:HB     | 6:e:59:GLU:H      | 1.68                     | 0.58              |
| 30:N:498:ILE:HG23 | 30:N:535:LEU:HD21 | 1.84                     | 0.58              |
| 32:o:924:LYS:HG2  | 32:o:953:THR:HG21 | 1.84                     | 0.58              |
| 10:C:233:GLN:CD   | 10:C:233:GLN:H    | 2.11                     | 0.58              |
| 20:R:27:SER:OG    | 20:R:320:LYS:NZ   | 2.36                     | 0.58              |
| 1:b:40:THR:HG22   | 1:b:45:ILE:HG12   | 1.85                     | 0.58              |
| 8:A:54:ILE:HD11   | 8:A:223:LEU:HB2   | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:a:250:MET:HA    | 7:a:250:MET:HE3   | 1.85                     | 0.58              |
| 28:Q:158:ILE:HG12 | 28:Q:177:VAL:HG23 | 1.84                     | 0.58              |
| 29:U:119:LEU:HD11 | 29:U:136:ALA:HB1  | 1.85                     | 0.58              |
| 3:3:101:GLY:O     | 4:4:93:ARG:NH1    | 2.36                     | 0.58              |
| 20:R:285:ALA:HB1  | 20:R:315:VAL:HG22 | 1.85                     | 0.58              |
| 23:W:68:GLU:HB2   | 23:W:71:LYS:HZ2   | 1.68                     | 0.58              |
| 25:J:264:GLY:HA2  | 25:J:267:GLU:HB3  | 1.85                     | 0.58              |
| 26:H:174:VAL:HG11 | 26:H:183:ILE:HG12 | 1.86                     | 0.58              |
| 4:4:83:PHE:O      | 4:4:87:GLU:HG2    | 2.03                     | 0.58              |
| 6:6:26:ASP:OD2    | 6:6:27:ASN:N      | 2.37                     | 0.58              |
| 15:I:236:VAL:O    | 15:I:240:THR:OG1  | 2.22                     | 0.58              |
| 21:S:261:HIS:ND1  | 21:S:269:GLU:OE2  | 2.35                     | 0.58              |
| 7:a:139:LYS:NZ    | 7:a:141:ASN:O     | 2.36                     | 0.58              |
| 7:a:140:MET:H     | 7:a:140:MET:HE2   | 1.69                     | 0.58              |
| 3:h:113:ASN:O     | 3:h:192:LYS:NZ    | 2.37                     | 0.58              |
| 26:H:356:ASN:N    | 26:H:356:ASN:OD1  | 2.36                     | 0.58              |
| 28:Q:359:ILE:HD11 | 28:Q:390:LEU:HD11 | 1.84                     | 0.58              |
| 32:o:617:ILE:HD12 | 32:o:743:ILE:HG13 | 1.84                     | 0.58              |
| 9:B:222:LEU:HD13  | 9:B:232:GLY:HA2   | 1.85                     | 0.58              |
| 16:K:124:SER:HA   | 16:K:128:ARG:HH22 | 1.69                     | 0.58              |
| 21:S:256:LYS:NZ   | 30:N:40:SER:OG    | 2.30                     | 0.58              |
| 30:N:452:LEU:HD11 | 30:N:751:LEU:HD11 | 1.84                     | 0.58              |
| 32:o:938:GLN:HB2  | 32:o:942:PRO:HG3  | 1.85                     | 0.58              |
| 9:B:119:GLN:HG3   | 10:C:86:ILE:HD11  | 1.85                     | 0.58              |
| 10:C:59:GLN:NE2   | 10:C:209:ASP:O    | 2.35                     | 0.58              |
| 19:P:25:ASP:O     | 19:P:29:GLN:NE2   | 2.36                     | 0.58              |
| 6:6:97:ASP:OD1    | 6:6:98:HIS:ND1    | 2.37                     | 0.58              |
| 15:I:311:ASN:O    | 15:I:315:GLY:N    | 2.37                     | 0.58              |
| 20:R:222:ARG:NH1  | 24:Y:62:GLU:O     | 2.35                     | 0.58              |
| 2:i:63:LEU:HD13   | 2:i:205:CYS:HB2   | 1.85                     | 0.58              |
| 2:2:86:GLN:NE2    | 9:B:98:LYS:O      | 2.37                     | 0.58              |
| 6:6:47:ARG:NH1    | 6:6:215:ILE:O     | 2.37                     | 0.58              |
| 7:7:50:ASP:O      | 7:7:158:GLN:NE2   | 2.37                     | 0.58              |
| 17:L:246:SER:HB3  | 17:L:280:MET:HA   | 1.84                     | 0.58              |
| 18:O:92:PHE:HB2   | 18:O:140:LYS:HE2  | 1.86                     | 0.58              |
| 19:P:122:ILE:HG21 | 19:P:139:VAL:HG21 | 1.86                     | 0.58              |
| 23:W:3:LEU:HB3    | 23:W:106:GLN:HG2  | 1.85                     | 0.58              |
| 4:g:38:LEU:HD11   | 4:g:60:ILE:HG13   | 1.85                     | 0.58              |
| 3:h:84:PRO:HA     | 3:h:87:PHE:HB3    | 1.86                     | 0.58              |
| 29:U:186:LEU:HD21 | 31:T:267:ALA:HB1  | 1.85                     | 0.58              |
| 30:N:127:ASP:O    | 30:N:128:ILE:HD13 | 2.04                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:N:380:LEU:HG   | 30:N:381:GLU:HG2  | 1.86                     | 0.58              |
| 32:o:808:SER:O    | 32:o:812:ILE:HG23 | 2.04                     | 0.58              |
| 4:4:101:ASN:HB3   | 4:4:133:HIS:CD2   | 2.39                     | 0.57              |
| 15:I:130:VAL:HG11 | 15:I:156:ILE:HG13 | 1.86                     | 0.57              |
| 16:K:282:PHE:HE1  | 16:K:284:ALA:HB2  | 1.69                     | 0.57              |
| 17:L:277:ILE:HG22 | 17:L:277:ILE:O    | 2.03                     | 0.57              |
| 18:O:172:TYR:HB3  | 18:O:195:TYR:HB2  | 1.86                     | 0.57              |
| 18:O:186:ASN:HD21 | 18:O:225:ASP:H    | 1.51                     | 0.57              |
| 25:J:18:GLY:O     | 25:J:20:LYS:N     | 2.36                     | 0.57              |
| 32:o:157:LEU:HD11 | 32:o:207:ILE:HD11 | 1.86                     | 0.57              |
| 32:o:804:ASP:O    | 32:o:807:VAL:N    | 2.35                     | 0.57              |
| 8:A:218:PHE:HB3   | 8:A:223:LEU:HD22  | 1.86                     | 0.57              |
| 11:D:158:SER:HB3  | 12:E:63:SER:HB2   | 1.86                     | 0.57              |
| 13:F:54:ASP:O     | 13:F:57:SER:OG    | 2.21                     | 0.57              |
| 15:I:229:LYS:NZ   | 34:J:501:ATP:O2B  | 2.36                     | 0.57              |
| 22:V:301:ASN:O    | 22:V:305:ILE:HB   | 2.03                     | 0.57              |
| 28:Q:426:LEU:HD11 | 29:U:289:ASP:HB2  | 1.86                     | 0.57              |
| 30:N:772:GLN:NE2  | 30:N:869:ASP:OD1  | 2.37                     | 0.57              |
| 9:B:88:LYS:O      | 9:B:92:VAL:HG12   | 2.04                     | 0.57              |
| 26:H:51:GLN:N     | 26:H:51:GLN:OE1   | 2.33                     | 0.57              |
| 27:M:120:LYS:HG2  | 27:M:126:THR:HG22 | 1.86                     | 0.57              |
| 27:M:197:ILE:HG13 | 27:M:324:LEU:HD21 | 1.86                     | 0.57              |
| 30:N:314:LEU:HD21 | 30:N:336:ASN:HB2  | 1.87                     | 0.57              |
| 2:2:137:SER:O     | 2:2:138:HIS:ND1   | 2.36                     | 0.57              |
| 2:2:188:ILE:HD13  | 2:2:202:VAL:HG13  | 1.86                     | 0.57              |
| 4:4:9:VAL:HG23    | 4:4:11:ASP:H      | 1.69                     | 0.57              |
| 4:4:25:ILE:HD11   | 5:5:209:THR:HG21  | 1.86                     | 0.57              |
| 5:5:244:ALA:HB1   | 3:h:179:ALA:HB1   | 1.87                     | 0.57              |
| 11:D:117:GLN:NE2  | 11:D:151:GLU:O    | 2.36                     | 0.57              |
| 14:G:78:TYR:HD2   | 14:G:85:GLY:HA3   | 1.69                     | 0.57              |
| 20:R:38:VAL:O     | 20:R:43:ARG:NH2   | 2.37                     | 0.57              |
| 22:V:178:GLY:O    | 22:V:181:ASN:ND2  | 2.37                     | 0.57              |
| 7:a:131:THR:O     | 7:a:135:GLN:HG2   | 2.05                     | 0.57              |
| 9:B:148:TYR:HE1   | 9:B:158:PRO:HB3   | 1.70                     | 0.57              |
| 5:f:280:GLY:O     | 5:f:283:ASN:ND2   | 2.29                     | 0.57              |
| 25:J:89:GLN:OE1   | 25:J:89:GLN:N     | 2.29                     | 0.57              |
| 25:J:195:LYS:HE2  | 25:J:293:ALA:HB1  | 1.87                     | 0.57              |
| 25:J:306:ARG:NE   | 25:J:307:PRO:O    | 2.34                     | 0.57              |
| 29:U:70:HIS:ND1   | 29:U:113:TYR:OH   | 2.31                     | 0.57              |
| 1:1:57:HIS:ND1    | 1:1:58:ASP:OD1    | 2.37                     | 0.57              |
| 13:F:135:ILE:HD11 | 13:F:222:PHE:HE1  | 1.69                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:K:262:ARG:NH2  | 16:K:302:GLN:OE1  | 2.38                     | 0.57              |
| 30:N:120:ASP:OD2  | 30:N:125:THR:OG1  | 2.21                     | 0.57              |
| 3:3:28:ARG:HB2    | 3:3:183:TRP:HB2   | 1.86                     | 0.57              |
| 19:P:43:GLU:OE2   | 19:P:88:GLN:NE2   | 2.35                     | 0.57              |
| 20:R:277:LEU:HA   | 20:R:280:ILE:HD12 | 1.86                     | 0.57              |
| 22:V:71:MET:HE2   | 22:V:71:MET:HA    | 1.85                     | 0.57              |
| 22:V:153:ILE:HG22 | 22:V:201:ILE:HG13 | 1.86                     | 0.57              |
| 7:a:183:MET:HE2   | 7:a:183:MET:HA    | 1.86                     | 0.57              |
| 32:o:135:LEU:HD12 | 32:o:135:LEU:H    | 1.68                     | 0.57              |
| 4:4:49:GLU:OE2    | 4:4:51:GLY:N      | 2.35                     | 0.57              |
| 4:4:92:ILE:HD12   | 4:4:93:ARG:HG3    | 1.85                     | 0.57              |
| 11:D:216:LYS:HB2  | 11:D:220:ASP:HB3  | 1.87                     | 0.57              |
| 20:R:263:ARG:NH2  | 20:R:297:TYR:O    | 2.37                     | 0.57              |
| 18:O:246:SER:HA   | 18:O:249:ASP:HB2  | 1.87                     | 0.57              |
| 23:W:41:ARG:HD3   | 23:W:45:PRO:HA    | 1.86                     | 0.57              |
| 5:f:152:ALA:O     | 5:f:156:LYS:HG2   | 2.04                     | 0.57              |
| 25:J:103:ASN:N    | 25:J:103:ASN:OD1  | 2.38                     | 0.57              |
| 26:H:311:ILE:HG21 | 26:H:353:PHE:HD1  | 1.68                     | 0.57              |
| 30:N:536:ILE:HD12 | 30:N:555:ILE:HG12 | 1.86                     | 0.57              |
| 32:o:42:ASP:OD2   | 32:o:43:ALA:N     | 2.38                     | 0.57              |
| 6:6:116:LEU:HD23  | 6:6:124:TYR:HD2   | 1.70                     | 0.57              |
| 10:C:195:LYS:HG2  | 10:C:199:LYS:HZ2  | 1.69                     | 0.57              |
| 15:I:62:MET:O     | 15:I:66:LYS:HG3   | 2.04                     | 0.57              |
| 19:P:395:ARG:NH2  | 28:Q:358:GLU:OE1  | 2.38                     | 0.57              |
| 30:N:245:LEU:HD21 | 30:N:254:SER:HA   | 1.87                     | 0.57              |
| 2:2:235:PRO:O     | 2:2:238:THR:OG1   | 2.22                     | 0.56              |
| 5:5:134:LEU:HG    | 5:5:158:LEU:HD13  | 1.86                     | 0.56              |
| 5:5:266:HIS:HB3   | 5:5:271:LEU:HD11  | 1.87                     | 0.56              |
| 12:E:154:GLN:HG2  | 12:E:166:ARG:HH12 | 1.69                     | 0.56              |
| 17:L:286:ILE:O    | 17:L:286:ILE:HG13 | 2.05                     | 0.56              |
| 21:S:455:GLU:OE2  | 31:T:258:ASN:ND2  | 2.38                     | 0.56              |
| 6:e:125:TYR:HA    | 6:e:146:PRO:HB3   | 1.86                     | 0.56              |
| 30:N:605:ILE:HD12 | 30:N:605:ILE:H    | 1.69                     | 0.56              |
| 30:N:759:ILE:HG23 | 30:N:902:VAL:HG13 | 1.86                     | 0.56              |
| 5:5:241:HIS:ND1   | 3:h:204:GLN:O     | 2.38                     | 0.56              |
| 10:C:16:GLU:OE2   | 10:C:18:ARG:HG2   | 2.04                     | 0.56              |
| 23:W:125:LEU:HB3  | 23:W:157:PHE:CE1  | 2.40                     | 0.56              |
| 6:e:76:PHE:HB3    | 6:e:79:ASP:HB2    | 1.86                     | 0.56              |
| 26:H:411:CYS:SG   | 26:H:414:SER:OG   | 2.63                     | 0.56              |
| 27:M:379:LEU:HD21 | 27:M:415:PHE:HB3  | 1.85                     | 0.56              |
| 5:5:234:ARG:HH12  | 5:5:279:GLU:HG3   | 1.71                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:P:9:ALA:HB2    | 19:P:51:ASP:HB2   | 1.87                     | 0.56              |
| 19:P:69:ARG:HB2   | 19:P:71:LYS:HG2   | 1.87                     | 0.56              |
| 20:R:33:LEU:HD22  | 20:R:71:LEU:HD21  | 1.86                     | 0.56              |
| 6:e:47:ARG:HB2    | 6:e:219:ASP:HB2   | 1.87                     | 0.56              |
| 31:T:67:LEU:HA    | 31:T:70:ILE:HG22  | 1.87                     | 0.56              |
| 32:o:52:LEU:HD22  | 32:o:67:SER:HA    | 1.88                     | 0.56              |
| 7:7:103:LEU:HD21  | 7:7:125:ILE:HG22  | 1.87                     | 0.56              |
| 15:I:319:ARG:CZ   | 15:I:320:GLY:H    | 2.18                     | 0.56              |
| 18:O:307:MET:N    | 18:O:307:MET:SD   | 2.79                     | 0.56              |
| 21:S:52:TYR:O     | 21:S:56:SER:OG    | 2.22                     | 0.56              |
| 27:M:384:ASP:OD1  | 27:M:384:ASP:N    | 2.36                     | 0.56              |
| 30:N:127:ASP:N    | 30:N:127:ASP:OD1  | 2.38                     | 0.56              |
| 1:1:204:ARG:HG2   | 7:a:259:LYS:HE3   | 1.87                     | 0.56              |
| 3:3:104:PHE:HD1   | 3:3:126:LEU:HD11  | 1.71                     | 0.56              |
| 3:3:205:ASP:HB2   | 5:f:247:GLY:HA3   | 1.88                     | 0.56              |
| 4:4:147:HIS:HB3   | 4:4:160:LEU:HD21  | 1.88                     | 0.56              |
| 7:7:187:LEU:O     | 7:7:190:LYS:NZ    | 2.34                     | 0.56              |
| 11:D:121:THR:HG22 | 11:D:128:PRO:HB3  | 1.88                     | 0.56              |
| 13:F:118:LYS:HA   | 13:F:118:LYS:HE3  | 1.87                     | 0.56              |
| 16:K:356:ILE:HD11 | 34:K:501:ATP:H2   | 1.70                     | 0.56              |
| 5:f:134:LEU:HD22  | 5:f:158:LEU:HB2   | 1.88                     | 0.56              |
| 29:U:182:ALA:O    | 29:U:184:GLY:N    | 2.38                     | 0.56              |
| 2:2:240:ALA:HB2   | 6:e:185:GLY:HA3   | 1.87                     | 0.56              |
| 6:6:86:ARG:HE     | 6:6:115:LEU:HD22  | 1.71                     | 0.56              |
| 19:P:59:LEU:HB3   | 19:P:96:MET:HB2   | 1.87                     | 0.56              |
| 23:W:101:ARG:HH12 | 23:W:108:GLN:HE21 | 1.52                     | 0.56              |
| 2:i:47:THR:HG21   | 2:i:217:ARG:HH22  | 1.70                     | 0.56              |
| 27:M:167:VAL:HA   | 27:M:170:MET:SD   | 2.45                     | 0.56              |
| 30:N:638:ILE:HG23 | 30:N:660:LEU:HD21 | 1.87                     | 0.56              |
| 5:5:76:THR:O      | 5:5:206:SER:N     | 2.36                     | 0.56              |
| 8:A:64:LEU:HD22   | 14:G:160:TYR:HE2  | 1.70                     | 0.56              |
| 15:I:421:GLU:O    | 15:I:425:LYS:HG2  | 2.05                     | 0.56              |
| 1:b:79:GLN:O      | 1:b:83:GLU:HG2    | 2.06                     | 0.56              |
| 27:M:225:GLY:N    | 34:M:501:ATP:O1B  | 2.34                     | 0.56              |
| 32:o:778:LEU:HD11 | 32:o:888:LEU:HD23 | 1.88                     | 0.56              |
| 5:5:236:ILE:HD13  | 5:5:250:VAL:HG13  | 1.88                     | 0.56              |
| 5:5:283:ASN:ND2   | 4:g:148:TYR:O     | 2.39                     | 0.56              |
| 8:A:96:ARG:O      | 8:A:96:ARG:HD3    | 2.06                     | 0.56              |
| 8:A:135:ARG:NH1   | 14:G:124:THR:O    | 2.39                     | 0.56              |
| 13:F:82:ARG:HH21  | 13:F:86:ASN:ND2   | 2.04                     | 0.56              |
| 17:L:407:ARG:NH2  | 17:L:414:ASP:OD2  | 2.38                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:V:107:TRP:NE1  | 22:V:126:GLN:OE1  | 2.32                     | 0.56              |
| 31:T:79:GLU:O     | 31:T:83:ASN:ND2   | 2.39                     | 0.56              |
| 31:T:171:ILE:HD13 | 31:T:174:PHE:CE2  | 2.40                     | 0.56              |
| 32:o:256:LEU:HD21 | 32:o:260:GLU:HB2  | 1.87                     | 0.56              |
| 6:6:163:SER:HB2   | 3:h:145:GLN:HG2   | 1.88                     | 0.56              |
| 8:A:157:THR:OG1   | 8:A:158:ASP:N     | 2.38                     | 0.56              |
| 7:a:180:GLY:HA2   | 7:a:183:MET:HB2   | 1.87                     | 0.56              |
| 25:J:310:ILE:O    | 25:J:313:LYS:NZ   | 2.39                     | 0.56              |
| 27:M:356:SER:O    | 27:M:360:ILE:HG12 | 2.05                     | 0.56              |
| 1:1:23:MET:HE1    | 1:1:143:TYR:HB2   | 1.87                     | 0.56              |
| 13:F:80:ASP:OD1   | 13:F:126:ARG:NH2  | 2.34                     | 0.56              |
| 13:F:187:ASP:N    | 13:F:187:ASP:OD1  | 2.39                     | 0.56              |
| 32:o:304:PRO:O    | 32:o:308:LYS:HG3  | 2.07                     | 0.56              |
| 2:2:75:ALA:N      | 2:2:126:TYR:O     | 2.39                     | 0.55              |
| 10:C:15:PRO:HA    | 11:D:22:TYR:CZ    | 2.41                     | 0.55              |
| 16:K:357:ALA:HB2  | 16:K:387:MET:HE1  | 1.87                     | 0.55              |
| 18:O:228:TYR:HA   | 18:O:294:MET:HE1  | 1.88                     | 0.55              |
| 19:P:183:GLN:HB3  | 19:P:199:LEU:HD23 | 1.87                     | 0.55              |
| 22:V:35:LEU:HD12  | 29:U:16:LEU:HD12  | 1.88                     | 0.55              |
| 3:h:41:GLU:OE1    | 3:h:43:ILE:N      | 2.36                     | 0.55              |
| 3:h:177:ARG:HA    | 3:h:177:ARG:HH11  | 1.71                     | 0.55              |
| 28:Q:242:SER:HB2  | 28:Q:261:VAL:HG21 | 1.88                     | 0.55              |
| 31:T:59:LYS:NZ    | 31:T:98:GLU:O     | 2.40                     | 0.55              |
| 5:5:175:MET:HA    | 5:5:175:MET:HE3   | 1.89                     | 0.55              |
| 6:6:176:LYS:HD2   | 3:h:203:ARG:NH2   | 2.21                     | 0.55              |
| 20:R:222:ARG:NH1  | 24:Y:62:GLU:OE1   | 2.39                     | 0.55              |
| 5:f:112:ILE:HG23  | 5:f:135:GLY:HA2   | 1.88                     | 0.55              |
| 32:o:951:GLN:HB3  | 32:o:955:VAL:HG11 | 1.88                     | 0.55              |
| 7:7:90:ILE:HA     | 7:7:93:MET:HG2    | 1.87                     | 0.55              |
| 7:7:97:GLU:O      | 7:7:101:LYS:HG2   | 2.05                     | 0.55              |
| 7:7:105:THR:HA    | 14:G:72:ARG:HH21  | 1.70                     | 0.55              |
| 7:7:256:LYS:HB3   | 1:b:206:ILE:HG21  | 1.89                     | 0.55              |
| 9:B:174:PHE:HA    | 9:B:177:LYS:HE2   | 1.86                     | 0.55              |
| 22:V:291:ASN:O    | 22:V:295:VAL:HG23 | 2.06                     | 0.55              |
| 29:U:70:HIS:HD1   | 29:U:113:TYR:HH   | 1.46                     | 0.55              |
| 1:1:23:MET:HG3    | 1:1:174:ILE:HD11  | 1.88                     | 0.55              |
| 2:2:153:TYR:HB2   | 2:2:167:LEU:HD13  | 1.88                     | 0.55              |
| 15:I:263:LEU:O    | 15:I:267:ILE:HG12 | 2.06                     | 0.55              |
| 18:O:325:GLU:O    | 18:O:329:MET:HG2  | 2.05                     | 0.55              |
| 23:W:100:HIS:CE1  | 29:U:57:GLU:HG3   | 2.41                     | 0.55              |
| 16:K:349:ARG:HH12 | 16:K:375:ASN:HA   | 1.72                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:h:172:LEU:HD22  | 3:h:202:MET:HB3   | 1.88                     | 0.55              |
| 30:N:657:MET:HG2  | 30:N:682:PHE:HE1  | 1.72                     | 0.55              |
| 1:1:23:MET:HE2    | 1:1:145:ILE:HG23  | 1.88                     | 0.55              |
| 5:5:96:THR:HG22   | 5:5:101:VAL:HG22  | 1.89                     | 0.55              |
| 7:7:58:ASP:HA     | 7:7:228:PHE:HA    | 1.89                     | 0.55              |
| 7:7:111:ASN:HB3   | 7:7:114:ALA:HB2   | 1.87                     | 0.55              |
| 10:C:44:ILE:HB    | 10:C:216:ILE:HD12 | 1.88                     | 0.55              |
| 10:C:76:ALA:HB3   | 10:C:136:ILE:HB   | 1.89                     | 0.55              |
| 14:G:109:ILE:HG21 | 14:G:147:HIS:HB2  | 1.89                     | 0.55              |
| 15:I:254:GLN:NE2  | 25:J:228:ARG:O    | 2.32                     | 0.55              |
| 15:I:308:GLU:OE1  | 26:H:277:SER:OG   | 2.24                     | 0.55              |
| 21:S:60:LEU:HD11  | 21:S:144:LEU:HD13 | 1.89                     | 0.55              |
| 21:S:125:LYS:HB2  | 21:S:127:THR:HG22 | 1.89                     | 0.55              |
| 5:f:83:PHE:HE1    | 5:f:88:ILE:HG12   | 1.72                     | 0.55              |
| 32:o:301:THR:HG21 | 32:o:306:MET:HB2  | 1.89                     | 0.55              |
| 1:1:50:THR:OG1    | 1:1:51:ASP:N      | 2.40                     | 0.55              |
| 12:E:146:GLY:HA2  | 12:E:222:ILE:HG12 | 1.88                     | 0.55              |
| 18:O:343:GLN:HE22 | 19:P:364:ARG:HG2  | 1.71                     | 0.55              |
| 19:P:52:LEU:H     | 19:P:52:LEU:HD23  | 1.72                     | 0.55              |
| 21:S:157:GLU:O    | 21:S:161:LYS:HB2  | 2.07                     | 0.55              |
| 21:S:254:ILE:HD13 | 21:S:276:LEU:HD11 | 1.87                     | 0.55              |
| 5:f:145:GLU:HB3   | 5:f:147:GLU:HG2   | 1.88                     | 0.55              |
| 2:i:188:ILE:HG21  | 2:i:202:VAL:HG13  | 1.89                     | 0.55              |
| 1:1:70:ASP:HB3    | 1:1:112:LEU:HD13  | 1.88                     | 0.55              |
| 6:6:27:ASN:HD22   | 6:6:77:ALA:HB2    | 1.71                     | 0.55              |
| 12:E:22:PHE:O     | 12:E:24:VAL:N     | 2.39                     | 0.55              |
| 19:P:24:ILE:HD11  | 19:P:35:ALA:HA    | 1.88                     | 0.55              |
| 19:P:72:TRP:HA    | 19:P:75:LEU:HB3   | 1.89                     | 0.55              |
| 7:a:101:LYS:HA    | 7:a:104:VAL:HG12  | 1.87                     | 0.55              |
| 32:o:867:PHE:HD2  | 32:o:871:HIS:HA   | 1.70                     | 0.55              |
| 12:E:72:ARG:HE    | 12:E:227:GLY:HA3  | 1.72                     | 0.55              |
| 30:N:375:HIS:CD2  | 30:N:385:VAL:HG11 | 2.42                     | 0.55              |
| 30:N:602:VAL:O    | 30:N:606:VAL:HG22 | 2.07                     | 0.55              |
| 1:1:192:ILE:HB    | 1:1:207:PHE:HB2   | 1.88                     | 0.55              |
| 1:1:194:MET:HA    | 1:1:194:MET:HE3   | 1.89                     | 0.55              |
| 3:3:144:ASP:OD1   | 3:3:144:ASP:N     | 2.36                     | 0.55              |
| 12:E:114:GLN:HE21 | 12:E:114:GLN:C    | 2.15                     | 0.55              |
| 7:a:81:ASN:ND2    | 7:a:152:VAL:O     | 2.40                     | 0.55              |
| 25:J:131:ASP:OD1  | 25:J:134:VAL:HG23 | 2.07                     | 0.55              |
| 27:M:299:ARG:HG3  | 27:M:303:ARG:HH21 | 1.70                     | 0.55              |
| 28:Q:14:LEU:HD23  | 28:Q:19:GLN:HG3   | 1.89                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:90:SER:OG     | 9:B:99:ARG:NH1    | 2.40                     | 0.54              |
| 6:6:119:LYS:NZ    | 6:6:122:PHE:O     | 2.38                     | 0.54              |
| 7:7:36:GLN:NE2    | 7:7:37:PRO:O      | 2.37                     | 0.54              |
| 10:C:44:ILE:HD11  | 10:C:146:TYR:HB3  | 1.88                     | 0.54              |
| 21:S:391:GLY:O    | 21:S:395:ILE:HG12 | 2.07                     | 0.54              |
| 7:a:204:GLN:H     | 7:a:204:GLN:CD    | 2.14                     | 0.54              |
| 5:f:156:LYS:HD3   | 5:f:196:ARG:HH12  | 1.72                     | 0.54              |
| 4:g:104:ILE:HB    | 4:g:117:TYR:HB2   | 1.87                     | 0.54              |
| 15:I:168:VAL:HG21 | 15:I:270:VAL:HG21 | 1.89                     | 0.54              |
| 17:L:109:MET:HE1  | 17:L:126:ARG:HE   | 1.72                     | 0.54              |
| 17:L:132:ARG:NH2  | 17:L:134:SER:OG   | 2.41                     | 0.54              |
| 6:e:147:VAL:HG22  | 5:f:125:ALA:HB3   | 1.89                     | 0.54              |
| 30:N:722:THR:OG1  | 30:N:723:GLY:N    | 2.40                     | 0.54              |
| 6:6:101:LYS:NZ    | 12:E:105:GLU:OE2  | 2.40                     | 0.54              |
| 16:K:119:VAL:N    | 25:J:70:SER:O     | 2.36                     | 0.54              |
| 19:P:104:LEU:O    | 19:P:115:ARG:NH2  | 2.41                     | 0.54              |
| 21:S:62:SER:O     | 21:S:66:GLN:NE2   | 2.40                     | 0.54              |
| 25:J:118:ASP:OD1  | 25:J:118:ASP:N    | 2.40                     | 0.54              |
| 30:N:387:ALA:HA   | 30:N:390:LEU:HD12 | 1.89                     | 0.54              |
| 32:o:575:MET:HA   | 32:o:607:ALA:HA   | 1.89                     | 0.54              |
| 8:A:194:ILE:HG22  | 8:A:196:GLU:H     | 1.72                     | 0.54              |
| 12:E:122:ARG:NH2  | 12:E:132:ARG:O    | 2.41                     | 0.54              |
| 7:a:191:VAL:HG12  | 7:a:192:VAL:HG23  | 1.90                     | 0.54              |
| 28:Q:159:ASN:HB3  | 28:Q:163:ARG:HH21 | 1.72                     | 0.54              |
| 3:3:188:TYR:HE1   | 3:3:197:LYS:HG3   | 1.72                     | 0.54              |
| 5:5:250:VAL:HB    | 5:5:266:HIS:HB2   | 1.88                     | 0.54              |
| 6:6:201:LYS:HB2   | 2:i:229:GLN:HG2   | 1.90                     | 0.54              |
| 7:7:131:THR:O     | 7:7:135:GLN:HG2   | 2.07                     | 0.54              |
| 17:L:313:ASP:OD1  | 17:L:342:ARG:NE   | 2.41                     | 0.54              |
| 5:f:165:TYR:HB3   | 5:f:170:LEU:HD12  | 1.89                     | 0.54              |
| 4:g:10:GLN:NE2    | 4:g:151:ASP:O     | 2.41                     | 0.54              |
| 3:h:53:ILE:HG22   | 3:h:60:VAL:HG22   | 1.89                     | 0.54              |
| 30:N:665:ILE:HD13 | 30:N:715:ILE:HG13 | 1.90                     | 0.54              |
| 9:B:46:ALA:HB2    | 9:B:211:LEU:HD13  | 1.89                     | 0.54              |
| 11:D:48:ARG:HE    | 11:D:209:ASN:HA   | 1.72                     | 0.54              |
| 14:G:126:TYR:HB2  | 14:G:129:VAL:HG12 | 1.89                     | 0.54              |
| 17:L:295:THR:OG1  | 17:L:296:SER:N    | 2.41                     | 0.54              |
| 19:P:60:ALA:HB2   | 19:P:95:TYR:HE2   | 1.72                     | 0.54              |
| 19:P:254:GLU:HA   | 19:P:257:TRP:NE1  | 2.23                     | 0.54              |
| 29:U:141:GLU:HA   | 29:U:152:LYS:HA   | 1.88                     | 0.54              |
| 31:T:104:LYS:HE2  | 31:T:171:ILE:HG23 | 1.89                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:I:230:THR:N    | 34:J:501:ATP:O1B  | 2.37                     | 0.54              |
| 16:K:87:LYS:HE3   | 16:K:125:THR:HG21 | 1.90                     | 0.54              |
| 18:O:152:ASP:HA   | 18:O:155:LYS:HD2  | 1.89                     | 0.54              |
| 21:S:136:CYS:HB3  | 21:S:179:ILE:HG21 | 1.90                     | 0.54              |
| 7:a:58:ASP:HA     | 7:a:228:PHE:HA    | 1.88                     | 0.54              |
| 3:h:199:TYR:HB2   | 2:i:243:LYS:H     | 1.72                     | 0.54              |
| 28:Q:20:TYR:HB2   | 28:Q:64:LEU:HD13  | 1.90                     | 0.54              |
| 28:Q:275:ILE:HG21 | 28:Q:307:ASN:HB2  | 1.90                     | 0.54              |
| 30:N:17:GLN:O     | 30:N:21:LYS:HG2   | 2.07                     | 0.54              |
| 32:o:797:THR:HG22 | 32:o:801:HIS:HE1  | 1.72                     | 0.54              |
| 5:5:82:ARG:NH1    | 5:5:185:PRO:O     | 2.41                     | 0.54              |
| 9:B:69:PRO:HB3    | 9:B:233:PRO:HB3   | 1.90                     | 0.54              |
| 9:B:213:ILE:HD12  | 9:B:238:LEU:HD21  | 1.88                     | 0.54              |
| 15:I:177:PRO:O    | 15:I:178:THR:OG1  | 2.20                     | 0.54              |
| 18:O:82:LEU:HD23  | 18:O:83:LEU:HD23  | 1.90                     | 0.54              |
| 18:O:231:GLY:O    | 18:O:235:HIS:ND1  | 2.41                     | 0.54              |
| 20:R:203:ASP:N    | 20:R:203:ASP:OD1  | 2.37                     | 0.54              |
| 20:R:312:TYR:HA   | 20:R:316:LEU:HD13 | 1.88                     | 0.54              |
| 23:W:180:LEU:HD12 | 23:W:182:TYR:CE2  | 2.42                     | 0.54              |
| 8:A:104:PHE:CD1   | 8:A:112:MET:HB3   | 2.43                     | 0.54              |
| 9:B:178:ARG:HB3   | 9:B:191:ILE:HD12  | 1.89                     | 0.54              |
| 16:K:131:LEU:HD23 | 16:K:149:ILE:HD12 | 1.88                     | 0.54              |
| 19:P:294:GLU:OE1  | 19:P:294:GLU:N    | 2.41                     | 0.54              |
| 20:R:117:ILE:HG12 | 20:R:133:ALA:HB1  | 1.90                     | 0.54              |
| 4:4:149:ARG:HH12  | 5:f:281:SER:HA    | 1.73                     | 0.54              |
| 7:7:42:THR:H      | 7:7:74:ARG:HH22   | 1.54                     | 0.54              |
| 7:7:139:LYS:HE3   | 7:7:141:ASN:HB3   | 1.89                     | 0.54              |
| 16:K:322:ASP:OD2  | 16:K:323:THR:N    | 2.40                     | 0.54              |
| 20:R:149:ASN:HA   | 20:R:152:LYS:HD2  | 1.90                     | 0.54              |
| 20:R:289:ILE:HG12 | 20:R:315:VAL:HG21 | 1.89                     | 0.54              |
| 1:b:78:VAL:HG22   | 1:b:100:VAL:HG12  | 1.90                     | 0.54              |
| 4:g:56:PHE:O      | 4:g:60:ILE:HG23   | 2.06                     | 0.54              |
| 28:Q:17:GLU:HB2   | 28:Q:19:GLN:HG2   | 1.88                     | 0.54              |
| 32:o:471:LEU:HB2  | 32:o:497:PHE:HZ   | 1.73                     | 0.54              |
| 5:5:140:LEU:HB3   | 5:5:144:ARG:HH22  | 1.74                     | 0.53              |
| 6:6:134:ASP:OD1   | 6:6:138:LYS:N     | 2.31                     | 0.53              |
| 7:7:248:GLU:OE1   | 7:7:248:GLU:N     | 2.41                     | 0.53              |
| 8:A:200:GLU:HG2   | 8:A:244:ARG:HH21  | 1.72                     | 0.53              |
| 15:I:167:MET:HE1  | 25:J:229:MET:H    | 1.72                     | 0.53              |
| 17:L:225:GLY:HA3  | 27:M:339:ARG:HD3  | 1.91                     | 0.53              |
| 17:L:435:GLN:NE2  | 17:L:436:LYS:O    | 2.41                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:U:66:TRP:CE2   | 29:U:106:ILE:HG12 | 2.42                     | 0.53              |
| 30:N:101:ILE:O    | 30:N:105:SER:OG   | 2.24                     | 0.53              |
| 32:o:280:ASP:OD1  | 32:o:280:ASP:N    | 2.40                     | 0.53              |
| 10:C:5:ARG:NH2    | 14:G:11:SER:OG    | 2.40                     | 0.53              |
| 15:I:72:GLU:HG2   | 32:o:760:HIS:CE1  | 2.44                     | 0.53              |
| 15:I:194:ILE:HG21 | 15:I:232:LEU:HD21 | 1.90                     | 0.53              |
| 16:K:242:PHE:HB3  | 16:K:295:ILE:HD13 | 1.89                     | 0.53              |
| 20:R:22:PRO:HG3   | 20:R:177:LEU:HD23 | 1.90                     | 0.53              |
| 20:R:189:GLU:HG3  | 20:R:190:LYS:HE2  | 1.90                     | 0.53              |
| 21:S:466:LYS:NZ   | 31:T:265:ASP:OD2  | 2.28                     | 0.53              |
| 26:H:98:GLN:O     | 26:H:176:VAL:N    | 2.41                     | 0.53              |
| 7:7:129:LEU:HA    | 7:7:132:VAL:HG12  | 1.91                     | 0.53              |
| 15:I:79:SER:O     | 15:I:83:LYS:HG2   | 2.09                     | 0.53              |
| 15:I:124:THR:HG21 | 25:J:91:GLU:HB3   | 1.90                     | 0.53              |
| 20:R:237:THR:O    | 20:R:237:THR:OG1  | 2.25                     | 0.53              |
| 6:e:50:THR:OG1    | 6:e:55:ASN:OD1    | 2.23                     | 0.53              |
| 6:e:156:ARG:HG2   | 6:e:166:MET:HE1   | 1.89                     | 0.53              |
| 4:4:66:LEU:HB2    | 11:D:94:GLN:HG3   | 1.91                     | 0.53              |
| 7:7:92:ASP:O      | 7:7:96:ILE:HG12   | 2.09                     | 0.53              |
| 20:R:17:THR:HG22  | 20:R:19:ASN:H     | 1.74                     | 0.53              |
| 21:S:28:GLU:O     | 21:S:32:GLN:HG2   | 2.08                     | 0.53              |
| 30:N:373:VAL:HG23 | 30:N:410:LEU:HD21 | 1.90                     | 0.53              |
| 32:o:809:MET:HE1  | 32:o:843:ASP:HB2  | 1.90                     | 0.53              |
| 5:5:89:VAL:HG22   | 5:5:253:TYR:HB2   | 1.91                     | 0.53              |
| 6:6:71:MET:HB2    | 6:6:130:ILE:HG22  | 1.90                     | 0.53              |
| 10:C:232:PRO:HA   | 10:C:235:ILE:HB   | 1.90                     | 0.53              |
| 12:E:16:SER:OG    | 12:E:20:ARG:O     | 2.23                     | 0.53              |
| 17:L:294:GLY:O    | 17:L:299:ARG:NH2  | 2.40                     | 0.53              |
| 17:L:373:GLU:H    | 17:L:373:GLU:CD   | 2.16                     | 0.53              |
| 3:h:11:ILE:HG21   | 3:h:142:ALA:HB3   | 1.91                     | 0.53              |
| 25:J:103:ASN:HB3  | 25:J:105:LYS:HE2  | 1.91                     | 0.53              |
| 27:M:364:HIS:NE2  | 34:M:501:ATP:O2'  | 2.42                     | 0.53              |
| 32:o:567:ALA:HB2  | 32:o:599:ILE:HD12 | 1.90                     | 0.53              |
| 2:2:101:ARG:NH2   | 8:A:115:ASP:OD2   | 2.41                     | 0.53              |
| 2:2:212:ASP:OD1   | 2:2:213:ALA:N     | 2.41                     | 0.53              |
| 4:4:82:SER:HA     | 4:4:85:ARG:HG2    | 1.90                     | 0.53              |
| 6:6:76:PHE:HB3    | 6:6:79:ASP:HB2    | 1.90                     | 0.53              |
| 8:A:164:VAL:HG13  | 8:A:166:TYR:HE1   | 1.74                     | 0.53              |
| 18:O:42:SER:HB3   | 18:O:73:ILE:HD13  | 1.91                     | 0.53              |
| 2:2:66:ILE:HB     | 2:2:70:ILE:HG23   | 1.91                     | 0.53              |
| 10:C:114:ARG:O    | 10:C:118:ILE:HG12 | 2.08                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:I:370:ASN:ND2  | 15:I:409:MET:O    | 2.41                     | 0.53              |
| 16:K:350:ARG:NH2  | 16:K:368:LEU:HB2  | 2.24                     | 0.53              |
| 17:L:339:ARG:NH2  | 17:L:342:ARG:HG3  | 2.22                     | 0.53              |
| 20:R:28:GLU:HA    | 20:R:320:LYS:HD2  | 1.90                     | 0.53              |
| 23:W:143:ASN:HB3  | 23:W:173:THR:HA   | 1.90                     | 0.53              |
| 4:g:107:TYR:HE2   | 4:g:186:LYS:HG3   | 1.74                     | 0.53              |
| 4:g:181:VAL:HB    | 4:g:192:VAL:HB    | 1.91                     | 0.53              |
| 26:H:384:GLY:O    | 26:H:388:ILE:HG12 | 2.07                     | 0.53              |
| 3:3:15:MET:HA     | 3:3:15:MET:HE3    | 1.89                     | 0.53              |
| 8:A:46:ARG:NH2    | 8:A:192:ASP:O     | 2.37                     | 0.53              |
| 14:G:54:ILE:O     | 14:G:210:LYS:NZ   | 2.30                     | 0.53              |
| 21:S:44:THR:HG21  | 21:S:53:ILE:HD11  | 1.91                     | 0.53              |
| 26:H:393:SER:O    | 26:H:393:SER:OG   | 2.24                     | 0.53              |
| 32:o:335:LEU:HD11 | 32:o:910:PRO:HG2  | 1.90                     | 0.53              |
| 5:5:269:GLY:HA3   | 3:h:203:ARG:HH11  | 1.74                     | 0.53              |
| 8:A:89:ASP:HA     | 14:G:121:GLN:HE22 | 1.74                     | 0.53              |
| 19:P:106:SER:HA   | 19:P:108:LYS:HE2  | 1.90                     | 0.53              |
| 19:P:242:GLN:N    | 19:P:264:ILE:HD11 | 2.24                     | 0.53              |
| 6:e:46:THR:OG1    | 6:e:219:ASP:O     | 2.27                     | 0.53              |
| 3:h:110:ALA:HA    | 3:h:121:ILE:HG22  | 1.91                     | 0.53              |
| 2:i:220:LEU:HG    | 2:i:222:PRO:HD3   | 1.91                     | 0.53              |
| 8:A:183:GLU:HG2   | 9:B:55:LEU:HG     | 1.91                     | 0.53              |
| 10:C:145:GLY:O    | 10:C:147:GLN:NE2  | 2.42                     | 0.53              |
| 10:C:238:ILE:H    | 10:C:238:ILE:HD12 | 1.72                     | 0.53              |
| 12:E:204:LEU:HA   | 12:E:207:VAL:HG12 | 1.91                     | 0.53              |
| 5:f:95:ALA:HB2    | 5:f:106:VAL:HG21  | 1.90                     | 0.53              |
| 27:M:55:ASN:HA    | 27:M:58:MET:HG3   | 1.90                     | 0.53              |
| 32:o:597:SER:O    | 32:o:601:VAL:HG22 | 2.09                     | 0.53              |
| 7:7:176:ALA:HB3   | 7:7:181:ALA:HA    | 1.91                     | 0.52              |
| 12:E:71:ASP:OD2   | 12:E:73:HIS:ND1   | 2.28                     | 0.52              |
| 13:F:98:VAL:HG12  | 13:F:99:PHE:HD2   | 1.74                     | 0.52              |
| 14:G:91:ARG:O     | 14:G:91:ARG:HD3   | 2.08                     | 0.52              |
| 15:I:55:CYS:SG    | 32:o:248:TYR:OH   | 2.65                     | 0.52              |
| 18:O:232:GLU:HA   | 18:O:235:HIS:HE1  | 1.74                     | 0.52              |
| 19:P:301:LYS:O    | 19:P:305:THR:OG1  | 2.28                     | 0.52              |
| 21:S:438:HIS:O    | 21:S:438:HIS:ND1  | 2.35                     | 0.52              |
| 30:N:227:LYS:HE2  | 30:N:722:THR:HA   | 1.91                     | 0.52              |
| 7:7:103:LEU:HD22  | 7:7:128:TYR:HD2   | 1.73                     | 0.52              |
| 14:G:60:VAL:HG13  | 14:G:63:LYS:HB2   | 1.92                     | 0.52              |
| 15:I:116:ASP:OD2  | 26:H:89:GLN:NE2   | 2.31                     | 0.52              |
| 18:O:165:LEU:O    | 18:O:167:ILE:N    | 2.41                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:P:13:TYR:O     | 19:P:17:LEU:N     | 2.33                     | 0.52              |
| 3:h:84:PRO:HB2    | 3:h:120:PHE:HE2   | 1.74                     | 0.52              |
| 30:N:76:GLU:OE2   | 30:N:76:GLU:N     | 2.39                     | 0.52              |
| 30:N:109:TYR:OH   | 30:N:162:ARG:NH1  | 2.32                     | 0.52              |
| 30:N:389:TYR:HB3  | 30:N:404:SER:HB2  | 1.92                     | 0.52              |
| 5:5:119:THR:OG1   | 5:5:175:MET:N     | 2.40                     | 0.52              |
| 12:E:214:GLU:HG3  | 12:E:233:ASN:HB3  | 1.91                     | 0.52              |
| 17:L:264:ARG:NE   | 17:L:307:GLU:OE2  | 2.39                     | 0.52              |
| 22:V:87:PHE:CZ    | 29:U:79:MET:HB3   | 2.44                     | 0.52              |
| 7:a:152:VAL:HG22  | 7:a:158:GLN:HG3   | 1.91                     | 0.52              |
| 30:N:533:ASP:OD1  | 30:N:559:TYR:OH   | 2.27                     | 0.52              |
| 3:3:84:PRO:HB2    | 3:3:120:PHE:HD2   | 1.74                     | 0.52              |
| 9:B:185:LEU:HD21  | 9:B:213:ILE:HG21  | 1.92                     | 0.52              |
| 10:C:72:LYS:HD2   | 10:C:140:TYR:HB3  | 1.91                     | 0.52              |
| 13:F:77:LEU:HG    | 13:F:79:PRO:HD2   | 1.90                     | 0.52              |
| 15:I:99:ILE:O     | 26:H:90:ARG:NH1   | 2.40                     | 0.52              |
| 16:K:361:SER:O    | 16:K:401:VAL:HG23 | 2.09                     | 0.52              |
| 20:R:226:GLU:O    | 20:R:230:LEU:HG   | 2.08                     | 0.52              |
| 21:S:484:ASP:HB2  | 25:J:46:ALA:HB2   | 1.89                     | 0.52              |
| 30:N:181:GLU:HA   | 30:N:184:LYS:HD2  | 1.90                     | 0.52              |
| 32:o:546:ILE:HG21 | 32:o:570:LEU:HB2  | 1.90                     | 0.52              |
| 6:6:192:LYS:NZ    | 6:6:193:TYR:O     | 2.42                     | 0.52              |
| 16:K:316:MET:HE3  | 16:K:334:LEU:HD11 | 1.90                     | 0.52              |
| 17:L:247:PRO:HG2  | 17:L:250:GLY:HA3  | 1.92                     | 0.52              |
| 6:6:137:GLY:O     | 6:6:228:LYS:NZ    | 2.43                     | 0.52              |
| 15:I:234:LYS:NZ   | 25:J:277:ASN:OD1  | 2.36                     | 0.52              |
| 17:L:108:VAL:HG22 | 17:L:119:VAL:HG12 | 1.92                     | 0.52              |
| 23:W:101:ARG:NH1  | 23:W:106:GLN:O    | 2.42                     | 0.52              |
| 30:N:572:LEU:O    | 30:N:576:VAL:HG23 | 2.09                     | 0.52              |
| 5:5:136:SER:OG    | 5:5:137:GLN:OE1   | 2.27                     | 0.52              |
| 7:7:80:ASP:OD2    | 7:7:81:ASN:N      | 2.43                     | 0.52              |
| 7:7:86:ILE:HD11   | 7:7:93:MET:HA     | 1.92                     | 0.52              |
| 15:I:150:HIS:CE1  | 15:I:152:LYS:H    | 2.28                     | 0.52              |
| 17:L:261:ARG:O    | 17:L:265:GLU:HG2  | 2.10                     | 0.52              |
| 22:V:94:MET:HE3   | 29:U:76:MET:HE2   | 1.92                     | 0.52              |
| 7:a:133:MET:HG3   | 7:a:165:LEU:HA    | 1.91                     | 0.52              |
| 4:g:193:ASP:OD1   | 4:g:193:ASP:N     | 2.43                     | 0.52              |
| 28:Q:153:ASP:N    | 28:Q:153:ASP:OD1  | 2.39                     | 0.52              |
| 30:N:773:MET:HG2  | 30:N:884:PHE:HA   | 1.90                     | 0.52              |
| 8:A:200:GLU:HG2   | 8:A:244:ARG:NH2   | 2.25                     | 0.52              |
| 16:K:368:LEU:HD12 | 16:K:368:LEU:H    | 1.73                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:e:117:TYR:OH    | 5:f:126:ASP:OD1   | 2.18                     | 0.52              |
| 6:e:152:ARG:HD3   | 6:e:153:GLU:N     | 2.25                     | 0.52              |
| 3:h:27:LEU:HG     | 3:h:185:ALA:HA    | 1.91                     | 0.52              |
| 28:Q:261:VAL:O    | 28:Q:265:MET:HG2  | 2.10                     | 0.52              |
| 28:Q:283:ASN:O    | 28:Q:288:LYS:NZ   | 2.42                     | 0.52              |
| 30:N:11:ALA:HB1   | 31:T:80:ASN:HB3   | 1.92                     | 0.52              |
| 32:o:776:VAL:O    | 32:o:780:MET:HG2  | 2.09                     | 0.52              |
| 32:o:862:MET:SD   | 32:o:908:ILE:HD11 | 2.50                     | 0.52              |
| 2:2:87:LEU:HD12   | 9:B:99:ARG:HH22   | 1.75                     | 0.52              |
| 3:3:25:CYS:HB2    | 3:3:43:ILE:HD11   | 1.92                     | 0.52              |
| 14:G:102:LEU:HD23 | 14:G:103:TYR:CD2  | 2.44                     | 0.52              |
| 17:L:219:LEU:HB2  | 17:L:343:LEU:HD12 | 1.92                     | 0.52              |
| 20:R:19:ASN:HB3   | 20:R:21:VAL:HG22  | 1.90                     | 0.52              |
| 21:S:458:GLN:NE2  | 29:U:270:ASN:OD1  | 2.43                     | 0.52              |
| 21:S:482:PRO:O    | 21:S:486:LYS:N    | 2.43                     | 0.52              |
| 6:e:220:GLY:HA2   | 6:e:238:LEU:H     | 1.75                     | 0.52              |
| 25:J:98:VAL:HA    | 25:J:122:LEU:HB2  | 1.92                     | 0.52              |
| 25:J:197:LEU:HD22 | 36:J:502:ADP:H2'  | 1.92                     | 0.52              |
| 26:H:395:SER:OG   | 26:H:396:MET:N    | 2.42                     | 0.52              |
| 30:N:735:MET:HG3  | 30:N:748:PHE:CD2  | 2.45                     | 0.52              |
| 31:T:32:ILE:HG22  | 31:T:36:LYS:HE3   | 1.92                     | 0.52              |
| 8:A:123:ASN:O     | 8:A:127:ILE:HG12  | 2.09                     | 0.52              |
| 10:C:215:THR:O    | 10:C:227:GLN:NE2  | 2.43                     | 0.52              |
| 13:F:157:TYR:HE1  | 14:G:60:VAL:HA    | 1.74                     | 0.52              |
| 15:I:83:LYS:HB3   | 15:I:88:LYS:HG3   | 1.91                     | 0.52              |
| 1:b:117:ILE:HD11  | 1:b:129:VAL:HG13  | 1.91                     | 0.52              |
| 25:J:112:ARG:HH21 | 25:J:126:LEU:HD23 | 1.74                     | 0.52              |
| 28:Q:11:ALA:HA    | 28:Q:14:LEU:HD12  | 1.92                     | 0.52              |
| 30:N:55:PHE:HB3   | 30:N:58:ARG:HG2   | 1.92                     | 0.52              |
| 31:T:4:LEU:O      | 31:T:8:THR:HG23   | 2.10                     | 0.52              |
| 31:T:76:ASP:OD1   | 31:T:76:ASP:N     | 2.41                     | 0.52              |
| 5:5:96:THR:HA     | 5:5:101:VAL:HA    | 1.92                     | 0.51              |
| 15:I:218:GLY:HA3  | 15:I:344:ILE:HG22 | 1.92                     | 0.51              |
| 20:R:131:ALA:O    | 20:R:135:ILE:HG12 | 2.10                     | 0.51              |
| 21:S:271:ARG:NE   | 24:Y:37:ASP:OD2   | 2.35                     | 0.51              |
| 22:V:160:ASP:O    | 22:V:161:THR:HG23 | 2.10                     | 0.51              |
| 32:o:95:THR:O     | 32:o:99:LEU:HD22  | 2.10                     | 0.51              |
| 10:C:136:ILE:HD11 | 10:C:165:VAL:HG22 | 1.93                     | 0.51              |
| 14:G:99:PHE:CG    | 14:G:107:ILE:HD13 | 2.46                     | 0.51              |
| 21:S:239:ARG:NH1  | 21:S:243:ASN:OD1  | 2.44                     | 0.51              |
| 23:W:20:ASP:OD1   | 23:W:21:PHE:N     | 2.41                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:i:153:TYR:HB2   | 2:i:167:LEU:HD13  | 1.91                     | 0.51              |
| 2:i:177:LYS:HE3   | 2:i:206:VAL:HG11  | 1.93                     | 0.51              |
| 32:o:381:LEU:HD21 | 32:o:898:HIS:CD2  | 2.45                     | 0.51              |
| 2:2:51:GLN:OE1    | 2:2:51:GLN:N      | 2.41                     | 0.51              |
| 6:6:161:ALA:HB2   | 6:6:214:HIS:HD2   | 1.74                     | 0.51              |
| 18:O:232:GLU:HA   | 18:O:235:HIS:CE1  | 2.46                     | 0.51              |
| 21:S:393:ARG:HA   | 21:S:432:ILE:HD11 | 1.93                     | 0.51              |
| 5:f:138:CYS:HB2   | 5:f:149:ILE:HG21  | 1.92                     | 0.51              |
| 27:M:284:ASP:OD1  | 27:M:284:ASP:N    | 2.35                     | 0.51              |
| 3:3:31:SER:N      | 3:3:34:LEU:O      | 2.43                     | 0.51              |
| 4:4:160:LEU:HD23  | 4:4:163:LEU:HD12  | 1.92                     | 0.51              |
| 7:7:160:LEU:HG    | 7:7:175:LEU:HD23  | 1.92                     | 0.51              |
| 12:E:205:LYS:HA   | 12:E:208:MET:HG2  | 1.92                     | 0.51              |
| 15:I:242:ALA:HB2  | 15:I:276:PRO:HG2  | 1.91                     | 0.51              |
| 7:7:122:PRO:HB2   | 7:7:159:PHE:HD2   | 1.76                     | 0.51              |
| 8:A:219:SER:N     | 8:A:222:ASP:OD2   | 2.38                     | 0.51              |
| 19:P:310:ARG:NH1  | 19:P:367:GLU:O    | 2.37                     | 0.51              |
| 1:b:214:GLN:OE1   | 1:b:214:GLN:N     | 2.43                     | 0.51              |
| 4:g:95:ARG:HH11   | 4:g:96:ARG:HB2    | 1.75                     | 0.51              |
| 26:H:282:LYS:HG2  | 26:H:283:TYR:CD2  | 2.46                     | 0.51              |
| 26:H:343:PHE:HD2  | 27:M:245:LYS:HD3  | 1.76                     | 0.51              |
| 28:Q:52:ASN:HA    | 28:Q:55:GLU:HG2   | 1.92                     | 0.51              |
| 3:3:203:ARG:O     | 3:3:203:ARG:NH1   | 2.43                     | 0.51              |
| 15:I:316:PHE:HD2  | 26:H:273:ARG:HD2  | 1.76                     | 0.51              |
| 17:L:293:GLU:OE1  | 17:L:293:GLU:N    | 2.43                     | 0.51              |
| 20:R:218:CYS:HG   | 20:R:223:ASN:ND2  | 2.07                     | 0.51              |
| 24:Y:77:LEU:HD23  | 24:Y:77:LEU:H     | 1.75                     | 0.51              |
| 1:b:48:ARG:NE     | 2:i:168:GLU:OE2   | 2.43                     | 0.51              |
| 2:i:30:THR:HG21   | 2:i:75:ALA:HA     | 1.93                     | 0.51              |
| 28:Q:410:ASP:O    | 28:Q:414:GLU:HG2  | 2.10                     | 0.51              |
| 32:o:737:ALA:CA   | 32:o:775:MET:HE1  | 2.38                     | 0.51              |
| 32:o:761:PHE:HB3  | 32:o:776:VAL:HG13 | 1.92                     | 0.51              |
| 4:4:5:LEU:HD21    | 4:4:140:THR:HG21  | 1.92                     | 0.51              |
| 15:I:339:ILE:HA   | 15:I:344:ILE:HD11 | 1.92                     | 0.51              |
| 18:O:22:LEU:HD13  | 18:O:57:LEU:HD11  | 1.93                     | 0.51              |
| 20:R:54:ILE:HG12  | 20:R:59:MET:HB2   | 1.93                     | 0.51              |
| 21:S:433:GLU:OE1  | 21:S:446:THR:OG1  | 2.26                     | 0.51              |
| 7:a:260:GLY:HA2   | 7:a:264:GLN:HE21  | 1.76                     | 0.51              |
| 25:J:160:ILE:HD11 | 25:J:187:LEU:HD21 | 1.92                     | 0.51              |
| 26:H:98:GLN:HB3   | 26:H:149:LEU:HD21 | 1.92                     | 0.51              |
| 30:N:330:THR:HG23 | 30:N:366:THR:HG21 | 1.93                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:125:ALA:HB1   | 2:2:127:LEU:HD21  | 1.93                     | 0.51              |
| 6:6:140:ALA:HA    | 6:6:152:ARG:HH12  | 1.76                     | 0.51              |
| 7:7:122:PRO:HG3   | 7:7:151:GLY:HA3   | 1.92                     | 0.51              |
| 11:D:67:ILE:HG21  | 11:D:109:LEU:HD11 | 1.92                     | 0.51              |
| 17:L:95:ILE:O     | 17:L:99:GLN:HG2   | 2.11                     | 0.51              |
| 17:L:165:PRO:HD3  | 27:M:83:VAL:HG13  | 1.92                     | 0.51              |
| 17:L:258:GLU:OE1  | 17:L:258:GLU:HA   | 2.11                     | 0.51              |
| 30:N:427:ILE:HD13 | 30:N:443:LEU:HD13 | 1.93                     | 0.51              |
| 31:T:39:LEU:HB3   | 31:T:58:THR:HG21  | 1.93                     | 0.51              |
| 32:o:812:ILE:HD12 | 32:o:848:THR:HA   | 1.92                     | 0.51              |
| 1:1:159:LYS:HG3   | 1:b:180:GLN:HE21  | 1.75                     | 0.51              |
| 7:7:34:THR:N      | 7:7:140:MET:O     | 2.44                     | 0.51              |
| 11:D:116:VAL:HA   | 11:D:119:ARG:NH1  | 2.26                     | 0.51              |
| 15:I:380:LEU:HD21 | 15:I:416:PHE:CD2  | 2.45                     | 0.51              |
| 20:R:348:LEU:HD12 | 20:R:349:SER:H    | 1.76                     | 0.51              |
| 25:J:96:VAL:HG11  | 25:J:115:LEU:HD22 | 1.92                     | 0.51              |
| 30:N:104:LYS:HA   | 30:N:107:GLU:HG2  | 1.93                     | 0.51              |
| 32:o:309:GLN:HG3  | 32:o:982:ILE:HG13 | 1.92                     | 0.51              |
| 15:I:56:LYS:HE2   | 32:o:226:GLU:HB3  | 1.93                     | 0.51              |
| 23:W:141:ILE:HD13 | 23:W:154:LEU:HD22 | 1.93                     | 0.51              |
| 4:g:184:VAL:HG22  | 4:g:189:ILE:HG12  | 1.93                     | 0.51              |
| 25:J:188:TYR:CE1  | 25:J:297:LEU:HD11 | 2.45                     | 0.51              |
| 25:J:213:VAL:HG11 | 25:J:233:LEU:HD22 | 1.93                     | 0.51              |
| 2:2:54:ILE:HD11   | 3:3:147:PHE:HD2   | 1.77                     | 0.50              |
| 15:I:290:LYS:HB3  | 15:I:292:TYR:CE1  | 2.46                     | 0.50              |
| 17:L:279:PHE:HD1  | 17:L:324:ILE:HB   | 1.75                     | 0.50              |
| 22:V:127:LYS:O    | 22:V:131:GLN:HG2  | 2.11                     | 0.50              |
| 28:Q:344:GLU:HG2  | 28:Q:376:LYS:HE3  | 1.92                     | 0.50              |
| 32:o:279:THR:OG1  | 32:o:280:ASP:OD1  | 2.29                     | 0.50              |
| 32:o:387:ASN:ND2  | 32:o:397:ASP:OD2  | 2.36                     | 0.50              |
| 32:o:751:ASP:OD1  | 32:o:751:ASP:N    | 2.40                     | 0.50              |
| 1:1:78:VAL:HG22   | 1:1:100:VAL:HG23  | 1.93                     | 0.50              |
| 8:A:125:SER:O     | 8:A:129:THR:HG23  | 2.11                     | 0.50              |
| 15:I:244:PHE:HD1  | 15:I:278:ILE:HB   | 1.76                     | 0.50              |
| 16:K:109:ILE:HG12 | 16:K:119:VAL:HG22 | 1.92                     | 0.50              |
| 20:R:171:MET:HA   | 20:R:174:ILE:CD1  | 2.41                     | 0.50              |
| 20:R:224:PHE:O    | 20:R:260:THR:HG21 | 2.11                     | 0.50              |
| 21:S:404:LEU:N    | 21:S:441:GLY:O    | 2.45                     | 0.50              |
| 26:H:102:CYS:SG   | 26:H:103:THR:N    | 2.84                     | 0.50              |
| 32:o:74:SER:O     | 32:o:78:SER:N     | 2.43                     | 0.50              |
| 4:4:44:MET:HE2    | 4:4:44:MET:HA     | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:A:189:SER:O     | 8:A:190:LYS:HG3   | 2.10                     | 0.50              |
| 8:A:228:ALA:HB2   | 8:A:233:PHE:HD1   | 1.76                     | 0.50              |
| 11:D:148:TYR:CE1  | 11:D:158:SER:HB2  | 2.43                     | 0.50              |
| 12:E:86:ARG:HG2   | 12:E:86:ARG:HH11  | 1.77                     | 0.50              |
| 12:E:122:ARG:O    | 12:E:122:ARG:NE   | 2.43                     | 0.50              |
| 13:F:177:ASP:OD1  | 13:F:177:ASP:N    | 2.39                     | 0.50              |
| 20:R:66:LEU:HD22  | 20:R:92:ILE:HG21  | 1.94                     | 0.50              |
| 21:S:183:LEU:O    | 21:S:187:ILE:HG12 | 2.10                     | 0.50              |
| 22:V:296:LEU:HD23 | 29:U:190:LEU:HD22 | 1.93                     | 0.50              |
| 4:g:49:GLU:O      | 4:g:53:THR:HG23   | 2.11                     | 0.50              |
| 26:H:93:GLU:O     | 26:H:96:PRO:HD2   | 2.11                     | 0.50              |
| 6:6:240:ARG:HD3   | 2:i:193:TRP:HB3   | 1.94                     | 0.50              |
| 9:B:217:GLU:HB2   | 9:B:231:LYS:HE2   | 1.93                     | 0.50              |
| 12:E:184:LEU:HA   | 13:F:56:LEU:HD11  | 1.93                     | 0.50              |
| 15:I:273:GLU:HG3  | 15:I:274:ASN:HD22 | 1.77                     | 0.50              |
| 16:K:171:TYR:O    | 16:K:181:LYS:NZ   | 2.37                     | 0.50              |
| 20:R:148:ASP:OD1  | 20:R:148:ASP:N    | 2.45                     | 0.50              |
| 21:S:307:LEU:HD21 | 21:S:337:ASN:HB2  | 1.94                     | 0.50              |
| 2:i:206:VAL:HB    | 2:i:214:GLU:HB2   | 1.93                     | 0.50              |
| 27:M:246:LEU:HD11 | 27:M:251:LEU:HG   | 1.93                     | 0.50              |
| 29:U:15:LEU:C     | 29:U:15:LEU:HD23  | 2.35                     | 0.50              |
| 1:1:163:GLU:N     | 1:1:163:GLU:OE2   | 2.43                     | 0.50              |
| 3:3:99:ARG:NH2    | 3:3:127:ILE:HG23  | 2.25                     | 0.50              |
| 6:6:32:LEU:HD23   | 6:6:203:VAL:HG13  | 1.92                     | 0.50              |
| 7:7:152:VAL:HG11  | 7:7:235:LYS:HB3   | 1.92                     | 0.50              |
| 15:I:76:VAL:HB    | 26:H:66:LYS:HZ1   | 1.74                     | 0.50              |
| 15:I:262:ARG:NH2  | 26:H:281:GLN:OE1  | 2.44                     | 0.50              |
| 18:O:75:GLN:HB3   | 18:O:122:HIS:CD2  | 2.45                     | 0.50              |
| 3:h:108:VAL:HA    | 3:h:123:GLY:HA2   | 1.94                     | 0.50              |
| 25:J:112:ARG:HE   | 25:J:126:LEU:HD23 | 1.77                     | 0.50              |
| 27:M:203:ARG:HE   | 27:M:206:LYS:HD2  | 1.76                     | 0.50              |
| 32:o:609:THR:HG21 | 32:o:878:LEU:HD21 | 1.92                     | 0.50              |
| 1:1:176:HIS:HA    | 1:b:159:LYS:HZ3   | 1.77                     | 0.50              |
| 1:1:194:MET:HB2   | 1:1:205:LEU:HB3   | 1.94                     | 0.50              |
| 3:3:66:MET:O      | 3:3:70:LYS:HG2    | 2.11                     | 0.50              |
| 8:A:101:ALA:HA    | 8:A:112:MET:SD    | 2.51                     | 0.50              |
| 11:D:43:VAL:HG22  | 11:D:214:VAL:HG22 | 1.94                     | 0.50              |
| 21:S:59:ASP:O     | 21:S:63:LEU:HG    | 2.11                     | 0.50              |
| 7:a:204:GLN:O     | 7:a:208:GLU:HG2   | 2.11                     | 0.50              |
| 7:a:215:ARG:NH1   | 7:a:249:ASN:OD1   | 2.44                     | 0.50              |
| 1:b:163:GLU:HG3   | 1:b:164:ASN:OD1   | 2.11                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:H:501:ATP:H5'2 | 34:H:501:ATP:C8   | 2.47                     | 0.50              |
| 28:Q:85:MET:SD    | 28:Q:89:ALA:HB3   | 2.51                     | 0.50              |
| 30:N:256:GLN:HE22 | 30:N:903:VAL:HA   | 1.75                     | 0.50              |
| 4:4:104:ILE:HG23  | 4:4:117:TYR:HB2   | 1.93                     | 0.50              |
| 5:5:208:GLN:OE1   | 5:5:208:GLN:N     | 2.41                     | 0.50              |
| 32:o:973:TYR:HE1  | 32:o:984:LYS:HB3  | 1.77                     | 0.50              |
| 4:4:13:VAL:HG13   | 4:4:184:VAL:HB    | 1.94                     | 0.50              |
| 5:5:210:PHE:HB3   | 5:5:239:ALA:HA    | 1.94                     | 0.50              |
| 8:A:143:PHE:N     | 8:A:155:TYR:O     | 2.42                     | 0.50              |
| 16:K:221:MET:HE1  | 34:K:501:ATP:H2'  | 1.93                     | 0.50              |
| 19:P:173:MET:HE2  | 19:P:173:MET:HA   | 1.94                     | 0.50              |
| 20:R:202:GLY:HA2  | 20:R:207:ARG:HH21 | 1.77                     | 0.50              |
| 20:R:317:ILE:HG13 | 20:R:318:PRO:HD3  | 1.94                     | 0.50              |
| 22:V:90:LYS:O     | 22:V:94:MET:HG2   | 2.12                     | 0.50              |
| 22:V:154:ASP:OD1  | 22:V:154:ASP:N    | 2.44                     | 0.50              |
| 22:V:265:GLU:O    | 22:V:269:ARG:N    | 2.45                     | 0.50              |
| 23:W:19:GLY:HA2   | 23:W:24:THR:HA    | 1.94                     | 0.50              |
| 25:J:217:GLU:OE1  | 25:J:217:GLU:N    | 2.45                     | 0.50              |
| 26:H:173:ARG:HD2  | 26:H:190:ARG:HB2  | 1.94                     | 0.50              |
| 28:Q:328:ASP:O    | 28:Q:331:THR:N    | 2.40                     | 0.50              |
| 30:N:654:GLN:HE22 | 30:N:694:LEU:HD12 | 1.77                     | 0.50              |
| 32:o:117:ASP:O    | 32:o:121:ILE:HG12 | 2.12                     | 0.50              |
| 5:5:109:VAL:HG11  | 5:5:253:TYR:CE2   | 2.47                     | 0.50              |
| 14:G:147:HIS:HB3  | 14:G:149:TYR:CE1  | 2.47                     | 0.50              |
| 15:I:110:GLU:OE1  | 15:I:111:GLU:HB2  | 2.12                     | 0.50              |
| 18:O:49:PHE:O     | 18:O:58:ARG:NH2   | 2.41                     | 0.50              |
| 18:O:389:GLN:HA   | 18:O:392:TRP:CD1  | 2.47                     | 0.50              |
| 20:R:179:PHE:CZ   | 20:R:187:VAL:HG11 | 2.47                     | 0.50              |
| 23:W:125:LEU:HD22 | 23:W:157:PHE:HZ   | 1.77                     | 0.50              |
| 28:Q:198:LEU:HD12 | 28:Q:221:MET:HG3  | 1.93                     | 0.50              |
| 30:N:657:MET:HE2  | 30:N:681:ASN:HD21 | 1.77                     | 0.50              |
| 32:o:774:ARG:HB2  | 32:o:810:ASN:ND2  | 2.27                     | 0.50              |
| 1:1:85:TYR:HE2    | 1:1:92:PRO:HA     | 1.77                     | 0.49              |
| 5:5:220:LYS:HB3   | 5:5:223:LEU:HG    | 1.93                     | 0.49              |
| 13:F:4:ASN:OD1    | 13:F:6:TYR:N      | 2.32                     | 0.49              |
| 13:F:6:TYR:CE2    | 13:F:15:PRO:HD3   | 2.46                     | 0.49              |
| 16:K:210:LEU:HB2  | 16:K:334:LEU:HD23 | 1.94                     | 0.49              |
| 17:L:88:TYR:CE1   | 27:M:62:ILE:HG13  | 2.46                     | 0.49              |
| 30:N:119:LYS:HG3  | 30:N:120:ASP:H    | 1.77                     | 0.49              |
| 30:N:297:ASP:O    | 30:N:301:THR:HG23 | 2.12                     | 0.49              |
| 30:N:594:VAL:HG12 | 30:N:595:LEU:HD23 | 1.93                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:5:117:LEU:HB2   | 5:5:177:CYS:HB2   | 1.92                     | 0.49              |
| 17:L:79:GLN:HA    | 17:L:82:ARG:HH11  | 1.76                     | 0.49              |
| 20:R:33:LEU:HA    | 20:R:43:ARG:HG3   | 1.94                     | 0.49              |
| 23:W:123:ASP:N    | 23:W:123:ASP:OD1  | 2.43                     | 0.49              |
| 7:a:59:ASN:O      | 7:a:72:VAL:N      | 2.44                     | 0.49              |
| 3:h:68:ARG:NH1    | 3:h:72:ASN:OD1    | 2.45                     | 0.49              |
| 3:h:162:ASP:HA    | 2:i:236:ARG:CZ    | 2.42                     | 0.49              |
| 29:U:75:ASN:O     | 29:U:79:MET:HG2   | 2.12                     | 0.49              |
| 31:T:258:ASN:O    | 31:T:260:ILE:N    | 2.44                     | 0.49              |
| 32:o:826:ARG:HH22 | 32:o:830:LEU:HD11 | 1.77                     | 0.49              |
| 5:5:114:PRO:HA    | 5:5:260:TRP:NE1   | 2.27                     | 0.49              |
| 9:B:217:GLU:HB3   | 9:B:231:LYS:HB2   | 1.94                     | 0.49              |
| 21:S:329:GLU:OE2  | 21:S:331:SER:OG   | 2.30                     | 0.49              |
| 5:f:82:ARG:HE     | 5:f:221:TRP:HZ3   | 1.58                     | 0.49              |
| 25:J:52:ASN:ND2   | 30:N:611:LYS:O    | 2.45                     | 0.49              |
| 30:N:111:GLN:O    | 30:N:115:LYS:HG2  | 2.12                     | 0.49              |
| 30:N:158:LEU:HD21 | 30:N:206:ILE:HD12 | 1.93                     | 0.49              |
| 1:1:155:GLY:O     | 1:b:180:GLN:NE2   | 2.46                     | 0.49              |
| 15:I:126:PRO:HG2  | 26:H:98:GLN:HE22  | 1.77                     | 0.49              |
| 17:L:229:THR:HG21 | 27:M:314:GLY:HA2  | 1.93                     | 0.49              |
| 18:O:10:ILE:HG21  | 18:O:64:ASN:HB3   | 1.95                     | 0.49              |
| 21:S:141:LEU:HA   | 21:S:144:LEU:HD12 | 1.93                     | 0.49              |
| 7:a:194:ARG:NE    | 7:a:195:GLU:OE1   | 2.45                     | 0.49              |
| 4:g:111:LYS:HD2   | 4:g:113:LYS:HB2   | 1.95                     | 0.49              |
| 30:N:438:ASP:OD1  | 30:N:438:ASP:N    | 2.44                     | 0.49              |
| 30:N:750:SER:HA   | 30:N:753:PHE:HD2  | 1.76                     | 0.49              |
| 9:B:38:LYS:HG3    | 9:B:43:VAL:HG22   | 1.94                     | 0.49              |
| 11:D:66:LYS:HA    | 11:D:72:VAL:HG23  | 1.93                     | 0.49              |
| 14:G:52:LYS:NZ    | 14:G:215:GLU:HB2  | 2.27                     | 0.49              |
| 16:K:137:VAL:HB   | 16:K:146:LEU:HD21 | 1.95                     | 0.49              |
| 18:O:299:THR:HG21 | 18:O:316:ALA:HB1  | 1.95                     | 0.49              |
| 22:V:37:MET:HB3   | 22:V:141:VAL:HG11 | 1.94                     | 0.49              |
| 23:W:3:LEU:HG     | 23:W:106:GLN:HE21 | 1.77                     | 0.49              |
| 7:a:204:GLN:HA    | 7:a:207:GLU:OE1   | 2.12                     | 0.49              |
| 7:a:218:TYR:CD2   | 7:a:247:VAL:HG21  | 2.48                     | 0.49              |
| 1:b:69:ALA:HB3    | 2:i:145:HIS:CD2   | 2.47                     | 0.49              |
| 5:f:82:ARG:HG2    | 5:f:200:ASP:HB3   | 1.93                     | 0.49              |
| 2:i:137:SER:HB3   | 2:i:209:ILE:HD11  | 1.94                     | 0.49              |
| 28:Q:65:TYR:CE2   | 28:Q:73:LYS:HB3   | 2.47                     | 0.49              |
| 1:1:85:TYR:HA     | 1:1:89:TYR:HD1    | 1.77                     | 0.49              |
| 1:1:85:TYR:CD1    | 14:G:103:TYR:HE1  | 2.29                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:4:174:MET:HE2   | 4:4:174:MET:HA    | 1.93                     | 0.49              |
| 5:5:78:THR:HG22   | 5:5:91:VAL:HG13   | 1.95                     | 0.49              |
| 5:5:232:GLY:O     | 5:5:236:ILE:HG22  | 2.11                     | 0.49              |
| 8:A:185:HIS:O     | 8:A:188:LYS:HG3   | 2.13                     | 0.49              |
| 11:D:39:LYS:HD3   | 11:D:184:PRO:HG2  | 1.94                     | 0.49              |
| 13:F:203:ASP:OD1  | 13:F:204:GLU:N    | 2.45                     | 0.49              |
| 21:S:399:TYR:HB3  | 21:S:402:ILE:HB   | 1.94                     | 0.49              |
| 7:a:221:ASP:OD1   | 7:a:223:ARG:NH2   | 2.45                     | 0.49              |
| 26:H:192:ASP:OD1  | 26:H:194:SER:N    | 2.39                     | 0.49              |
| 28:Q:114:GLN:HB3  | 28:Q:144:LEU:HD13 | 1.95                     | 0.49              |
| 29:U:40:ASP:OD2   | 29:U:47:ARG:NH1   | 2.45                     | 0.49              |
| 32:o:928:ARG:HG3  | 32:o:966:GLU:HB2  | 1.94                     | 0.49              |
| 5:5:83:PHE:HE1    | 5:5:88:ILE:HG12   | 1.78                     | 0.49              |
| 5:5:97:ALA:HB2    | 5:5:102:ALA:HB2   | 1.94                     | 0.49              |
| 12:E:205:LYS:NZ   | 12:E:212:LEU:H    | 2.11                     | 0.49              |
| 15:I:216:PRO:HG3  | 15:I:346:ARG:HD2  | 1.94                     | 0.49              |
| 17:L:309:LEU:HG   | 17:L:342:ARG:CZ   | 2.43                     | 0.49              |
| 3:h:168:SER:O     | 3:h:172:LEU:HG    | 2.12                     | 0.49              |
| 26:H:251:PRO:O    | 26:H:254:THR:OG1  | 2.22                     | 0.49              |
| 26:H:416:GLY:HA2  | 26:H:419:LEU:HD23 | 1.94                     | 0.49              |
| 30:N:894:ARG:HH21 | 30:N:897:LYS:HZ3  | 1.59                     | 0.49              |
| 32:o:405:ASN:HA   | 32:o:408:TYR:HD2  | 1.77                     | 0.49              |
| 5:5:108:LYS:HB3   | 5:5:120:MET:HB2   | 1.94                     | 0.49              |
| 6:6:83:LEU:HD21   | 6:6:124:TYR:CD2   | 2.47                     | 0.49              |
| 11:D:79:ASN:O     | 11:D:83:ARG:NH1   | 2.45                     | 0.49              |
| 12:E:142:LEU:HB2  | 12:E:158:ALA:HB3  | 1.95                     | 0.49              |
| 19:P:357:TYR:CD2  | 19:P:360:ILE:HB   | 2.44                     | 0.49              |
| 23:W:113:PHE:CE1  | 23:W:142:ILE:HD12 | 2.47                     | 0.49              |
| 27:M:317:SER:C    | 27:M:319:ASP:H    | 2.20                     | 0.49              |
| 28:Q:89:ALA:O     | 28:Q:91:SER:N     | 2.44                     | 0.49              |
| 28:Q:326:MET:HB3  | 28:Q:332:ARG:HD3  | 1.95                     | 0.49              |
| 30:N:750:SER:HA   | 30:N:753:PHE:CD2  | 2.48                     | 0.49              |
| 32:o:391:ASN:ND2  | 32:o:397:ASP:OD1  | 2.45                     | 0.49              |
| 32:o:924:LYS:HA   | 32:o:953:THR:HB   | 1.95                     | 0.49              |
| 3:3:41:GLU:OE2    | 3:3:41:GLU:N      | 2.35                     | 0.49              |
| 9:B:220:ASP:N     | 9:B:220:ASP:OD1   | 2.46                     | 0.49              |
| 14:G:151:LEU:HD13 | 14:G:157:TYR:HB3  | 1.94                     | 0.49              |
| 16:K:179:MET:HA   | 16:K:179:MET:HE3  | 1.94                     | 0.49              |
| 19:P:72:TRP:H     | 19:P:72:TRP:CD1   | 2.31                     | 0.49              |
| 21:S:80:VAL:O     | 21:S:111:ARG:NH2  | 2.46                     | 0.49              |
| 21:S:411:LEU:HB3  | 21:S:413:LEU:HD12 | 1.95                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:V:94:MET:HE3   | 29:U:76:MET:CE    | 2.43                     | 0.49              |
| 1:b:56:VAL:HG12   | 1:b:79:GLN:HB2    | 1.93                     | 0.49              |
| 2:i:32:ILE:HD11   | 2:i:156:LEU:HB3   | 1.95                     | 0.49              |
| 26:H:46:ALA:HA    | 26:H:49:LEU:HB2   | 1.95                     | 0.49              |
| 32:o:616:LEU:O    | 32:o:620:LEU:HD23 | 2.13                     | 0.49              |
| 1:1:23:MET:SD     | 1:1:25:VAL:HG23   | 2.52                     | 0.49              |
| 3:3:65:GLU:OE1    | 10:C:100:LYS:HD3  | 2.13                     | 0.49              |
| 8:A:24:ARG:HH21   | 8:A:26:TYR:HE1    | 1.61                     | 0.49              |
| 9:B:204:PHE:CE1   | 9:B:209:ILE:HD11  | 2.48                     | 0.49              |
| 12:E:204:LEU:O    | 12:E:208:MET:N    | 2.46                     | 0.49              |
| 19:P:344:ARG:HA   | 19:P:344:ARG:HD3  | 1.57                     | 0.49              |
| 20:R:312:TYR:CE1  | 20:R:326:ALA:HB1  | 2.48                     | 0.49              |
| 21:S:41:ILE:HG22  | 21:S:56:SER:HB3   | 1.95                     | 0.49              |
| 21:S:481:TYR:HB2  | 21:S:482:PRO:HD3  | 1.95                     | 0.49              |
| 23:W:109:ARG:HD2  | 23:W:138:ALA:HB3  | 1.95                     | 0.49              |
| 2:i:124:GLY:HA2   | 2:i:144:ALA:HB1   | 1.95                     | 0.49              |
| 26:H:197:MET:SD   | 26:H:197:MET:N    | 2.85                     | 0.49              |
| 26:H:314:VAL:HG23 | 26:H:314:VAL:O    | 2.13                     | 0.49              |
| 26:H:402:ILE:HG13 | 26:H:440:GLU:HB2  | 1.95                     | 0.49              |
| 27:M:149:ASN:OD1  | 27:M:150:LYS:N    | 2.46                     | 0.49              |
| 28:Q:322:GLU:OE1  | 28:Q:322:GLU:N    | 2.41                     | 0.49              |
| 2:2:115:HIS:C     | 2:2:115:HIS:HD1   | 2.19                     | 0.48              |
| 9:B:211:LEU:HD23  | 9:B:243:ILE:HD13  | 1.94                     | 0.48              |
| 13:F:117:GLN:HB3  | 13:F:118:LYS:HD2  | 1.95                     | 0.48              |
| 15:I:316:PHE:CD2  | 26:H:273:ARG:HD2  | 2.47                     | 0.48              |
| 16:K:370:SER:OG   | 16:K:404:GLN:NE2  | 2.36                     | 0.48              |
| 19:P:254:GLU:HA   | 19:P:257:TRP:CD1  | 2.48                     | 0.48              |
| 20:R:40:ILE:HG12  | 20:R:43:ARG:HH12  | 1.77                     | 0.48              |
| 20:R:154:LEU:HD13 | 20:R:170:VAL:HG13 | 1.95                     | 0.48              |
| 20:R:154:LEU:HD12 | 20:R:174:ILE:HG13 | 1.95                     | 0.48              |
| 20:R:190:LYS:O    | 20:R:194:VAL:HG23 | 2.12                     | 0.48              |
| 21:S:188:TYR:CZ   | 21:S:192:GLU:HG3  | 2.47                     | 0.48              |
| 22:V:34:LEU:HD23  | 29:U:174:LEU:HD21 | 1.95                     | 0.48              |
| 5:f:94:ARG:H      | 5:f:108:LYS:NZ    | 2.10                     | 0.48              |
| 5:f:243:ASP:HB3   | 5:f:246:SER:HB3   | 1.95                     | 0.48              |
| 26:H:101:ARG:NH1  | 27:M:165:SER:OG   | 2.41                     | 0.48              |
| 32:o:309:GLN:OE1  | 32:o:973:TYR:HB2  | 2.13                     | 0.48              |
| 1:1:182:ILE:HG23  | 1:1:189:GLY:HA2   | 1.95                     | 0.48              |
| 3:3:13:VAL:HA     | 3:3:138:VAL:HG12  | 1.95                     | 0.48              |
| 3:3:160:PRO:HA    | 3:3:163:LEU:HD23  | 1.96                     | 0.48              |
| 7:7:82:THR:HG21   | 7:7:125:ILE:HD11  | 1.94                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:K:350:ARG:HH22 | 16:K:368:LEU:HB2  | 1.76                     | 0.48              |
| 19:P:141:LYS:O    | 19:P:144:VAL:HG12 | 2.14                     | 0.48              |
| 19:P:198:VAL:HA   | 19:P:201:ARG:HH22 | 1.77                     | 0.48              |
| 21:S:336:SER:OG   | 21:S:337:ASN:N    | 2.40                     | 0.48              |
| 23:W:110:ILE:HB   | 23:W:139:VAL:HG12 | 1.95                     | 0.48              |
| 7:a:168:VAL:HG22  | 6:e:77:ALA:HB3    | 1.95                     | 0.48              |
| 3:h:15:MET:HE2    | 3:h:15:MET:HA     | 1.95                     | 0.48              |
| 25:J:248:ASP:OD1  | 25:J:248:ASP:N    | 2.32                     | 0.48              |
| 25:J:328:LEU:O    | 25:J:332:SER:HB3  | 2.12                     | 0.48              |
| 29:U:100:ARG:N    | 29:U:103:ASP:OD2  | 2.41                     | 0.48              |
| 30:N:650:ASP:OD1  | 30:N:651:PHE:N    | 2.44                     | 0.48              |
| 31:T:258:ASN:C    | 31:T:259:ILE:HD12 | 2.37                     | 0.48              |
| 32:o:617:ILE:HD11 | 32:o:746:ILE:HB   | 1.94                     | 0.48              |
| 4:4:86:GLN:OE1    | 10:C:101:THR:HA   | 2.13                     | 0.48              |
| 6:6:47:ARG:NH2    | 6:6:241:ASP:O     | 2.47                     | 0.48              |
| 6:6:67:ASP:OD2    | 6:6:103:LEU:N     | 2.38                     | 0.48              |
| 7:7:255:ALA:O     | 1:b:193:ARG:NH2   | 2.46                     | 0.48              |
| 11:D:50:SER:HB2   | 11:D:209:ASN:HD21 | 1.78                     | 0.48              |
| 11:D:212:ILE:HD12 | 11:D:229:ILE:HD12 | 1.94                     | 0.48              |
| 12:E:75:GLY:HA3   | 12:E:228:PHE:CE2  | 2.48                     | 0.48              |
| 12:E:185:ASN:OD1  | 12:E:185:ASN:N    | 2.45                     | 0.48              |
| 21:S:479:MET:O    | 21:S:482:PRO:HD2  | 2.13                     | 0.48              |
| 22:V:147:VAL:HA   | 29:U:169:ILE:HD11 | 1.94                     | 0.48              |
| 5:f:254:HIS:O     | 5:f:261:ILE:N     | 2.45                     | 0.48              |
| 27:M:205:ASP:N    | 27:M:205:ASP:OD1  | 2.45                     | 0.48              |
| 28:Q:189:ARG:HD3  | 28:Q:189:ARG:HA   | 1.61                     | 0.48              |
| 30:N:10:LEU:HD11  | 30:N:42:GLU:OE2   | 2.13                     | 0.48              |
| 32:o:765:MET:HE1  | 32:o:773:ARG:HG2  | 1.95                     | 0.48              |
| 8:A:158:ASP:OD1   | 8:A:162:TYR:N     | 2.45                     | 0.48              |
| 9:B:45:ILE:HB     | 9:B:74:VAL:HG21   | 1.95                     | 0.48              |
| 16:K:52:LYS:HE3   | 30:N:196:THR:HG23 | 1.94                     | 0.48              |
| 18:O:358:ILE:HG23 | 18:O:362:GLN:HB2  | 1.96                     | 0.48              |
| 20:R:348:LEU:HD12 | 20:R:349:SER:N    | 2.29                     | 0.48              |
| 21:S:78:VAL:HG21  | 21:S:92:LEU:HD22  | 1.94                     | 0.48              |
| 27:M:164:ASP:HB3  | 27:M:167:VAL:HG23 | 1.95                     | 0.48              |
| 27:M:339:ARG:NH1  | 27:M:340:SER:O    | 2.46                     | 0.48              |
| 28:Q:212:THR:HA   | 28:Q:215:VAL:HG12 | 1.95                     | 0.48              |
| 29:U:68:LEU:HD21  | 29:U:73:ILE:HD11  | 1.94                     | 0.48              |
| 32:o:254:PRO:HG2  | 32:o:255:LEU:HD12 | 1.95                     | 0.48              |
| 1:1:145:ILE:HB    | 1:1:150:SER:HB2   | 1.95                     | 0.48              |
| 2:2:123:ILE:HG22  | 2:2:125:ALA:H     | 1.79                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:234:PHE:O     | 2:2:236:ARG:NH1   | 2.46                     | 0.48              |
| 15:I:290:LYS:NZ   | 15:I:292:TYR:OH   | 2.46                     | 0.48              |
| 15:I:386:ASP:C    | 15:I:387:LEU:HD22 | 2.39                     | 0.48              |
| 18:O:240:GLU:HA   | 18:O:243:VAL:HB   | 1.95                     | 0.48              |
| 19:P:250:ILE:HG23 | 19:P:256:LYS:HB3  | 1.96                     | 0.48              |
| 22:V:262:THR:OG1  | 22:V:264:GLU:OE1  | 2.19                     | 0.48              |
| 32:o:155:ARG:O    | 32:o:159:LEU:HG   | 2.13                     | 0.48              |
| 32:o:303:ASP:HB3  | 32:o:306:MET:HG3  | 1.95                     | 0.48              |
| 32:o:502:ASN:HB3  | 32:o:505:VAL:HB   | 1.95                     | 0.48              |
| 1:1:16:VAL:HG21   | 2:2:143:HIS:ND1   | 2.28                     | 0.48              |
| 6:6:74:ASN:O      | 6:6:127:HIS:N     | 2.37                     | 0.48              |
| 11:D:68:ASP:OD2   | 11:D:97:ARG:NH2   | 2.45                     | 0.48              |
| 11:D:227:GLU:HA   | 11:D:230:ASN:HD21 | 1.77                     | 0.48              |
| 13:F:86:ASN:O     | 13:F:90:GLN:HG2   | 2.13                     | 0.48              |
| 15:I:256:TYR:HE1  | 16:K:281:ARG:NH2  | 2.11                     | 0.48              |
| 4:g:122:LEU:H     | 4:g:122:LEU:HD12  | 1.78                     | 0.48              |
| 3:h:28:ARG:NH2    | 3:h:205:ASP:OXT   | 2.46                     | 0.48              |
| 2:i:88:ILE:HD12   | 2:i:111:MET:SD    | 2.54                     | 0.48              |
| 2:i:140:PHE:HB3   | 2:i:150:VAL:HG22  | 1.95                     | 0.48              |
| 25:J:193:THR:N    | 36:J:502:ADP:O1A  | 2.45                     | 0.48              |
| 30:N:625:LEU:HD12 | 30:N:641:LEU:HG   | 1.95                     | 0.48              |
| 32:o:117:ASP:OD2  | 32:o:138:ARG:NH1  | 2.46                     | 0.48              |
| 1:1:137:SER:OG    | 1:1:139:HIS:NE2   | 2.44                     | 0.48              |
| 2:2:152:TYR:OH    | 7:a:257:ASP:HB2   | 2.14                     | 0.48              |
| 7:7:37:PRO:HD3    | 7:7:144:TRP:CD1   | 2.49                     | 0.48              |
| 11:D:97:ARG:HH12  | 11:D:103:PRO:HG3  | 1.78                     | 0.48              |
| 11:D:118:GLN:NE2  | 12:E:84:ASP:HA    | 2.28                     | 0.48              |
| 15:I:167:MET:HE3  | 25:J:228:ARG:HB2  | 1.96                     | 0.48              |
| 16:K:169:VAL:O    | 16:K:228:ASN:ND2  | 2.31                     | 0.48              |
| 16:K:399:ARG:HG2  | 19:P:128:ASN:O    | 2.13                     | 0.48              |
| 21:S:267:SER:OG   | 21:S:271:ARG:NH1  | 2.47                     | 0.48              |
| 23:W:127:ARG:O    | 23:W:131:THR:OG1  | 2.31                     | 0.48              |
| 7:a:49:TYR:CE1    | 7:a:54:ILE:HG13   | 2.49                     | 0.48              |
| 29:U:52:PHE:CD1   | 29:U:76:MET:HG3   | 2.49                     | 0.48              |
| 32:o:138:ARG:CZ   | 32:o:146:PHE:HB3  | 2.44                     | 0.48              |
| 32:o:453:LEU:HD11 | 32:o:491:LEU:HD23 | 1.96                     | 0.48              |
| 32:o:740:VAL:HA   | 32:o:743:ILE:HG22 | 1.94                     | 0.48              |
| 32:o:815:MET:HB3  | 32:o:827:LEU:HD21 | 1.95                     | 0.48              |
| 1:1:180:GLN:O     | 1:1:184:TRP:HB2   | 2.13                     | 0.48              |
| 13:F:46:LEU:HD13  | 13:F:73:SER:HB2   | 1.95                     | 0.48              |
| 14:G:194:LYS:HB3  | 14:G:242:PHE:CE2  | 2.48                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:O:44:SER:HA    | 18:O:47:LYS:HB2   | 1.95                     | 0.48              |
| 21:S:126:LYS:HD3  | 21:S:126:LYS:HA   | 1.70                     | 0.48              |
| 7:a:36:GLN:HE21   | 7:a:38:ILE:HD11   | 1.79                     | 0.48              |
| 1:b:18:LEU:O      | 1:b:20:THR:HG23   | 2.13                     | 0.48              |
| 3:h:31:SER:O      | 3:h:32:GLN:NE2    | 2.47                     | 0.48              |
| 2:i:186:ASP:HA    | 2:i:189:GLN:HE21  | 1.78                     | 0.48              |
| 26:H:155:PHE:CE1  | 27:M:78:LEU:HD13  | 2.48                     | 0.48              |
| 27:M:364:HIS:CD2  | 27:M:392:LYS:HB2  | 2.49                     | 0.48              |
| 29:U:126:LYS:HB2  | 29:U:128:GLN:NE2  | 2.18                     | 0.48              |
| 30:N:473:ASP:OD1  | 30:N:504:TYR:OH   | 2.26                     | 0.48              |
| 32:o:224:LEU:HA   | 32:o:227:ILE:HG22 | 1.96                     | 0.48              |
| 32:o:324:GLU:OE1  | 32:o:324:GLU:N    | 2.45                     | 0.48              |
| 1:l:65:SER:OG     | 1:l:115:GLY:O     | 2.22                     | 0.48              |
| 2:2:101:ARG:NH1   | 8:A:149:GLU:OE1   | 2.47                     | 0.48              |
| 3:3:30:GLY:HA2    | 3:3:35:GLY:HA2    | 1.96                     | 0.48              |
| 15:I:125:MET:SD   | 15:I:125:MET:N    | 2.86                     | 0.48              |
| 19:P:104:LEU:HD22 | 19:P:115:ARG:HH21 | 1.79                     | 0.48              |
| 19:P:123:ARG:NH1  | 19:P:140:THR:OG1  | 2.39                     | 0.48              |
| 21:S:480:ARG:NH2  | 25:J:44:LEU:HD23  | 2.29                     | 0.48              |
| 23:W:101:ARG:NH1  | 23:W:108:GLN:HE21 | 2.10                     | 0.48              |
| 5:f:119:THR:OG1   | 5:f:175:MET:N     | 2.46                     | 0.48              |
| 4:g:34:LYS:HZ1    | 4:g:47:ALA:HA     | 1.78                     | 0.48              |
| 30:N:90:ASP:OD1   | 30:N:93:GLU:N     | 2.36                     | 0.48              |
| 30:N:735:MET:HE2  | 30:N:735:MET:HA   | 1.96                     | 0.48              |
| 31:T:90:PHE:HB3   | 31:T:132:HIS:CD2  | 2.41                     | 0.48              |
| 32:o:400:ILE:HD12 | 32:o:406:TRP:HE1  | 1.79                     | 0.48              |
| 6:6:164:LEU:HD22  | 3:h:148:GLY:H     | 1.79                     | 0.48              |
| 11:D:79:ASN:ND2   | 15:I:437:LEU:O    | 2.47                     | 0.48              |
| 11:D:81:ASP:N     | 11:D:81:ASP:OD1   | 2.47                     | 0.48              |
| 5:f:93:SER:HB2    | 5:f:106:VAL:H     | 1.78                     | 0.48              |
| 27:M:118:VAL:HG22 | 27:M:128:PHE:HD1  | 1.78                     | 0.48              |
| 30:N:697:PHE:HE1  | 30:N:739:PHE:HE2  | 1.61                     | 0.48              |
| 1:l:153:ILE:HD11  | 1:l:181:ALA:HB2   | 1.95                     | 0.47              |
| 14:G:141:VAL:HG11 | 14:G:221:LEU:HG   | 1.95                     | 0.47              |
| 15:I:111:GLU:HG2  | 15:I:113:ILE:HG23 | 1.95                     | 0.47              |
| 16:K:223:VAL:HG13 | 16:K:234:PHE:HZ   | 1.79                     | 0.47              |
| 30:N:411:ILE:HG22 | 30:N:412:TYR:HD1  | 1.78                     | 0.47              |
| 32:o:139:LEU:O    | 32:o:141:SER:N    | 2.47                     | 0.47              |
| 32:o:597:SER:HB2  | 32:o:623:ARG:NH2  | 2.23                     | 0.47              |
| 2:2:59:ASN:N      | 2:2:59:ASN:OD1    | 2.47                     | 0.47              |
| 2:2:171:TRP:O     | 7:a:251:LYS:NZ    | 2.38                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:4:130:TYR:OH    | 4:4:145:ASP:OD1   | 2.32                     | 0.47              |
| 23:W:14:GLU:OE2   | 23:W:83:GLY:N     | 2.45                     | 0.47              |
| 23:W:16:SER:O     | 23:W:25:ARG:HB2   | 2.14                     | 0.47              |
| 4:g:41:HIS:HD2    | 4:g:109:LYS:HD3   | 1.79                     | 0.47              |
| 25:J:186:ILE:HD13 | 25:J:292:MET:HB3  | 1.96                     | 0.47              |
| 29:U:211:LEU:O    | 29:U:215:ILE:HG23 | 2.14                     | 0.47              |
| 30:N:760:GLY:H    | 30:N:870:ASN:HD21 | 1.61                     | 0.47              |
| 1:1:180:GLN:HA    | 1:1:183:LYS:HG2   | 1.95                     | 0.47              |
| 8:A:178:ILE:HD11  | 8:A:214:LEU:HD21  | 1.96                     | 0.47              |
| 12:E:114:GLN:O    | 12:E:114:GLN:NE2  | 2.39                     | 0.47              |
| 14:G:8:TYR:CD2    | 14:G:17:PRO:HD3   | 2.49                     | 0.47              |
| 15:I:246:ARG:HH22 | 25:J:278:GLN:HB2  | 1.78                     | 0.47              |
| 18:O:42:SER:O     | 18:O:81:TYR:OH    | 2.31                     | 0.47              |
| 19:P:379:TYR:O    | 19:P:383:LEU:HG   | 2.14                     | 0.47              |
| 19:P:395:ARG:HG3  | 28:Q:354:PHE:HE1  | 1.80                     | 0.47              |
| 21:S:82:TYR:OH    | 21:S:135:ASN:OD1  | 2.28                     | 0.47              |
| 22:V:170:PRO:C    | 22:V:171:ARG:HG2  | 2.38                     | 0.47              |
| 1:b:32:ILE:HG12   | 1:b:196:VAL:HA    | 1.96                     | 0.47              |
| 26:H:163:VAL:HG21 | 26:H:168:ILE:HD11 | 1.97                     | 0.47              |
| 30:N:450:ILE:HD11 | 30:N:462:VAL:HG22 | 1.97                     | 0.47              |
| 3:3:172:LEU:HD22  | 3:3:202:MET:SD    | 2.53                     | 0.47              |
| 4:4:36:ARG:HG3    | 4:4:57:ALA:HB1    | 1.95                     | 0.47              |
| 7:7:126:PHE:O     | 7:7:129:LEU:HD12  | 2.14                     | 0.47              |
| 12:E:69:GLU:N     | 12:E:69:GLU:OE2   | 2.48                     | 0.47              |
| 13:F:140:SER:OG   | 13:F:143:HIS:NE2  | 2.41                     | 0.47              |
| 18:O:358:ILE:HD12 | 29:U:226:LEU:HB3  | 1.96                     | 0.47              |
| 22:V:232:GLU:OE1  | 22:V:232:GLU:N    | 2.43                     | 0.47              |
| 6:e:76:PHE:HD2    | 6:e:79:ASP:H      | 1.63                     | 0.47              |
| 3:h:89:GLN:OE1    | 3:h:89:GLN:N      | 2.45                     | 0.47              |
| 2:i:192:ILE:HG12  | 2:i:199:GLY:HA2   | 1.96                     | 0.47              |
| 26:H:224:VAL:HG12 | 26:H:225:VAL:HG23 | 1.95                     | 0.47              |
| 26:H:428:MET:HE2  | 26:H:428:MET:HB2  | 1.74                     | 0.47              |
| 30:N:302:PHE:CE2  | 30:N:712:ASN:HB3  | 2.48                     | 0.47              |
| 32:o:752:ILE:O    | 32:o:756:MET:HG2  | 2.14                     | 0.47              |
| 4:4:60:ILE:HG12   | 4:4:84:VAL:HG12   | 1.97                     | 0.47              |
| 5:5:92:ASP:OD1    | 5:5:92:ASP:N      | 2.42                     | 0.47              |
| 6:6:55:ASN:HB3    | 7:7:170:TYR:CE2   | 2.50                     | 0.47              |
| 9:B:163:ALA:O     | 9:B:168:SER:OG    | 2.32                     | 0.47              |
| 14:G:78:TYR:H     | 14:G:78:TYR:HD1   | 1.63                     | 0.47              |
| 16:K:293:GLN:NE2  | 25:J:221:LYS:O    | 2.48                     | 0.47              |
| 17:L:325:MET:SD   | 17:L:343:LEU:HD21 | 2.54                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:R:212:THR:OG1  | 20:R:234:SER:OG   | 2.32                     | 0.47              |
| 22:V:225:LEU:HD12 | 29:U:196:SER:HB3  | 1.96                     | 0.47              |
| 30:N:20:VAL:HG23  | 31:T:35:ILE:HD11  | 1.95                     | 0.47              |
| 30:N:262:VAL:HG23 | 30:N:290:LEU:HD23 | 1.96                     | 0.47              |
| 30:N:593:PHE:CZ   | 30:N:734:VAL:HG23 | 2.49                     | 0.47              |
| 31:T:258:ASN:HB3  | 31:T:259:ILE:HD12 | 1.97                     | 0.47              |
| 3:3:105:VAL:HG23  | 3:3:107:PRO:HD3   | 1.96                     | 0.47              |
| 7:7:230:LEU:O     | 7:7:242:LYS:NZ    | 2.48                     | 0.47              |
| 8:A:52:VAL:HG21   | 8:A:203:VAL:HG22  | 1.95                     | 0.47              |
| 12:E:177:GLU:N    | 12:E:177:GLU:OE1  | 2.47                     | 0.47              |
| 15:I:193:GLU:HB3  | 15:I:346:ARG:HH12 | 1.79                     | 0.47              |
| 15:I:326:MET:HE3  | 15:I:344:ILE:HG21 | 1.96                     | 0.47              |
| 16:K:152:PRO:HG2  | 16:K:263:GLU:OE2  | 2.14                     | 0.47              |
| 21:S:408:CYS:HB2  | 21:S:419:VAL:HG21 | 1.96                     | 0.47              |
| 21:S:428:ARG:HD3  | 31:T:192:ASN:HA   | 1.97                     | 0.47              |
| 23:W:172:LEU:HD13 | 23:W:189:PRO:HG3  | 1.97                     | 0.47              |
| 1:b:51:ASP:O      | 1:b:64:ARG:NH2    | 2.48                     | 0.47              |
| 3:h:169:GLN:NE2   | 2:i:239:THR:OG1   | 2.45                     | 0.47              |
| 27:M:78:LEU:HB3   | 27:M:148:VAL:HG13 | 1.95                     | 0.47              |
| 30:N:102:VAL:O    | 30:N:106:ILE:HG13 | 2.14                     | 0.47              |
| 32:o:321:PHE:O    | 32:o:330:ILE:HD12 | 2.13                     | 0.47              |
| 1:1:23:MET:SD     | 1:1:24:ALA:N      | 2.87                     | 0.47              |
| 1:1:172:ASP:OD2   | 1:1:176:HIS:HD2   | 1.98                     | 0.47              |
| 2:2:154:LEU:HD12  | 2:2:154:LEU:HA    | 1.80                     | 0.47              |
| 2:2:163:ALA:HB1   | 2:2:187:ALA:HB1   | 1.95                     | 0.47              |
| 3:3:9:GLY:HA2     | 3:3:141:THR:HG21  | 1.95                     | 0.47              |
| 6:6:178:GLN:HE22  | 6:6:189:LYS:HD2   | 1.80                     | 0.47              |
| 6:6:213:ARG:HE    | 3:h:151:GLU:HG3   | 1.79                     | 0.47              |
| 7:7:252:TRP:HH2   | 1:b:48:ARG:HB2    | 1.79                     | 0.47              |
| 10:C:43:GLY:HA2   | 10:C:146:TYR:CZ   | 2.49                     | 0.47              |
| 15:I:211:MET:O    | 26:H:396:MET:HA   | 2.14                     | 0.47              |
| 17:L:316:ASP:OD1  | 17:L:316:ASP:N    | 2.47                     | 0.47              |
| 18:O:38:TRP:HA    | 18:O:41:LEU:HB3   | 1.96                     | 0.47              |
| 21:S:107:SER:HB3  | 21:S:110:LEU:HB2  | 1.97                     | 0.47              |
| 23:W:190:ILE:HG22 | 23:W:191:ILE:HG23 | 1.97                     | 0.47              |
| 5:f:105:THR:O     | 5:f:105:THR:OG1   | 2.29                     | 0.47              |
| 3:h:21:VAL:HG23   | 3:h:190:ILE:HB    | 1.95                     | 0.47              |
| 25:J:162:GLU:HA   | 25:J:166:LEU:HB2  | 1.97                     | 0.47              |
| 28:Q:173:SER:O    | 28:Q:177:VAL:HG12 | 2.15                     | 0.47              |
| 28:Q:311:LEU:HD13 | 28:Q:343:LEU:HD13 | 1.96                     | 0.47              |
| 29:U:94:HIS:NE2   | 29:U:122:ILE:HG22 | 2.30                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:4:103:LEU:HD13  | 4:4:133:HIS:CE1   | 2.41                     | 0.47              |
| 18:O:270:ILE:O    | 18:O:274:ILE:HB   | 2.14                     | 0.47              |
| 19:P:73:ASP:N     | 19:P:73:ASP:OD1   | 2.44                     | 0.47              |
| 20:R:227:ALA:O    | 20:R:231:LEU:HD23 | 2.15                     | 0.47              |
| 21:S:200:GLU:O    | 31:T:92:ASN:ND2   | 2.48                     | 0.47              |
| 22:V:23:THR:HA    | 22:V:171:ARG:CZ   | 2.45                     | 0.47              |
| 26:H:46:ALA:HA    | 26:H:49:LEU:HD13  | 1.97                     | 0.47              |
| 28:Q:322:GLU:O    | 28:Q:326:MET:HG3  | 2.15                     | 0.47              |
| 32:o:60:ASP:OD2   | 32:o:62:SER:OG    | 2.33                     | 0.47              |
| 1:1:16:VAL:HG13   | 1:1:41:THR:HG22   | 1.96                     | 0.47              |
| 6:6:114:HIS:NE2   | 12:E:102:TYR:HA   | 2.29                     | 0.47              |
| 8:A:22:GLU:HB2    | 8:A:24:ARG:HG3    | 1.96                     | 0.47              |
| 9:B:95:THR:HA     | 9:B:99:ARG:HG3    | 1.97                     | 0.47              |
| 10:C:156:ASN:ND2  | 15:I:434:GLY:O    | 2.47                     | 0.47              |
| 20:R:419:ALA:HA   | 20:R:422:ARG:HD3  | 1.96                     | 0.47              |
| 21:S:163:VAL:HG21 | 21:S:187:ILE:HD11 | 1.96                     | 0.47              |
| 24:Y:40:ILE:HD12  | 24:Y:41:ASP:H     | 1.80                     | 0.47              |
| 7:a:58:ASP:OD1    | 7:a:74:ARG:NH2    | 2.48                     | 0.47              |
| 7:a:140:MET:HE2   | 7:a:140:MET:N     | 2.28                     | 0.47              |
| 1:b:23:MET:HB3    | 1:b:145:ILE:HG22  | 1.96                     | 0.47              |
| 3:h:96:TYR:CZ     | 3:h:99:ARG:HD2    | 2.50                     | 0.47              |
| 3:h:184:GLY:N     | 3:h:202:MET:HE2   | 2.30                     | 0.47              |
| 26:H:281:GLN:HE21 | 26:H:290:MET:HE3  | 1.80                     | 0.47              |
| 28:Q:95:LYS:O     | 28:Q:99:THR:HG22  | 2.15                     | 0.47              |
| 6:6:176:LYS:HA    | 6:6:176:LYS:HD3   | 1.64                     | 0.47              |
| 13:F:117:GLN:HE22 | 14:G:83:PRO:HB2   | 1.80                     | 0.47              |
| 14:G:75:GLY:HA3   | 14:G:228:HIS:CE1  | 2.50                     | 0.47              |
| 15:I:284:ILE:HG22 | 15:I:328:THR:HB   | 1.96                     | 0.47              |
| 16:K:188:VAL:O    | 16:K:192:LEU:HG   | 2.15                     | 0.47              |
| 16:K:200:GLN:HE21 | 25:J:336:ASN:HD22 | 1.62                     | 0.47              |
| 18:O:204:SER:C    | 18:O:205:ILE:HG13 | 2.40                     | 0.47              |
| 20:R:222:ARG:HH12 | 20:R:324:ARG:HH12 | 1.63                     | 0.47              |
| 20:R:333:MET:HA   | 20:R:333:MET:HE2  | 1.96                     | 0.47              |
| 6:e:86:ARG:NH1    | 6:e:115:LEU:O     | 2.48                     | 0.47              |
| 26:H:100:ALA:HB2  | 26:H:149:LEU:HD23 | 1.97                     | 0.47              |
| 27:M:384:ASP:HB2  | 27:M:385:GLU:OE2  | 2.15                     | 0.47              |
| 1:1:26:THR:HG22   | 1:1:31:VAL:HB     | 1.96                     | 0.46              |
| 5:5:274:LYS:HG3   | 5:5:275:VAL:N     | 2.30                     | 0.46              |
| 14:G:102:LEU:HD23 | 14:G:103:TYR:HD2  | 1.80                     | 0.46              |
| 15:I:180:SER:OG   | 15:I:181:TYR:N    | 2.48                     | 0.46              |
| 16:K:276:SER:HB3  | 17:L:306:MET:HG3  | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:O:358:ILE:HG21 | 29:U:226:LEU:HD12 | 1.96                     | 0.46              |
| 22:V:27:VAL:HB    | 22:V:201:ILE:HD13 | 1.97                     | 0.46              |
| 22:V:206:THR:O    | 22:V:210:THR:HG22 | 2.15                     | 0.46              |
| 22:V:262:THR:OG1  | 22:V:265:GLU:OE1  | 2.33                     | 0.46              |
| 6:e:47:ARG:HH21   | 6:e:218:GLY:HA3   | 1.80                     | 0.46              |
| 25:J:227:SER:HB2  | 25:J:232:GLU:HG3  | 1.97                     | 0.46              |
| 27:M:329:ARG:NH2  | 27:M:331:ASP:OD2  | 2.48                     | 0.46              |
| 29:U:25:THR:OG1   | 29:U:27:THR:HG23  | 2.15                     | 0.46              |
| 29:U:90:ILE:HG13  | 29:U:90:ILE:O     | 2.15                     | 0.46              |
| 32:o:601:VAL:HG11 | 32:o:623:ARG:HD2  | 1.97                     | 0.46              |
| 5:5:283:ASN:HD21  | 4:g:149:ARG:HD3   | 1.80                     | 0.46              |
| 6:6:197:GLU:HA    | 6:6:200:ILE:HG12  | 1.96                     | 0.46              |
| 14:G:12:ASN:ND2   | 14:G:131:PRO:HD3  | 2.30                     | 0.46              |
| 15:I:199:GLU:O    | 15:I:203:THR:HG22 | 2.15                     | 0.46              |
| 18:O:345:ASN:OD1  | 18:O:345:ASN:N    | 2.49                     | 0.46              |
| 20:R:22:PRO:HD2   | 20:R:176:ARG:HD2  | 1.95                     | 0.46              |
| 20:R:385:ASN:N    | 20:R:385:ASN:OD1  | 2.49                     | 0.46              |
| 21:S:460:VAL:O    | 21:S:464:ARG:HG2  | 2.15                     | 0.46              |
| 1:b:35:ALA:O      | 1:b:193:ARG:N     | 2.41                     | 0.46              |
| 26:H:212:GLY:O    | 34:H:501:ATP:N6   | 2.47                     | 0.46              |
| 26:H:376:GLU:O    | 26:H:376:GLU:HG2  | 2.16                     | 0.46              |
| 32:o:826:ARG:HH12 | 32:o:830:LEU:HG   | 1.80                     | 0.46              |
| 32:o:877:THR:HA   | 32:o:907:GLY:HA3  | 1.96                     | 0.46              |
| 3:3:177:ARG:HA    | 3:3:177:ARG:HD3   | 1.69                     | 0.46              |
| 4:4:135:TYR:HA    | 4:4:138:PHE:HE1   | 1.80                     | 0.46              |
| 6:6:34:ILE:HG12   | 6:6:155:CYS:HB3   | 1.98                     | 0.46              |
| 16:K:378:LEU:HD11 | 16:K:411:TYR:HE1  | 1.80                     | 0.46              |
| 19:P:165:VAL:HA   | 19:P:168:TYR:CD2  | 2.44                     | 0.46              |
| 21:S:256:LYS:HD3  | 30:N:72:LEU:HD21  | 1.98                     | 0.46              |
| 23:W:73:LEU:HA    | 23:W:76:LEU:HD12  | 1.97                     | 0.46              |
| 1:b:145:ILE:HD12  | 1:b:150:SER:HB3   | 1.97                     | 0.46              |
| 2:i:84:VAL:O      | 2:i:88:ILE:HG12   | 2.15                     | 0.46              |
| 25:J:338:THR:O    | 25:J:341:ILE:HG12 | 2.14                     | 0.46              |
| 26:H:436:LYS:HZ3  | 32:o:952:SER:HB2  | 1.80                     | 0.46              |
| 32:o:528:LEU:HD21 | 32:o:565:PHE:HB3  | 1.98                     | 0.46              |
| 7:7:127:GLU:O     | 7:7:131:THR:OG1   | 2.25                     | 0.46              |
| 8:A:77:ARG:NH2    | 8:A:231:ASP:O     | 2.37                     | 0.46              |
| 13:F:98:VAL:HG12  | 13:F:99:PHE:CD2   | 2.51                     | 0.46              |
| 14:G:38:ILE:HD12  | 14:G:40:ILE:HD11  | 1.98                     | 0.46              |
| 17:L:352:PRO:HB2  | 17:L:357:ARG:HG2  | 1.97                     | 0.46              |
| 19:P:77:GLU:OE1   | 19:P:77:GLU:N     | 2.48                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:R:54:ILE:HD13  | 20:R:63:TYR:CD1   | 2.48                     | 0.46              |
| 20:R:138:GLY:HA3  | 20:R:154:LEU:CD2  | 2.43                     | 0.46              |
| 22:V:244:MET:HE1  | 22:V:287:THR:HG21 | 1.97                     | 0.46              |
| 7:a:160:LEU:HG    | 7:a:175:LEU:HD12  | 1.98                     | 0.46              |
| 6:e:119:LYS:HD2   | 6:e:124:TYR:CE2   | 2.50                     | 0.46              |
| 4:g:81:SER:HB3    | 4:g:104:ILE:HG21  | 1.97                     | 0.46              |
| 27:M:271:LYS:HG3  | 27:M:318:ASP:OD2  | 2.15                     | 0.46              |
| 32:o:138:ARG:HE   | 32:o:144:SER:HA   | 1.80                     | 0.46              |
| 32:o:378:GLN:HB3  | 32:o:842:GLN:NE2  | 2.31                     | 0.46              |
| 32:o:394:TYR:OH   | 32:o:858:GLY:O    | 2.27                     | 0.46              |
| 7:7:243:LYS:HB3   | 7:7:243:LYS:HE3   | 1.72                     | 0.46              |
| 17:L:242:ASN:HD22 | 17:L:273:HIS:HB3  | 1.80                     | 0.46              |
| 17:L:305:LEU:O    | 17:L:309:LEU:HB2  | 2.15                     | 0.46              |
| 21:S:37:VAL:HG21  | 21:S:63:LEU:HD11  | 1.98                     | 0.46              |
| 22:V:251:TYR:HD1  | 22:V:276:PRO:O    | 1.99                     | 0.46              |
| 7:a:124:TYR:O     | 7:a:127:GLU:HG2   | 2.16                     | 0.46              |
| 3:h:168:SER:HB2   | 2:i:239:THR:HG21  | 1.98                     | 0.46              |
| 27:M:57:VAL:HG12  | 27:M:61:LYS:HE3   | 1.97                     | 0.46              |
| 27:M:383:THR:HG23 | 27:M:419:ILE:HD12 | 1.97                     | 0.46              |
| 30:N:393:SER:OG   | 30:N:394:ARG:N    | 2.47                     | 0.46              |
| 32:o:811:SER:O    | 32:o:815:MET:HG2  | 2.16                     | 0.46              |
| 2:2:155:SER:HB3   | 2:2:164:MET:HB2   | 1.96                     | 0.46              |
| 11:D:158:SER:N    | 12:E:63:SER:OG    | 2.32                     | 0.46              |
| 16:K:188:VAL:HG21 | 16:K:315:ILE:HD11 | 1.97                     | 0.46              |
| 16:K:200:GLN:NE2  | 25:J:375:ILE:HG23 | 2.31                     | 0.46              |
| 18:O:120:LYS:C    | 18:O:122:HIS:H    | 2.24                     | 0.46              |
| 18:O:192:SER:HB2  | 18:O:217:LEU:HD13 | 1.97                     | 0.46              |
| 18:O:387:ARG:NE   | 31:T:261:GLU:OE2  | 2.32                     | 0.46              |
| 20:R:267:LYS:HA   | 20:R:267:LYS:HD2  | 1.76                     | 0.46              |
| 22:V:213:LEU:HD11 | 29:U:16:LEU:HD11  | 1.96                     | 0.46              |
| 7:a:172:SER:OG    | 7:a:174:THR:O     | 2.33                     | 0.46              |
| 4:g:43:LEU:HB2    | 4:g:189:ILE:HD13  | 1.98                     | 0.46              |
| 26:H:249:TYR:HB2  | 26:H:358:PRO:HG3  | 1.97                     | 0.46              |
| 30:N:713:VAL:HG21 | 30:N:753:PHE:HB3  | 1.97                     | 0.46              |
| 1:i:159:LYS:CG    | 1:b:180:GLN:HE21  | 2.29                     | 0.46              |
| 7:7:220:ARG:NE    | 2:i:168:GLU:OE2   | 2.49                     | 0.46              |
| 8:A:134:MET:HA    | 8:A:134:MET:HE3   | 1.96                     | 0.46              |
| 10:C:198:SER:HB3  | 10:C:206:LEU:HD22 | 1.98                     | 0.46              |
| 13:F:52:ASN:HB2   | 13:F:57:SER:OG    | 2.16                     | 0.46              |
| 14:G:86:ARG:HG2   | 14:G:86:ARG:HH11  | 1.81                     | 0.46              |
| 20:R:158:LEU:O    | 20:R:158:LEU:HD12 | 2.16                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:R:171:MET:HA   | 20:R:174:ILE:HD12 | 1.97                     | 0.46              |
| 1:b:78:VAL:HG13   | 1:b:100:VAL:HB    | 1.98                     | 0.46              |
| 1:b:82:LEU:HD21   | 1:b:97:ALA:HA     | 1.97                     | 0.46              |
| 4:g:101:ASN:HD22  | 4:g:133:HIS:HB3   | 1.80                     | 0.46              |
| 25:J:105:LYS:H    | 25:J:105:LYS:HD3  | 1.81                     | 0.46              |
| 25:J:379:GLN:O    | 25:J:383:GLU:HG2  | 2.16                     | 0.46              |
| 32:o:888:LEU:N    | 32:o:894:MET:HE3  | 2.31                     | 0.46              |
| 4:4:158:LEU:O     | 4:4:162:LYS:HG2   | 2.16                     | 0.46              |
| 6:6:50:THR:OG1    | 6:6:55:ASN:ND2    | 2.28                     | 0.46              |
| 9:B:66:LEU:HD12   | 9:B:235:PHE:CD2   | 2.51                     | 0.46              |
| 9:B:108:LYS:HA    | 9:B:148:TYR:HE2   | 1.80                     | 0.46              |
| 15:I:100:ARG:O    | 15:I:150:HIS:HD2  | 1.99                     | 0.46              |
| 15:I:340:ARG:HH12 | 15:I:343:ARG:CZ   | 2.29                     | 0.46              |
| 18:O:123:GLY:O    | 18:O:127:LEU:HG   | 2.16                     | 0.46              |
| 19:P:107:SER:O    | 19:P:109:SER:N    | 2.48                     | 0.46              |
| 19:P:310:ARG:HH22 | 19:P:368:LEU:HA   | 1.80                     | 0.46              |
| 22:V:99:GLY:HA3   | 29:U:24:ARG:HD3   | 1.97                     | 0.46              |
| 1:b:27:PHE:HB2    | 1:b:165:MET:O     | 2.15                     | 0.46              |
| 6:e:194:LEU:HB3   | 6:e:198:GLU:HB2   | 1.97                     | 0.46              |
| 6:e:226:VAL:HG22  | 6:e:231:VAL:HG22  | 1.97                     | 0.46              |
| 4:g:158:LEU:O     | 4:g:161:LEU:HG    | 2.15                     | 0.46              |
| 2:i:43:ILE:HG12   | 2:i:207:MET:HE1   | 1.96                     | 0.46              |
| 2:i:74:GLY:HA2    | 2:i:127:LEU:HD23  | 1.97                     | 0.46              |
| 25:J:196:THR:HG22 | 36:J:502:ADP:O2A  | 2.16                     | 0.46              |
| 26:H:83:ASP:OD1   | 26:H:83:ASP:N     | 2.47                     | 0.46              |
| 27:M:299:ARG:HG3  | 27:M:303:ARG:NH2  | 2.30                     | 0.46              |
| 29:U:185:GLY:O    | 29:U:188:ILE:HG22 | 2.16                     | 0.46              |
| 32:o:970:TYR:HD2  | 32:o:983:LEU:HD13 | 1.80                     | 0.46              |
| 10:C:22:VAL:HG21  | 15:I:435:LEU:HD11 | 1.97                     | 0.46              |
| 10:C:197:LEU:HA   | 10:C:200:THR:HG22 | 1.98                     | 0.46              |
| 16:K:87:LYS:O     | 22:V:147:VAL:HG21 | 2.15                     | 0.46              |
| 18:O:222:LEU:HD23 | 18:O:222:LEU:HA   | 1.77                     | 0.46              |
| 20:R:120:LEU:HD13 | 20:R:129:GLU:HG3  | 1.97                     | 0.46              |
| 21:S:138:MET:HA   | 21:S:138:MET:HE3  | 1.98                     | 0.46              |
| 7:a:135:GLN:O     | 7:a:139:LYS:HG2   | 2.14                     | 0.46              |
| 5:f:152:ALA:HA    | 5:f:188:TYR:HE2   | 1.81                     | 0.46              |
| 3:h:50:PHE:HE2    | 3:h:195:VAL:HG21  | 1.81                     | 0.46              |
| 3:h:109:VAL:N     | 3:h:122:ALA:O     | 2.43                     | 0.46              |
| 28:Q:178:HIS:HB3  | 28:Q:201:ALA:HB2  | 1.97                     | 0.46              |
| 29:U:10:ILE:HD13  | 29:U:121:LEU:HD21 | 1.97                     | 0.46              |
| 30:N:285:ALA:HA   | 30:N:288:ASN:HD21 | 1.81                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:T:255:GLN:OE1  | 31:T:256:LYS:N    | 2.48                     | 0.46              |
| 2:2:109:LEU:HD22  | 2:2:140:PHE:CD2   | 2.51                     | 0.46              |
| 3:3:80:ARG:NH2    | 3:3:81:ALA:O      | 2.40                     | 0.46              |
| 5:5:241:HIS:HE1   | 3:h:204:GLN:HB3   | 1.77                     | 0.46              |
| 7:7:226:ARG:HD3   | 7:7:247:VAL:HB    | 1.97                     | 0.46              |
| 15:I:400:GLY:HA3  | 25:J:179:ILE:HG21 | 1.97                     | 0.46              |
| 16:K:52:LYS:HD3   | 16:K:52:LYS:HA    | 1.66                     | 0.46              |
| 18:O:324:VAL:O    | 18:O:328:VAL:HG23 | 2.16                     | 0.46              |
| 19:P:412:LEU:HD12 | 29:U:268:LYS:HG3  | 1.97                     | 0.46              |
| 19:P:440:HIS:ND1  | 29:U:220:PRO:HG3  | 2.30                     | 0.46              |
| 21:S:336:SER:O    | 21:S:338:MET:N    | 2.49                     | 0.46              |
| 22:V:250:GLN:HA   | 22:V:253:LYS:NZ   | 2.30                     | 0.46              |
| 1:b:94:THR:HG21   | 1:b:128:GLU:HG2   | 1.98                     | 0.46              |
| 6:e:128:THR:HB    | 6:e:144:PHE:HB2   | 1.98                     | 0.46              |
| 25:J:241:ALA:HB1  | 25:J:287:ASN:HD21 | 1.81                     | 0.46              |
| 25:J:298:ASP:OD1  | 25:J:298:ASP:N    | 2.49                     | 0.46              |
| 26:H:181:TYR:H    | 26:H:181:TYR:HD2  | 1.64                     | 0.46              |
| 32:o:278:LEU:H    | 32:o:278:LEU:HD12 | 1.80                     | 0.46              |
| 3:3:28:ARG:HH21   | 3:3:183:TRP:CD1   | 2.34                     | 0.45              |
| 4:4:183:ILE:HG12  | 4:4:190:ARG:HE    | 1.82                     | 0.45              |
| 8:A:135:ARG:HH12  | 14:G:125:LEU:HD12 | 1.80                     | 0.45              |
| 15:I:133:LEU:HD12 | 15:I:157:VAL:HG12 | 1.98                     | 0.45              |
| 16:K:245:LYS:HG3  | 16:K:246:TYR:N    | 2.30                     | 0.45              |
| 16:K:325:ASP:OD1  | 25:J:222:TYR:OH   | 2.32                     | 0.45              |
| 19:P:166:GLU:OE1  | 19:P:166:GLU:N    | 2.26                     | 0.45              |
| 20:R:189:GLU:O    | 20:R:192:GLU:HG3  | 2.16                     | 0.45              |
| 20:R:279:LEU:O    | 20:R:282:THR:OG1  | 2.28                     | 0.45              |
| 25:J:341:ILE:HD12 | 25:J:379:GLN:HB2  | 1.97                     | 0.45              |
| 28:Q:158:ILE:HD11 | 28:Q:180:LEU:HB3  | 1.97                     | 0.45              |
| 30:N:173:LYS:HA   | 30:N:176:GLN:HE21 | 1.80                     | 0.45              |
| 30:N:493:GLY:HA2  | 30:N:524:ILE:HG23 | 1.98                     | 0.45              |
| 30:N:765:ASP:OD1  | 30:N:765:ASP:N    | 2.48                     | 0.45              |
| 3:3:172:LEU:HD11  | 3:3:200:LEU:HD13  | 1.98                     | 0.45              |
| 15:I:72:GLU:OE1   | 32:o:763:HIS:ND1  | 2.48                     | 0.45              |
| 15:I:234:LYS:NZ   | 25:J:277:ASN:O    | 2.37                     | 0.45              |
| 16:K:288:SER:HA   | 17:L:256:ILE:HD13 | 1.96                     | 0.45              |
| 18:O:71:ASP:OD1   | 18:O:109:LEU:HD22 | 2.17                     | 0.45              |
| 18:O:336:LEU:HB2  | 18:O:337:LEU:HD12 | 1.98                     | 0.45              |
| 21:S:100:HIS:CE1  | 21:S:102:SER:HB2  | 2.51                     | 0.45              |
| 21:S:188:TYR:HE2  | 21:S:239:ARG:HD3  | 1.81                     | 0.45              |
| 21:S:323:LEU:HD23 | 21:S:323:LEU:HA   | 1.79                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:W:7:VAL:HG11   | 23:W:94:ALA:HB1   | 1.98                     | 0.45              |
| 7:a:39:VAL:HG12   | 7:a:90:ILE:HD12   | 1.97                     | 0.45              |
| 7:a:78:VAL:HG11   | 7:a:100:LEU:HD12  | 1.99                     | 0.45              |
| 5:f:188:TYR:HE1   | 5:f:198:LYS:HD3   | 1.80                     | 0.45              |
| 25:J:333:ARG:HE   | 25:J:333:ARG:HB2  | 1.57                     | 0.45              |
| 29:U:33:CYS:O     | 29:U:95:SER:N     | 2.50                     | 0.45              |
| 31:T:63:GLU:OE2   | 31:T:89:TYR:OH    | 2.33                     | 0.45              |
| 32:o:358:TYR:CE1  | 32:o:849:ARG:HG2  | 2.50                     | 0.45              |
| 4:4:10:GLN:NE2    | 4:4:152:MET:O     | 2.50                     | 0.45              |
| 8:A:115:ASP:HB3   | 8:A:155:TYR:CZ    | 2.51                     | 0.45              |
| 8:A:237:SER:OG    | 8:A:239:GLU:OE2   | 2.34                     | 0.45              |
| 9:B:69:PRO:HD2    | 9:B:104:TYR:CE2   | 2.51                     | 0.45              |
| 9:B:172:LYS:HE2   | 9:B:172:LYS:HB2   | 1.82                     | 0.45              |
| 12:E:235:LYS:HA   | 12:E:238:GLU:HG3  | 1.98                     | 0.45              |
| 14:G:52:LYS:HZ2   | 14:G:215:GLU:HB2  | 1.80                     | 0.45              |
| 16:K:199:GLU:OE2  | 16:K:308:GLN:NE2  | 2.47                     | 0.45              |
| 19:P:93:ILE:HD13  | 19:P:93:ILE:HA    | 1.87                     | 0.45              |
| 6:e:225:ILE:O     | 6:e:232:ARG:NH1   | 2.49                     | 0.45              |
| 5:f:83:PHE:CE1    | 5:f:88:ILE:HG12   | 2.51                     | 0.45              |
| 5:f:166:LYS:HE3   | 4:g:96:ARG:NH1    | 2.32                     | 0.45              |
| 5:f:240:ALA:HB1   | 5:f:247:GLY:HA2   | 1.97                     | 0.45              |
| 3:h:144:ASP:N     | 3:h:144:ASP:OD1   | 2.49                     | 0.45              |
| 26:H:147:ILE:HG21 | 26:H:176:VAL:HG21 | 1.98                     | 0.45              |
| 30:N:331:ALA:HB2  | 30:N:697:PHE:HD2  | 1.81                     | 0.45              |
| 31:T:28:PRO:HA    | 31:T:31:LYS:HD3   | 1.99                     | 0.45              |
| 32:o:287:ARG:NH2  | 32:o:870:ALA:O    | 2.34                     | 0.45              |
| 32:o:964:GLU:HA   | 32:o:977:ILE:HD12 | 1.97                     | 0.45              |
| 3:3:29:LEU:HD13   | 3:3:40:PHE:HD1    | 1.82                     | 0.45              |
| 5:5:96:THR:HA     | 5:5:102:ALA:H     | 1.81                     | 0.45              |
| 13:F:217:GLY:N    | 13:F:220:THR:O    | 2.50                     | 0.45              |
| 14:G:8:TYR:HD2    | 14:G:17:PRO:HD3   | 1.80                     | 0.45              |
| 15:I:256:TYR:HB3  | 26:H:282:LYS:HD3  | 1.98                     | 0.45              |
| 15:I:295:ASN:ND2  | 15:I:298:GLY:O    | 2.49                     | 0.45              |
| 16:K:353:PHE:HD1  | 16:K:387:MET:HE3  | 1.81                     | 0.45              |
| 19:P:107:SER:HB3  | 19:P:110:LEU:HD13 | 1.98                     | 0.45              |
| 20:R:59:MET:O     | 20:R:63:TYR:N     | 2.44                     | 0.45              |
| 22:V:306:LYS:HA   | 29:U:236:LEU:HD11 | 1.98                     | 0.45              |
| 23:W:181:LEU:O    | 23:W:185:ILE:HG13 | 2.16                     | 0.45              |
| 23:W:185:ILE:HG23 | 23:W:189:PRO:HG2  | 1.97                     | 0.45              |
| 26:H:248:LEU:HD22 | 26:H:377:PHE:CE2  | 2.48                     | 0.45              |
| 27:M:83:VAL:HG23  | 27:M:120:LYS:HB2  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:N:53:ASP:OD2   | 30:N:53:ASP:N     | 2.35                     | 0.45              |
| 30:N:397:SER:O    | 30:N:400:ILE:HG22 | 2.17                     | 0.45              |
| 30:N:526:TYR:HE1  | 30:N:730:VAL:HG11 | 1.80                     | 0.45              |
| 30:N:578:ASP:OD1  | 30:N:580:ASN:N    | 2.48                     | 0.45              |
| 32:o:292:ASP:OD1  | 32:o:292:ASP:N    | 2.47                     | 0.45              |
| 1:1:82:LEU:O      | 1:1:86:THR:HG22   | 2.16                     | 0.45              |
| 1:1:153:ILE:H     | 1:1:153:ILE:HD12  | 1.81                     | 0.45              |
| 2:2:211:LYS:HE2   | 2:2:211:LYS:HB2   | 1.82                     | 0.45              |
| 7:7:44:VAL:H      | 7:7:177:THR:HB    | 1.81                     | 0.45              |
| 9:B:135:LEU:HG    | 9:B:164:ILE:HD11  | 1.99                     | 0.45              |
| 13:F:87:TYR:HE2   | 13:F:115:LYS:HD3  | 1.82                     | 0.45              |
| 15:I:71:LEU:HG    | 32:o:621:LEU:HD12 | 1.99                     | 0.45              |
| 15:I:153:THR:O    | 26:H:96:PRO:HG3   | 2.17                     | 0.45              |
| 16:K:240:SER:OG   | 17:L:307:GLU:OE1  | 2.34                     | 0.45              |
| 16:K:283:ASP:OD2  | 17:L:296:SER:OG   | 2.34                     | 0.45              |
| 19:P:276:LEU:HD23 | 19:P:276:LEU:HA   | 1.82                     | 0.45              |
| 21:S:41:ILE:O     | 21:S:44:THR:HG22  | 2.16                     | 0.45              |
| 21:S:154:GLN:HA   | 21:S:157:GLU:HB2  | 1.97                     | 0.45              |
| 7:a:128:TYR:CD2   | 7:a:129:LEU:HD23  | 2.51                     | 0.45              |
| 7:a:265:LYS:C     | 7:a:265:LYS:HD3   | 2.41                     | 0.45              |
| 4:g:172:MET:SD    | 4:g:174:MET:HE1   | 2.57                     | 0.45              |
| 26:H:167:ASP:C    | 26:H:168:ILE:HD13 | 2.42                     | 0.45              |
| 28:Q:263:LYS:NZ   | 28:Q:324:GLU:HB3  | 2.31                     | 0.45              |
| 30:N:285:ALA:HA   | 30:N:288:ASN:ND2  | 2.31                     | 0.45              |
| 6:6:110:ARG:NH1   | 12:E:101:LEU:O    | 2.48                     | 0.45              |
| 8:A:14:ARG:O      | 8:A:27:GLN:NE2    | 2.40                     | 0.45              |
| 15:I:214:LYS:HE3  | 26:H:420:ARG:HD3  | 1.99                     | 0.45              |
| 16:K:96:ILE:HD11  | 17:L:118:ILE:HD13 | 1.99                     | 0.45              |
| 16:K:420:THR:O    | 16:K:423:LYS:NZ   | 2.49                     | 0.45              |
| 18:O:75:GLN:NE2   | 18:O:124:ASP:OD1  | 2.50                     | 0.45              |
| 18:O:82:LEU:HD13  | 18:O:102:LEU:HD11 | 1.99                     | 0.45              |
| 18:O:258:LEU:HD22 | 18:O:291:ILE:HD11 | 1.98                     | 0.45              |
| 23:W:35:PHE:CD2   | 23:W:182:TYR:HB2  | 2.52                     | 0.45              |
| 5:f:181:ARG:NH1   | 5:f:257:GLU:HG3   | 2.32                     | 0.45              |
| 3:h:99:ARG:NH2    | 3:h:127:ILE:HG13  | 2.31                     | 0.45              |
| 2:i:69:LYS:NZ     | 2:i:103:PRO:O     | 2.43                     | 0.45              |
| 25:J:100:LYS:HB2  | 25:J:100:LYS:HE3  | 1.75                     | 0.45              |
| 28:Q:78:ILE:HD12  | 28:Q:117:VAL:HG11 | 1.97                     | 0.45              |
| 29:U:271:ASP:O    | 29:U:274:MET:HE3  | 2.16                     | 0.45              |
| 30:N:114:SER:O    | 30:N:118:THR:OG1  | 2.26                     | 0.45              |
| 32:o:509:LEU:O    | 32:o:513:ALA:N    | 2.28                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:o:740:VAL:HB   | 32:o:775:MET:SD   | 2.57                     | 0.45              |
| 5:5:279:GLU:OE1   | 5:5:281:SER:OG    | 2.25                     | 0.45              |
| 7:7:127:GLU:CD    | 13:F:100:ASN:HB2  | 2.42                     | 0.45              |
| 10:C:14:SER:OG    | 10:C:18:ARG:O     | 2.34                     | 0.45              |
| 15:I:106:ILE:HB   | 25:J:93:LYS:HG3   | 1.97                     | 0.45              |
| 16:K:376:ASP:OD1  | 16:K:376:ASP:N    | 2.49                     | 0.45              |
| 17:L:390:ASP:OD2  | 17:L:426:LYS:NZ   | 2.47                     | 0.45              |
| 18:O:358:ILE:HD11 | 29:U:230:GLN:HB2  | 1.99                     | 0.45              |
| 2:i:37:PHE:HE1    | 2:i:42:VAL:HG23   | 1.82                     | 0.45              |
| 29:U:56:PHE:CD1   | 29:U:56:PHE:C     | 2.95                     | 0.45              |
| 30:N:381:GLU:HB3  | 30:N:384:LYS:HE3  | 1.98                     | 0.45              |
| 31:T:68:ALA:O     | 31:T:72:THR:OG1   | 2.30                     | 0.45              |
| 32:o:269:TYR:OH   | 32:o:296:SER:OG   | 2.34                     | 0.45              |
| 5:5:107:LYS:HE2   | 5:5:107:LYS:HB2   | 1.86                     | 0.45              |
| 6:6:161:ALA:HB2   | 6:6:214:HIS:CD2   | 2.51                     | 0.45              |
| 9:B:97:TYR:CD1    | 9:B:105:PRO:HB3   | 2.52                     | 0.45              |
| 9:B:193:LEU:HD21  | 9:B:243:ILE:HD11  | 1.98                     | 0.45              |
| 15:I:355:LEU:HD12 | 15:I:355:LEU:HA   | 1.81                     | 0.45              |
| 18:O:24:PRO:HA    | 18:O:27:GLU:HG2   | 1.98                     | 0.45              |
| 18:O:51:ASP:O     | 18:O:58:ARG:NH2   | 2.49                     | 0.45              |
| 18:O:136:THR:O    | 18:O:140:LYS:N    | 2.49                     | 0.45              |
| 21:S:37:VAL:O     | 21:S:41:ILE:HG23  | 2.17                     | 0.45              |
| 21:S:278:LYS:O    | 21:S:282:ILE:HG13 | 2.17                     | 0.45              |
| 24:Y:37:ASP:N     | 24:Y:37:ASP:OD1   | 2.48                     | 0.45              |
| 1:b:56:VAL:HB     | 1:b:82:LEU:HD12   | 1.99                     | 0.45              |
| 6:e:227:THR:HG22  | 6:e:228:LYS:N     | 2.32                     | 0.45              |
| 5:f:108:LYS:H     | 5:f:108:LYS:HG2   | 1.62                     | 0.45              |
| 27:M:81:ASN:OD1   | 27:M:81:ASN:N     | 2.48                     | 0.45              |
| 27:M:121:THR:HG21 | 27:M:153:TYR:HE1  | 1.81                     | 0.45              |
| 27:M:377:GLN:O    | 27:M:381:ARG:HG3  | 2.16                     | 0.45              |
| 27:M:411:LYS:N    | 27:M:414:ASP:OD2  | 2.42                     | 0.45              |
| 30:N:132:LYS:O    | 30:N:136:ILE:HG12 | 2.17                     | 0.45              |
| 30:N:782:PHE:HB3  | 30:N:875:LEU:HD13 | 1.98                     | 0.45              |
| 32:o:337:GLU:HA   | 32:o:340:LEU:HG   | 1.99                     | 0.45              |
| 32:o:558:LEU:HD22 | 32:o:595:MET:HE1  | 1.99                     | 0.45              |
| 32:o:977:ILE:HG23 | 32:o:981:VAL:HG21 | 1.98                     | 0.45              |
| 6:6:50:THR:HG1    | 6:6:55:ASN:HD21   | 1.55                     | 0.45              |
| 6:6:221:LEU:N     | 6:6:236:TYR:O     | 2.48                     | 0.45              |
| 10:C:120:GLN:HG2  | 11:D:84:ILE:HD11  | 1.97                     | 0.45              |
| 12:E:68:VAL:HB    | 12:E:93:ARG:HH21  | 1.82                     | 0.45              |
| 18:O:9:THR:O      | 18:O:13:THR:HG23  | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:P:24:ILE:HG12  | 19:P:39:LEU:HG    | 1.98                     | 0.45              |
| 23:W:120:ASP:HB2  | 23:W:125:LEU:HD11 | 1.98                     | 0.45              |
| 28:Q:262:LEU:HD23 | 28:Q:296:ILE:HG13 | 1.99                     | 0.45              |
| 30:N:194:ILE:HA   | 30:N:203:ARG:NH1  | 2.29                     | 0.45              |
| 30:N:418:ASP:OD1  | 30:N:419:THR:N    | 2.50                     | 0.45              |
| 32:o:119:LEU:HB3  | 32:o:137:TYR:CE2  | 2.52                     | 0.45              |
| 2:2:116:LEU:HD23  | 2:2:116:LEU:HA    | 1.82                     | 0.45              |
| 4:4:106:GLY:HA2   | 4:4:184:VAL:HG11  | 1.99                     | 0.45              |
| 7:7:127:GLU:OE1   | 13:F:100:ASN:HB2  | 2.16                     | 0.45              |
| 11:D:177:LYS:HB3  | 11:D:177:LYS:HE2  | 1.80                     | 0.45              |
| 17:L:161:ARG:NE   | 17:L:272:GLU:OE2  | 2.50                     | 0.45              |
| 17:L:382:MET:HE2  | 17:L:382:MET:HB2  | 1.83                     | 0.45              |
| 20:R:232:VAL:HG11 | 20:R:269:LYS:HD2  | 1.97                     | 0.45              |
| 5:f:82:ARG:HH21   | 5:f:221:TRP:HH2   | 1.65                     | 0.45              |
| 5:f:89:VAL:HB     | 5:f:253:TYR:HB2   | 1.99                     | 0.45              |
| 4:g:166:GLN:O     | 4:g:170:LYS:HG2   | 2.17                     | 0.45              |
| 3:h:51:LEU:HD21   | 3:h:107:PRO:HB3   | 1.99                     | 0.45              |
| 28:Q:150:GLN:HB3  | 28:Q:153:ASP:OD1  | 2.16                     | 0.45              |
| 30:N:581:ASP:OD2  | 30:N:614:ASN:ND2  | 2.34                     | 0.45              |
| 1:1:142:PRO:HB2   | 1:1:161:PHE:CZ    | 2.51                     | 0.44              |
| 2:2:178:GLU:HA    | 2:2:181:ILE:HG22  | 1.99                     | 0.44              |
| 6:6:229:ASP:OD1   | 6:6:230:GLY:N     | 2.50                     | 0.44              |
| 8:A:22:GLU:OE1    | 8:A:22:GLU:N      | 2.49                     | 0.44              |
| 9:B:49:LYS:HE3    | 9:B:49:LYS:HB2    | 1.83                     | 0.44              |
| 13:F:206:LEU:HD13 | 13:F:211:LEU:HD22 | 1.98                     | 0.44              |
| 15:I:54:ARG:HH12  | 32:o:155:ARG:HH21 | 1.64                     | 0.44              |
| 17:L:98:LEU:HD21  | 27:M:72:ASN:HD22  | 1.82                     | 0.44              |
| 18:O:40:GLN:HA    | 18:O:43:GLU:CD    | 2.42                     | 0.44              |
| 18:O:156:THR:HA   | 18:O:159:LYS:HG2  | 1.98                     | 0.44              |
| 18:O:211:GLN:NE2  | 18:O:241:THR:O    | 2.51                     | 0.44              |
| 22:V:59:ASP:OD1   | 22:V:59:ASP:C     | 2.60                     | 0.44              |
| 5:f:153:ALA:O     | 5:f:157:ILE:HG12  | 2.16                     | 0.44              |
| 27:M:54:GLU:O     | 27:M:58:MET:HG3   | 2.17                     | 0.44              |
| 31:T:256:LYS:HD3  | 31:T:262:LYS:HE2  | 2.00                     | 0.44              |
| 32:o:528:LEU:HD11 | 32:o:565:PHE:HB3  | 1.99                     | 0.44              |
| 32:o:913:ILE:HD11 | 32:o:957:LEU:HD21 | 2.00                     | 0.44              |
| 2:2:32:ILE:HG22   | 2:2:45:ALA:HB2    | 1.98                     | 0.44              |
| 4:4:146:HIS:O     | 4:4:149:ARG:NH2   | 2.50                     | 0.44              |
| 5:5:216:ASP:N     | 5:5:216:ASP:OD1   | 2.49                     | 0.44              |
| 6:6:198:GLU:O     | 6:6:202:LEU:HG    | 2.18                     | 0.44              |
| 7:7:48:LYS:HA     | 7:7:53:VAL:HA     | 1.98                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:A:24:ARG:NH2    | 8:A:29:GLU:OE1    | 2.50                     | 0.44              |
| 9:B:141:GLU:H     | 9:B:141:GLU:CD    | 2.26                     | 0.44              |
| 13:F:52:ASN:ND2   | 13:F:59:TYR:OH    | 2.50                     | 0.44              |
| 15:I:161:GLN:HG2  | 15:I:163:ASP:HB2  | 1.99                     | 0.44              |
| 15:I:281:ILE:O    | 15:I:326:MET:HA   | 2.17                     | 0.44              |
| 18:O:292:CYS:HB3  | 18:O:327:LEU:HD11 | 1.99                     | 0.44              |
| 21:S:371:LEU:HD23 | 21:S:371:LEU:HA   | 1.86                     | 0.44              |
| 23:W:29:GLN:HG3   | 23:W:144:PHE:HZ   | 1.81                     | 0.44              |
| 7:a:226:ARG:NH1   | 7:a:246:GLN:HE21  | 2.15                     | 0.44              |
| 7:a:234:ASP:OD2   | 7:a:237:THR:N     | 2.37                     | 0.44              |
| 27:M:415:PHE:O    | 27:M:419:ILE:HG12 | 2.17                     | 0.44              |
| 28:Q:63:GLN:HB2   | 28:Q:103:LYS:HZ3  | 1.81                     | 0.44              |
| 30:N:394:ARG:HG3  | 30:N:394:ARG:O    | 2.18                     | 0.44              |
| 32:o:787:ASP:OD1  | 32:o:787:ASP:N    | 2.49                     | 0.44              |
| 6:6:30:THR:HA     | 6:6:74:ASN:HD21   | 1.81                     | 0.44              |
| 6:6:39:PHE:HE2    | 6:6:199:VAL:HG21  | 1.82                     | 0.44              |
| 7:7:164:ASN:HD21  | 7:7:166:LEU:HB2   | 1.82                     | 0.44              |
| 12:E:86:ARG:HG2   | 12:E:86:ARG:NH1   | 2.32                     | 0.44              |
| 14:G:90:ASN:O     | 14:G:94:GLU:HG2   | 2.17                     | 0.44              |
| 14:G:95:GLU:HB3   | 14:G:115:ARG:HH11 | 1.82                     | 0.44              |
| 15:I:93:LYS:O     | 15:I:97:GLU:HG2   | 2.18                     | 0.44              |
| 16:K:132:LYS:O    | 16:K:135:MET:HB2  | 2.17                     | 0.44              |
| 19:P:113:ASN:O    | 19:P:116:ILE:HG22 | 2.17                     | 0.44              |
| 21:S:159:ASN:N    | 21:S:159:ASN:HD22 | 2.15                     | 0.44              |
| 21:S:278:LYS:HG2  | 21:S:316:LEU:HD11 | 1.99                     | 0.44              |
| 6:e:134:ASP:OD1   | 6:e:138:LYS:N     | 2.49                     | 0.44              |
| 27:M:139:LYS:HD3  | 27:M:139:LYS:HA   | 1.74                     | 0.44              |
| 30:N:10:LEU:HD12  | 30:N:10:LEU:HA    | 1.69                     | 0.44              |
| 30:N:528:ARG:HB3  | 30:N:531:LEU:HB2  | 1.99                     | 0.44              |
| 1:1:102:LYS:HD3   | 14:G:104:LYS:NZ   | 2.33                     | 0.44              |
| 1:1:151:THR:HA    | 1:1:154:TYR:CE1   | 2.52                     | 0.44              |
| 1:1:159:LYS:HZ1   | 1:b:176:HIS:HB3   | 1.82                     | 0.44              |
| 13:F:191:LYS:HE2  | 13:F:191:LYS:HB2  | 1.86                     | 0.44              |
| 14:G:95:GLU:HB3   | 14:G:115:ARG:NH1  | 2.33                     | 0.44              |
| 15:I:255:LYS:HZ3  | 25:J:217:GLU:HB3  | 1.83                     | 0.44              |
| 16:K:129:GLU:H    | 16:K:129:GLU:HG2  | 1.57                     | 0.44              |
| 16:K:160:VAL:HG22 | 16:K:235:ILE:HG12 | 1.99                     | 0.44              |
| 17:L:165:PRO:HB2  | 27:M:143:ASN:OD1  | 2.18                     | 0.44              |
| 18:O:328:VAL:O    | 18:O:332:ILE:HG12 | 2.17                     | 0.44              |
| 18:O:392:TRP:HZ3  | 29:U:190:LEU:HB3  | 1.83                     | 0.44              |
| 1:b:172:ASP:O     | 1:b:176:HIS:ND1   | 2.34                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:e:109:ALA:HA    | 6:e:144:PHE:HZ    | 1.81                     | 0.44              |
| 25:J:197:LEU:HD12 | 25:J:197:LEU:HA   | 1.86                     | 0.44              |
| 28:Q:376:LYS:O    | 28:Q:380:MET:HG2  | 2.16                     | 0.44              |
| 29:U:50:ASN:OD1   | 29:U:51:SER:N     | 2.50                     | 0.44              |
| 30:N:511:GLY:O    | 30:N:514:THR:OG1  | 2.35                     | 0.44              |
| 30:N:664:LEU:HB2  | 30:N:706:MET:HE1  | 1.99                     | 0.44              |
| 1:1:151:THR:HA    | 1:1:154:TYR:HE1   | 1.82                     | 0.44              |
| 2:2:236:ARG:NH2   | 3:3:162:ASP:HA    | 2.33                     | 0.44              |
| 3:3:44:PHE:CE2    | 3:3:64:ASN:HB2    | 2.52                     | 0.44              |
| 5:5:250:VAL:N     | 5:5:266:HIS:O     | 2.48                     | 0.44              |
| 6:6:49:ILE:HG21   | 2:i:196:LEU:HD21  | 2.00                     | 0.44              |
| 6:6:176:LYS:HD2   | 3:h:203:ARG:HH22  | 1.80                     | 0.44              |
| 12:E:54:ALA:HA    | 12:E:59:LEU:HD23  | 1.99                     | 0.44              |
| 13:F:162:GLY:N    | 13:F:165:SER:OG   | 2.50                     | 0.44              |
| 14:G:148:LEU:C    | 14:G:149:TYR:HD1  | 2.26                     | 0.44              |
| 16:K:134:SER:O    | 16:K:134:SER:OG   | 2.30                     | 0.44              |
| 16:K:221:MET:O    | 16:K:221:MET:HG3  | 2.16                     | 0.44              |
| 17:L:396:THR:HA   | 27:M:212:ILE:HD11 | 1.99                     | 0.44              |
| 19:P:311:TRP:CE3  | 19:P:345:VAL:HG11 | 2.53                     | 0.44              |
| 22:V:25:GLU:CD    | 22:V:157:ARG:HH22 | 2.25                     | 0.44              |
| 7:a:122:PRO:HB2   | 7:a:159:PHE:HD2   | 1.82                     | 0.44              |
| 7:a:134:TYR:HE2   | 6:e:82:ALA:HB2    | 1.83                     | 0.44              |
| 6:e:102:LYS:NZ    | 6:e:103:LEU:O     | 2.44                     | 0.44              |
| 6:e:227:THR:HG22  | 6:e:228:LYS:H     | 1.83                     | 0.44              |
| 2:i:129:VAL:HB    | 2:i:140:PHE:CE1   | 2.52                     | 0.44              |
| 2:i:195:ASP:HB3   | 2:i:198:SER:HB3   | 1.99                     | 0.44              |
| 26:H:95:HIS:HB2   | 26:H:96:PRO:HD3   | 1.98                     | 0.44              |
| 26:H:360:THR:O    | 26:H:360:THR:OG1  | 2.30                     | 0.44              |
| 30:N:186:ILE:HG21 | 30:N:214:LEU:HD21 | 1.99                     | 0.44              |
| 30:N:475:ALA:HB2  | 30:N:510:HIS:CD2  | 2.52                     | 0.44              |
| 30:N:492:THR:HG21 | 30:N:494:LYS:HE2  | 1.99                     | 0.44              |
| 30:N:858:LYS:HD2  | 30:N:859:ASN:H    | 1.82                     | 0.44              |
| 32:o:293:MET:O    | 32:o:297:VAL:HG23 | 2.18                     | 0.44              |
| 32:o:357:ILE:HG13 | 32:o:390:LEU:HD11 | 2.00                     | 0.44              |
| 15:I:150:HIS:CD2  | 26:H:90:ARG:HH22  | 2.35                     | 0.44              |
| 15:I:194:ILE:HG12 | 15:I:348:ILE:HD13 | 1.98                     | 0.44              |
| 16:K:304:ASP:OD2  | 16:K:333:ARG:NH2  | 2.42                     | 0.44              |
| 17:L:141:LYS:HE2  | 17:L:141:LYS:HB2  | 1.77                     | 0.44              |
| 19:P:63:VAL:HG23  | 19:P:75:LEU:HD11  | 2.00                     | 0.44              |
| 19:P:362:LEU:HD23 | 19:P:398:LYS:C    | 2.43                     | 0.44              |
| 20:R:149:ASN:OD1  | 20:R:150:ALA:N    | 2.50                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:V:118:LEU:HD22 | 22:V:122:ASP:HB3  | 1.99                     | 0.44              |
| 25:J:249:GLU:HG3  | 25:J:250:ILE:H    | 1.82                     | 0.44              |
| 26:H:86:GLY:O     | 26:H:90:ARG:HB2   | 2.18                     | 0.44              |
| 27:M:320:ARG:HE   | 27:M:320:ARG:HB2  | 1.66                     | 0.44              |
| 30:N:374:ILE:HG22 | 30:N:375:HIS:ND1  | 2.32                     | 0.44              |
| 2:2:87:LEU:HD22   | 2:2:115:HIS:HD2   | 1.83                     | 0.44              |
| 3:3:109:VAL:O     | 3:3:121:ILE:HD12  | 2.18                     | 0.44              |
| 3:3:121:ILE:HG13  | 3:3:137:ILE:HD13  | 1.99                     | 0.44              |
| 4:4:149:ARG:HD3   | 4:4:149:ARG:HA    | 1.74                     | 0.44              |
| 7:7:228:PHE:N     | 7:7:245:LEU:O     | 2.40                     | 0.44              |
| 15:I:233:ALA:HA   | 15:I:236:VAL:HG12 | 1.99                     | 0.44              |
| 18:O:15:ARG:HH21  | 18:O:23:HIS:CD2   | 2.36                     | 0.44              |
| 18:O:151:ASP:HA   | 18:O:154:GLU:HG3  | 1.99                     | 0.44              |
| 18:O:373:TRP:CE3  | 29:U:204:LEU:HD11 | 2.53                     | 0.44              |
| 19:P:326:ASP:O    | 19:P:328:ALA:N    | 2.48                     | 0.44              |
| 23:W:5:ALA:H      | 23:W:106:GLN:HB3  | 1.82                     | 0.44              |
| 23:W:9:VAL:HA     | 23:W:52:ILE:HG23  | 2.00                     | 0.44              |
| 4:g:168:LEU:O     | 4:g:172:MET:HB2   | 2.17                     | 0.44              |
| 3:h:159:GLU:OE1   | 3:h:161:GLU:HB3   | 2.18                     | 0.44              |
| 2:i:48:ARG:NH2    | 2:i:196:LEU:O     | 2.51                     | 0.44              |
| 25:J:327:ILE:HG22 | 25:J:358:VAL:HG11 | 1.98                     | 0.44              |
| 26:H:82:TRP:CD1   | 26:H:82:TRP:H     | 2.34                     | 0.44              |
| 26:H:395:SER:O    | 26:H:396:MET:HB2  | 2.18                     | 0.44              |
| 28:Q:77:PHE:O     | 28:Q:80:HIS:ND1   | 2.46                     | 0.44              |
| 30:N:193:ALA:HB2  | 30:N:206:ILE:HD13 | 1.99                     | 0.44              |
| 30:N:301:THR:HG22 | 30:N:920:VAL:H    | 1.83                     | 0.44              |
| 30:N:536:ILE:O    | 30:N:540:LEU:HB2  | 2.17                     | 0.44              |
| 30:N:559:TYR:CD2  | 30:N:567:ALA:HB2  | 2.53                     | 0.44              |
| 31:T:112:ASN:O    | 31:T:116:GLN:HG2  | 2.18                     | 0.44              |
| 32:o:279:THR:HB   | 32:o:974:THR:HG23 | 2.00                     | 0.44              |
| 32:o:945:ILE:HD11 | 32:o:962:ARG:HB2  | 1.99                     | 0.44              |
| 11:D:66:LYS:NZ    | 11:D:69:SER:HA    | 2.33                     | 0.44              |
| 19:P:423:LEU:O    | 19:P:426:ILE:HG22 | 2.17                     | 0.44              |
| 20:R:31:PHE:HB3   | 20:R:320:LYS:HG2  | 2.00                     | 0.44              |
| 21:S:159:ASN:OD1  | 21:S:187:ILE:HA   | 2.18                     | 0.44              |
| 7:a:49:TYR:HE1    | 7:a:54:ILE:HG13   | 1.83                     | 0.44              |
| 4:g:29:LYS:HE2    | 4:g:31:SER:HB2    | 1.99                     | 0.44              |
| 4:g:167:GLU:HG3   | 4:g:168:LEU:N     | 2.32                     | 0.44              |
| 26:H:320:ASP:OD1  | 26:H:321:ASP:N    | 2.51                     | 0.44              |
| 26:H:439:THR:OG1  | 26:H:440:GLU:N    | 2.51                     | 0.44              |
| 27:M:76:PRO:HG2   | 27:M:150:LYS:NZ   | 2.33                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:N:202:PHE:O    | 30:N:206:ILE:HG22 | 2.18                     | 0.44              |
| 30:N:443:LEU:HD12 | 30:N:469:VAL:HG21 | 2.00                     | 0.44              |
| 30:N:646:LYS:HD3  | 30:N:646:LYS:HA   | 1.69                     | 0.44              |
| 31:T:59:LYS:NZ    | 31:T:96:LEU:O     | 2.49                     | 0.44              |
| 32:o:620:LEU:HD12 | 32:o:739:ALA:HA   | 1.99                     | 0.44              |
| 2:2:233:LYS:HA    | 2:2:233:LYS:HD2   | 1.90                     | 0.44              |
| 7:7:214:MET:HE2   | 7:7:214:MET:HA    | 2.00                     | 0.44              |
| 16:K:396:ARG:NH2  | 17:L:195:GLU:OE1  | 2.51                     | 0.44              |
| 20:R:59:MET:SD    | 20:R:59:MET:N     | 2.91                     | 0.44              |
| 21:S:437:ASN:HB3  | 21:S:442:PHE:CE1  | 2.52                     | 0.44              |
| 7:a:44:VAL:HG23   | 7:a:87:SER:HB2    | 1.99                     | 0.44              |
| 4:g:4:ILE:HG22    | 4:g:103:LEU:HD12  | 1.99                     | 0.44              |
| 3:h:45:HIS:CE1    | 2:i:247:VAL:HG11  | 2.53                     | 0.44              |
| 26:H:223:GLU:HG2  | 26:H:227:LEU:HD12 | 2.00                     | 0.44              |
| 26:H:389:PHE:O    | 26:H:393:SER:HB3  | 2.18                     | 0.44              |
| 28:Q:195:LYS:HD2  | 28:Q:225:LEU:HD13 | 1.98                     | 0.44              |
| 29:U:71:ASN:OD1   | 29:U:71:ASN:N     | 2.51                     | 0.44              |
| 29:U:211:LEU:O    | 29:U:214:VAL:HG12 | 2.17                     | 0.44              |
| 32:o:278:LEU:HA   | 32:o:281:ALA:HB3  | 1.99                     | 0.44              |
| 6:6:177:ASN:ND2   | 3:h:176:ASP:OD2   | 2.25                     | 0.43              |
| 7:7:49:TYR:CE1    | 7:7:54:ILE:HG13   | 2.52                     | 0.43              |
| 14:G:73:HIS:CE1   | 14:G:106:PRO:HB3  | 2.53                     | 0.43              |
| 15:I:304:ARG:HH21 | 26:H:329:VAL:HG21 | 1.83                     | 0.43              |
| 17:L:147:THR:OG1  | 17:L:156:MET:HB2  | 2.18                     | 0.43              |
| 17:L:248:ALA:HB1  | 17:L:285:ALA:HB3  | 2.00                     | 0.43              |
| 19:P:107:SER:HB3  | 19:P:110:LEU:HB2  | 1.99                     | 0.43              |
| 19:P:384:VAL:CG1  | 28:Q:353:PRO:HB3  | 2.46                     | 0.43              |
| 7:a:190:LYS:HA    | 7:a:190:LYS:HD2   | 1.73                     | 0.43              |
| 4:g:115:GLU:HG2   | 4:g:117:TYR:CZ    | 2.53                     | 0.43              |
| 30:N:143:LYS:HA   | 30:N:146:LYS:HD2  | 2.00                     | 0.43              |
| 32:o:497:PHE:CG   | 32:o:505:VAL:HG21 | 2.53                     | 0.43              |
| 1:1:166:SER:OG    | 1:1:169:GLU:HG3   | 2.17                     | 0.43              |
| 4:4:103:LEU:HD12  | 4:4:103:LEU:HA    | 1.86                     | 0.43              |
| 5:5:286:ILE:HD12  | 5:5:286:ILE:HA    | 1.91                     | 0.43              |
| 6:6:153:GLU:OE1   | 6:6:156:ARG:NE    | 2.49                     | 0.43              |
| 8:A:65:ASP:OD2    | 8:A:67:THR:OG1    | 2.35                     | 0.43              |
| 8:A:76:SER:OG     | 8:A:77:ARG:N      | 2.51                     | 0.43              |
| 9:B:37:ILE:HG22   | 9:B:161:ALA:HB1   | 1.99                     | 0.43              |
| 10:C:4:ARG:HH12   | 12:E:10:ARG:HA    | 1.82                     | 0.43              |
| 10:C:181:LYS:HA   | 10:C:181:LYS:HD3  | 1.89                     | 0.43              |
| 11:D:113:VAL:HG12 | 11:D:150:THR:HG21 | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:F:155:GLU:O    | 14:G:60:VAL:HG12  | 2.18                     | 0.43              |
| 14:G:83:PRO:O     | 14:G:86:ARG:HB3   | 2.18                     | 0.43              |
| 17:L:220:LEU:HD22 | 17:L:349:ILE:HD11 | 1.99                     | 0.43              |
| 18:O:38:TRP:HB3   | 18:O:69:PHE:CE2   | 2.52                     | 0.43              |
| 18:O:248:TYR:HB3  | 18:O:251:LEU:HD21 | 2.00                     | 0.43              |
| 18:O:287:LEU:HD12 | 18:O:287:LEU:HA   | 1.87                     | 0.43              |
| 19:P:33:ASN:OD1   | 19:P:33:ASN:N     | 2.50                     | 0.43              |
| 19:P:141:LYS:HD2  | 19:P:179:PHE:HE1  | 1.83                     | 0.43              |
| 21:S:33:GLU:O     | 21:S:37:VAL:HG23  | 2.18                     | 0.43              |
| 22:V:229:ASP:C    | 22:V:229:ASP:OD2  | 2.61                     | 0.43              |
| 23:W:34:GLU:HG3   | 23:W:69:PHE:CZ    | 2.53                     | 0.43              |
| 4:g:135:TYR:HD1   | 4:g:138:PHE:HE2   | 1.65                     | 0.43              |
| 32:o:457:ILE:HA   | 32:o:460:SER:HB3  | 1.98                     | 0.43              |
| 32:o:809:MET:HB3  | 32:o:847:ILE:HD13 | 2.00                     | 0.43              |
| 32:o:967:THR:HG22 | 32:o:969:GLU:H    | 1.82                     | 0.43              |
| 4:4:44:MET:HE1    | 4:4:104:ILE:HB    | 2.00                     | 0.43              |
| 5:5:120:MET:SD    | 5:5:127:CYS:HB2   | 2.58                     | 0.43              |
| 5:5:198:LYS:HA    | 5:5:198:LYS:HD2   | 1.82                     | 0.43              |
| 7:7:60:LEU:HD22   | 7:7:225:SER:HB3   | 2.00                     | 0.43              |
| 7:7:208:GLU:HA    | 7:7:211:VAL:HG12  | 2.01                     | 0.43              |
| 8:A:61:ASP:CG     | 17:L:420:ARG:HH21 | 2.23                     | 0.43              |
| 8:A:126:GLN:NE2   | 9:B:81:ASP:HA     | 2.31                     | 0.43              |
| 9:B:94:HIS:O      | 9:B:99:ARG:HG2    | 2.17                     | 0.43              |
| 13:F:163:ALA:O    | 13:F:164:ARG:HG2  | 2.18                     | 0.43              |
| 14:G:36:THR:HA    | 14:G:166:GLY:HA3  | 2.00                     | 0.43              |
| 15:I:150:HIS:O    | 15:I:154:MET:HG2  | 2.17                     | 0.43              |
| 19:P:300:VAL:O    | 19:P:304:THR:OG1  | 2.24                     | 0.43              |
| 6:e:180:GLU:O     | 6:e:183:THR:OG1   | 2.31                     | 0.43              |
| 3:h:24:ALA:HB2    | 3:h:187:VAL:HG22  | 1.99                     | 0.43              |
| 3:h:95:LEU:HD11   | 3:h:107:PRO:HG2   | 2.00                     | 0.43              |
| 2:i:47:THR:HB     | 2:i:59:ASN:HA     | 2.00                     | 0.43              |
| 28:Q:224:ILE:HD12 | 28:Q:330:LEU:HD22 | 2.01                     | 0.43              |
| 28:Q:275:ILE:H    | 28:Q:275:ILE:HG13 | 1.53                     | 0.43              |
| 28:Q:390:LEU:HD12 | 28:Q:391:ASP:H    | 1.84                     | 0.43              |
| 29:U:294:ASN:O    | 29:U:297:GLN:HG3  | 2.18                     | 0.43              |
| 31:T:202:LEU:HB3  | 31:T:231:SER:HB2  | 2.01                     | 0.43              |
| 32:o:154:ILE:O    | 32:o:157:LEU:HG   | 2.18                     | 0.43              |
| 32:o:375:ASP:HB3  | 32:o:842:GLN:HE22 | 1.83                     | 0.43              |
| 4:4:20:ALA:HB2    | 4:4:177:LYS:HG2   | 2.00                     | 0.43              |
| 9:B:186:GLU:HA    | 9:B:189:ILE:HG22  | 2.00                     | 0.43              |
| 11:D:50:SER:O     | 11:D:50:SER:OG    | 2.36                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:O:147:ARG:CZ   | 18:O:150:LEU:HD11 | 2.49                     | 0.43              |
| 22:V:175:SER:OG   | 30:N:741:TYR:HA   | 2.18                     | 0.43              |
| 24:Y:72:ASP:OD1   | 24:Y:74:THR:OG1   | 2.36                     | 0.43              |
| 7:a:98:ARG:HG3    | 7:a:101:LYS:HE2   | 1.99                     | 0.43              |
| 1:b:133:PRO:HD2   | 1:b:137:SER:O     | 2.18                     | 0.43              |
| 6:e:111:ASN:O     | 6:e:115:LEU:HG    | 2.18                     | 0.43              |
| 4:g:168:LEU:HB3   | 4:g:176:PHE:CE2   | 2.54                     | 0.43              |
| 3:h:10:GLY:HA3    | 3:h:42:LYS:HE2    | 2.00                     | 0.43              |
| 2:i:96:SER:OG     | 2:i:101:ARG:O     | 2.31                     | 0.43              |
| 27:M:50:ARG:O     | 27:M:53:HIS:ND1   | 2.49                     | 0.43              |
| 27:M:203:ARG:NE   | 27:M:206:LYS:HD2  | 2.34                     | 0.43              |
| 28:Q:251:THR:H    | 28:Q:254:SER:HB3  | 1.84                     | 0.43              |
| 30:N:319:SER:OG   | 30:N:320:SER:N    | 2.51                     | 0.43              |
| 3:3:18:LYS:NZ     | 3:3:157:ASN:HB3   | 2.33                     | 0.43              |
| 3:3:65:GLU:CD     | 10:C:100:LYS:HA   | 2.43                     | 0.43              |
| 3:3:165:GLU:O     | 3:3:169:GLN:HG2   | 2.18                     | 0.43              |
| 7:7:125:ILE:O     | 7:7:129:LEU:HG    | 2.18                     | 0.43              |
| 8:A:232:LYS:HA    | 8:A:232:LYS:HD2   | 1.81                     | 0.43              |
| 9:B:19:GLY:O      | 9:B:23:TYR:HD1    | 2.01                     | 0.43              |
| 9:B:176:GLU:HG3   | 10:C:56:LEU:HD23  | 2.01                     | 0.43              |
| 11:D:75:PHE:CE2   | 11:D:79:ASN:HA    | 2.53                     | 0.43              |
| 11:D:200:LEU:HA   | 11:D:203:VAL:HG12 | 1.99                     | 0.43              |
| 11:D:203:VAL:O    | 11:D:204:GLN:HG3  | 2.17                     | 0.43              |
| 18:O:211:GLN:HG2  | 18:O:241:THR:HB   | 1.99                     | 0.43              |
| 18:O:236:HIS:HB3  | 18:O:238:ILE:HG22 | 2.01                     | 0.43              |
| 18:O:296:LEU:HD22 | 18:O:327:LEU:HD22 | 2.00                     | 0.43              |
| 20:R:67:CYS:HB3   | 20:R:94:PHE:HB2   | 2.00                     | 0.43              |
| 20:R:410:LEU:HD22 | 29:U:281:LEU:HD21 | 2.00                     | 0.43              |
| 21:S:336:SER:OG   | 21:S:337:ASN:OD1  | 2.36                     | 0.43              |
| 21:S:423:VAL:O    | 21:S:427:ILE:HG23 | 2.18                     | 0.43              |
| 21:S:474:GLU:O    | 21:S:477:VAL:HG12 | 2.18                     | 0.43              |
| 1:b:122:ASP:OD1   | 1:b:123:ASP:N     | 2.51                     | 0.43              |
| 1:b:151:THR:HA    | 1:b:154:TYR:HE2   | 1.83                     | 0.43              |
| 1:b:151:THR:HA    | 1:b:154:TYR:CE2   | 2.54                     | 0.43              |
| 6:e:45:ASP:O      | 6:e:61:LYS:NZ     | 2.50                     | 0.43              |
| 5:f:107:LYS:HA    | 5:f:107:LYS:HD2   | 1.80                     | 0.43              |
| 4:g:149:ARG:HB2   | 4:g:152:MET:HG3   | 2.00                     | 0.43              |
| 4:g:178:GLY:HA3   | 4:g:195:PHE:CE1   | 2.53                     | 0.43              |
| 30:N:739:PHE:O    | 30:N:739:PHE:CG   | 2.71                     | 0.43              |
| 31:T:255:GLN:CD   | 31:T:256:LYS:H    | 2.27                     | 0.43              |
| 32:o:506:LEU:HD12 | 32:o:534:PHE:CE1  | 2.53                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:o:583:ASP:OD1  | 32:o:584:VAL:N    | 2.51                     | 0.43              |
| 32:o:854:LEU:HD12 | 32:o:854:LEU:O    | 2.18                     | 0.43              |
| 1:l:155:GLY:HA2   | 1:b:180:GLN:CD    | 2.42                     | 0.43              |
| 4:4:99:GLN:HA     | 4:4:121:TYR:HB2   | 2.00                     | 0.43              |
| 6:6:224:LEU:HD12  | 6:6:224:LEU:HA    | 1.81                     | 0.43              |
| 7:7:86:ILE:HG22   | 7:7:147:ILE:HG23  | 2.00                     | 0.43              |
| 7:7:121:GLU:HB2   | 7:7:124:TYR:CE2   | 2.54                     | 0.43              |
| 9:B:66:LEU:HD12   | 9:B:235:PHE:HD2   | 1.84                     | 0.43              |
| 9:B:66:LEU:HD11   | 9:B:69:PRO:HA     | 2.00                     | 0.43              |
| 17:L:159:LEU:HD11 | 27:M:128:PHE:CD1  | 2.54                     | 0.43              |
| 17:L:283:VAL:HG21 | 17:L:325:MET:HE3  | 1.99                     | 0.43              |
| 18:O:150:LEU:HA   | 18:O:153:LEU:HB2  | 2.01                     | 0.43              |
| 22:V:270:TYR:N    | 22:V:270:TYR:CD1  | 2.87                     | 0.43              |
| 1:b:20:THR:HG21   | 1:b:52:LYS:HD2    | 2.01                     | 0.43              |
| 1:b:23:MET:SD     | 1:b:174:ILE:HG12  | 2.59                     | 0.43              |
| 6:e:29:GLY:HA3    | 6:e:61:LYS:HE2    | 2.00                     | 0.43              |
| 5:f:82:ARG:HH22   | 5:f:185:PRO:HD2   | 1.83                     | 0.43              |
| 5:f:113:ASN:C     | 5:f:115:PHE:H     | 2.26                     | 0.43              |
| 5:f:156:LYS:HZ2   | 5:f:196:ARG:HH22  | 1.65                     | 0.43              |
| 4:g:81:SER:HB2    | 4:g:125:LYS:HD2   | 2.00                     | 0.43              |
| 4:g:100:VAL:HG12  | 4:g:102:VAL:HG13  | 1.99                     | 0.43              |
| 25:J:121:MET:HE2  | 25:J:121:MET:HB2  | 1.86                     | 0.43              |
| 26:H:168:ILE:HG13 | 26:H:183:ILE:HG21 | 2.01                     | 0.43              |
| 26:H:331:ARG:CZ   | 27:M:301:VAL:HG21 | 2.48                     | 0.43              |
| 27:M:354:GLU:OE1  | 27:M:354:GLU:C    | 2.61                     | 0.43              |
| 28:Q:23:ALA:HA    | 28:Q:26:VAL:HB    | 2.00                     | 0.43              |
| 30:N:126:LYS:HA   | 30:N:126:LYS:HD3  | 1.80                     | 0.43              |
| 32:o:509:LEU:HD23 | 32:o:530:LEU:HG   | 2.01                     | 0.43              |
| 2:2:48:ARG:O      | 2:2:62:LYS:NZ     | 2.51                     | 0.43              |
| 3:3:46:TYR:OH     | 3:3:64:ASN:O      | 2.33                     | 0.43              |
| 3:3:201:LYS:HE3   | 5:f:273:TRP:HE1   | 1.84                     | 0.43              |
| 6:6:55:ASN:HB3    | 7:7:170:TYR:CZ    | 2.54                     | 0.43              |
| 7:7:42:THR:OG1    | 7:7:43:SER:N      | 2.52                     | 0.43              |
| 8:A:88:PRO:HD3    | 14:G:156:SER:HB2  | 2.00                     | 0.43              |
| 18:O:308:LEU:HD23 | 18:O:308:LEU:HA   | 1.80                     | 0.43              |
| 19:P:257:TRP:CH2  | 19:P:289:ASN:HB3  | 2.54                     | 0.43              |
| 6:e:86:ARG:NE     | 6:e:115:LEU:HD22  | 2.34                     | 0.43              |
| 5:f:76:THR:O      | 5:f:206:SER:N     | 2.52                     | 0.43              |
| 3:h:66:MET:O      | 3:h:70:LYS:HE3    | 2.19                     | 0.43              |
| 26:H:85:MET:C     | 26:H:85:MET:HE2   | 2.43                     | 0.43              |
| 26:H:198:MET:HB2  | 26:H:273:ARG:O    | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:H:367:ARG:HH21 | 26:H:370:ARG:CZ   | 2.31                     | 0.43              |
| 32:o:52:LEU:HD23  | 32:o:55:ARG:HH11  | 1.83                     | 0.43              |
| 32:o:769:ASN:HB2  | 32:o:772:ILE:HD12 | 2.01                     | 0.43              |
| 32:o:789:GLN:OE1  | 32:o:791:LYS:N    | 2.43                     | 0.43              |
| 4:4:152:MET:H     | 4:4:152:MET:HG2   | 1.58                     | 0.43              |
| 7:7:144:TRP:HA    | 7:7:165:LEU:HD22  | 1.99                     | 0.43              |
| 10:C:43:GLY:HA2   | 10:C:146:TYR:CE1  | 2.54                     | 0.43              |
| 12:E:70:ILE:HD11  | 12:E:76:CYS:HB3   | 2.01                     | 0.43              |
| 15:I:81:ILE:HA    | 15:I:85:PHE:CZ    | 2.54                     | 0.43              |
| 15:I:232:LEU:HD13 | 15:I:350:PHE:HZ   | 1.84                     | 0.43              |
| 15:I:345:ASP:OD1  | 15:I:345:ASP:N    | 2.42                     | 0.43              |
| 17:L:186:LEU:HD11 | 17:L:349:ILE:HG23 | 2.00                     | 0.43              |
| 17:L:288:GLY:HA3  | 27:M:299:ARG:NH1  | 2.34                     | 0.43              |
| 20:R:235:LEU:HD21 | 20:R:250:ALA:HA   | 2.00                     | 0.43              |
| 21:S:136:CYS:HA   | 21:S:167:LEU:HD11 | 2.01                     | 0.43              |
| 3:h:66:MET:HE2    | 3:h:66:MET:HA     | 2.01                     | 0.43              |
| 27:M:228:LYS:HG2  | 27:M:349:PHE:CD2  | 2.54                     | 0.43              |
| 30:N:101:ILE:HD13 | 30:N:101:ILE:HA   | 1.84                     | 0.43              |
| 30:N:353:LEU:HD23 | 30:N:353:LEU:HA   | 1.82                     | 0.43              |
| 30:N:647:ASP:C    | 30:N:647:ASP:OD1  | 2.61                     | 0.43              |
| 32:o:756:MET:N    | 32:o:756:MET:HE2  | 2.33                     | 0.43              |
| 32:o:797:THR:HG22 | 32:o:801:HIS:CE1  | 2.53                     | 0.43              |
| 1:1:86:THR:HA     | 1:1:90:GLY:O      | 2.19                     | 0.43              |
| 7:7:215:ARG:NH2   | 7:7:249:ASN:HB3   | 2.33                     | 0.43              |
| 8:A:13:ASP:C      | 8:A:13:ASP:OD2    | 2.61                     | 0.43              |
| 15:I:300:ARG:O    | 15:I:304:ARG:HG2  | 2.18                     | 0.43              |
| 16:K:356:ILE:HD11 | 34:K:501:ATP:C2   | 2.54                     | 0.43              |
| 17:L:156:MET:HE3  | 17:L:156:MET:HB3  | 1.92                     | 0.43              |
| 17:L:233:LYS:HB2  | 17:L:233:LYS:HE3  | 1.79                     | 0.43              |
| 18:O:54:SER:OG    | 18:O:57:LEU:HB2   | 2.18                     | 0.43              |
| 18:O:228:TYR:CE2  | 18:O:334:LEU:HD13 | 2.54                     | 0.43              |
| 18:O:244:ASN:OD1  | 18:O:244:ASN:N    | 2.52                     | 0.43              |
| 18:O:387:ARG:O    | 18:O:387:ARG:NH1  | 2.52                     | 0.43              |
| 19:P:342:GLN:O    | 19:P:345:VAL:HG12 | 2.18                     | 0.43              |
| 20:R:309:LEU:HD23 | 20:R:309:LEU:HA   | 1.85                     | 0.43              |
| 4:g:95:ARG:HD2    | 4:g:95:ARG:C      | 2.43                     | 0.43              |
| 26:H:83:ASP:HB2   | 26:H:85:MET:HG3   | 2.00                     | 0.43              |
| 26:H:346:ARG:HG2  | 26:H:349:ILE:HB   | 2.01                     | 0.43              |
| 27:M:290:ARG:NH1  | 27:M:306:LEU:HD11 | 2.33                     | 0.43              |
| 29:U:138:VAL:HG12 | 29:U:140:ILE:HG23 | 2.01                     | 0.43              |
| 30:N:104:LYS:O    | 30:N:107:GLU:HB2  | 2.17                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:N:447:SER:HA   | 30:N:450:ILE:HG22 | 2.00                     | 0.43              |
| 30:N:534:ASP:O    | 30:N:535:LEU:HB2  | 2.18                     | 0.43              |
| 31:T:108:LEU:HD23 | 31:T:108:LEU:HA   | 1.87                     | 0.43              |
| 2:2:82:GLU:H      | 2:2:82:GLU:CD     | 2.27                     | 0.43              |
| 2:2:120:GLN:O     | 2:2:122:HIS:ND1   | 2.52                     | 0.43              |
| 2:2:166:VAL:O     | 2:2:169:SER:OG    | 2.37                     | 0.43              |
| 3:3:104:PHE:HA    | 3:3:126:LEU:HG    | 2.00                     | 0.43              |
| 5:5:172:MET:H     | 5:5:192:SER:HB3   | 1.83                     | 0.43              |
| 7:7:53:VAL:O      | 7:7:233:ILE:HG12  | 2.19                     | 0.43              |
| 7:7:137:ARG:HD3   | 7:7:166:LEU:HA    | 2.00                     | 0.43              |
| 11:D:53:LYS:HD3   | 11:D:53:LYS:HA    | 1.74                     | 0.43              |
| 11:D:193:LYS:HG3  | 11:D:236:ILE:HD11 | 2.00                     | 0.43              |
| 14:G:118:GLN:OE1  | 14:G:118:GLN:HA   | 2.19                     | 0.43              |
| 14:G:221:LEU:HA   | 14:G:225:ASN:HA   | 1.99                     | 0.43              |
| 16:K:378:LEU:HD23 | 16:K:378:LEU:HA   | 1.79                     | 0.43              |
| 19:P:281:ILE:HD11 | 19:P:300:VAL:HG22 | 2.00                     | 0.43              |
| 20:R:98:LEU:HD23  | 20:R:98:LEU:HA    | 1.86                     | 0.43              |
| 20:R:238:PHE:CE1  | 20:R:249:ILE:HG13 | 2.54                     | 0.43              |
| 23:W:124:GLU:OE1  | 23:W:127:ARG:NH1  | 2.51                     | 0.43              |
| 7:a:60:LEU:HD21   | 7:a:67:LEU:HD13   | 2.01                     | 0.43              |
| 3:h:67:PHE:CD1    | 3:h:70:LYS:HD2    | 2.54                     | 0.43              |
| 2:i:195:ASP:OD1   | 2:i:197:GLY:N     | 2.50                     | 0.43              |
| 30:N:442:LEU:HD12 | 30:N:442:LEU:HA   | 1.88                     | 0.43              |
| 30:N:517:LEU:HD23 | 30:N:517:LEU:HA   | 1.89                     | 0.43              |
| 30:N:561:GLY:O    | 30:N:597:ARG:HD2  | 2.18                     | 0.43              |
| 32:o:89:LEU:HA    | 32:o:92:LEU:HD12  | 2.00                     | 0.43              |
| 3:3:88:THR:HB     | 3:3:109:VAL:HG21  | 2.00                     | 0.42              |
| 5:5:206:SER:OG    | 5:5:243:ASP:OD2   | 2.28                     | 0.42              |
| 16:K:238:ASN:OD1  | 17:L:310:THR:HG21 | 2.19                     | 0.42              |
| 18:O:103:LYS:NZ   | 18:O:107:GLN:OE1  | 2.52                     | 0.42              |
| 19:P:38:GLN:O     | 19:P:42:LEU:HD12  | 2.19                     | 0.42              |
| 19:P:281:ILE:HD12 | 19:P:281:ILE:HA   | 1.92                     | 0.42              |
| 21:S:64:ARG:HD3   | 21:S:144:LEU:HD22 | 2.01                     | 0.42              |
| 21:S:178:LEU:HD12 | 21:S:178:LEU:H    | 1.84                     | 0.42              |
| 1:b:33:LEU:HD23   | 1:b:63:CYS:SG     | 2.59                     | 0.42              |
| 6:e:27:ASN:OD1    | 6:e:77:ALA:N      | 2.52                     | 0.42              |
| 5:f:139:ARG:HA    | 5:f:142:GLU:OE1   | 2.19                     | 0.42              |
| 5:f:229:LEU:HD11  | 5:f:263:HIS:CE1   | 2.54                     | 0.42              |
| 4:g:9:VAL:HG21    | 4:g:154:THR:HA    | 2.01                     | 0.42              |
| 25:J:230:VAL:HG22 | 25:J:233:LEU:HD23 | 2.01                     | 0.42              |
| 26:H:87:ASP:HA    | 26:H:90:ARG:HB3   | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:N:424:LYS:HE2  | 30:N:424:LYS:HB3  | 1.79                     | 0.42              |
| 30:N:873:ARG:NH1  | 30:N:875:LEU:HD11 | 2.34                     | 0.42              |
| 31:T:271:GLU:HA   | 31:T:271:GLU:OE2  | 2.18                     | 0.42              |
| 32:o:167:ASP:O    | 32:o:171:LYS:HB2  | 2.19                     | 0.42              |
| 32:o:769:ASN:O    | 32:o:773:ARG:HG3  | 2.19                     | 0.42              |
| 32:o:867:PHE:CD2  | 32:o:871:HIS:HA   | 2.52                     | 0.42              |
| 32:o:953:THR:OG1  | 32:o:954:PRO:HD3  | 2.19                     | 0.42              |
| 1:1:171:VAL:O     | 1:1:174:ILE:HG22  | 2.19                     | 0.42              |
| 12:E:102:TYR:C    | 12:E:103:TYR:HD2  | 2.27                     | 0.42              |
| 13:F:159:THR:OG1  | 13:F:160:ALA:N    | 2.51                     | 0.42              |
| 17:L:242:ASN:ND2  | 17:L:273:HIS:HB3  | 2.33                     | 0.42              |
| 17:L:356:GLY:O    | 17:L:360:ILE:HG12 | 2.19                     | 0.42              |
| 18:O:97:LYS:HD3   | 18:O:97:LYS:HA    | 1.90                     | 0.42              |
| 19:P:140:THR:HG21 | 19:P:163:LEU:HD13 | 2.01                     | 0.42              |
| 20:R:418:GLY:HA2  | 20:R:421:VAL:HG22 | 2.00                     | 0.42              |
| 3:h:15:MET:HG3    | 3:h:163:LEU:HD22  | 2.01                     | 0.42              |
| 25:J:164:ILE:HD13 | 25:J:164:ILE:HA   | 1.90                     | 0.42              |
| 25:J:247:MET:HE1  | 25:J:268:VAL:HB   | 2.00                     | 0.42              |
| 27:M:219:LEU:N    | 27:M:345:ARG:O    | 2.49                     | 0.42              |
| 30:N:379:LEU:HD21 | 30:N:415:PHE:HD2  | 1.84                     | 0.42              |
| 30:N:536:ILE:HG21 | 30:N:555:ILE:HD11 | 2.01                     | 0.42              |
| 30:N:858:LYS:HD2  | 30:N:859:ASN:N    | 2.33                     | 0.42              |
| 2:2:149:ASP:N     | 2:2:149:ASP:OD1   | 2.50                     | 0.42              |
| 3:3:175:ALA:O     | 3:3:181:SER:OG    | 2.37                     | 0.42              |
| 4:4:91:SER:HB3    | 4:4:98:TYR:HD1    | 1.85                     | 0.42              |
| 8:A:83:VAL:HG11   | 8:A:90:ALA:HB1    | 2.02                     | 0.42              |
| 9:B:171:ALA:O     | 9:B:175:LEU:HD23  | 2.20                     | 0.42              |
| 14:G:121:GLN:HA   | 14:G:124:THR:HG22 | 2.00                     | 0.42              |
| 15:I:317:ASP:OD1  | 15:I:317:ASP:N    | 2.53                     | 0.42              |
| 16:K:161:MET:HE2  | 16:K:161:MET:HB3  | 1.80                     | 0.42              |
| 34:K:501:ATP:O3G  | 17:L:342:ARG:NH2  | 2.44                     | 0.42              |
| 20:R:112:GLU:O    | 20:R:116:LYS:HG2  | 2.18                     | 0.42              |
| 21:S:375:ASP:N    | 21:S:375:ASP:OD1  | 2.53                     | 0.42              |
| 7:a:226:ARG:HG3   | 7:a:247:VAL:H     | 1.84                     | 0.42              |
| 3:h:50:PHE:CE2    | 3:h:195:VAL:HG21  | 2.54                     | 0.42              |
| 2:i:202:VAL:HG12  | 2:i:204:VAL:HG23  | 2.02                     | 0.42              |
| 26:H:349:ILE:HG22 | 26:H:349:ILE:O    | 2.20                     | 0.42              |
| 30:N:234:ASP:OD1  | 30:N:237:LEU:N    | 2.43                     | 0.42              |
| 30:N:331:ALA:HB2  | 30:N:697:PHE:CD2  | 2.54                     | 0.42              |
| 30:N:444:HIS:CE1  | 30:N:480:ALA:HB2  | 2.55                     | 0.42              |
| 32:o:793:PHE:O    | 32:o:797:THR:OG1  | 2.35                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:o:794:ASP:OD1  | 32:o:794:ASP:N    | 2.41                     | 0.42              |
| 1:1:99:SER:HB2    | 14:G:104:LYS:HG2  | 2.01                     | 0.42              |
| 4:4:159:ASP:O     | 4:4:163:LEU:HG    | 2.19                     | 0.42              |
| 6:6:153:GLU:HG2   | 6:6:154:GLN:N     | 2.34                     | 0.42              |
| 7:7:42:THR:N      | 7:7:74:ARG:HH22   | 2.16                     | 0.42              |
| 8:A:75:ILE:HD13   | 8:A:75:ILE:HA     | 1.82                     | 0.42              |
| 11:D:92:GLU:HG3   | 11:D:112:TYR:CG   | 2.55                     | 0.42              |
| 16:K:76:LYS:HE3   | 25:J:51:LEU:HD22  | 2.02                     | 0.42              |
| 17:L:280:MET:HE2  | 17:L:280:MET:HB3  | 1.94                     | 0.42              |
| 18:O:330:ARG:HG2  | 19:P:307:GLU:OE2  | 2.19                     | 0.42              |
| 18:O:382:LYS:HB3  | 18:O:382:LYS:HE2  | 1.62                     | 0.42              |
| 19:P:181:LEU:HD21 | 19:P:220:TYR:HB2  | 2.01                     | 0.42              |
| 21:S:326:ASP:OD2  | 21:S:326:ASP:C    | 2.62                     | 0.42              |
| 22:V:144:ILE:HD13 | 22:V:144:ILE:HA   | 1.84                     | 0.42              |
| 23:W:172:LEU:HB2  | 23:W:189:PRO:HG3  | 2.02                     | 0.42              |
| 7:a:35:GLN:HB3    | 7:a:144:TRP:HE1   | 1.85                     | 0.42              |
| 1:b:27:PHE:HE2    | 1:b:29:ASP:HB3    | 1.84                     | 0.42              |
| 3:h:56:LEU:O      | 3:h:60:VAL:HG23   | 2.19                     | 0.42              |
| 25:J:306:ARG:HD2  | 25:J:307:PRO:HD2  | 2.01                     | 0.42              |
| 26:H:99:VAL:HG23  | 26:H:187:LEU:HD12 | 2.01                     | 0.42              |
| 26:H:210:ASP:O    | 26:H:391:ILE:HG21 | 2.19                     | 0.42              |
| 26:H:274:VAL:HB   | 26:H:308:PHE:HD1  | 1.84                     | 0.42              |
| 27:M:360:ILE:HD12 | 34:M:501:ATP:N1   | 2.33                     | 0.42              |
| 28:Q:26:VAL:O     | 28:Q:29:SER:OG    | 2.34                     | 0.42              |
| 28:Q:179:LEU:O    | 28:Q:183:LYS:HG3  | 2.19                     | 0.42              |
| 28:Q:271:MET:HE1  | 28:Q:334:HIS:HB3  | 2.02                     | 0.42              |
| 30:N:217:MET:HE2  | 30:N:219:ASN:O    | 2.18                     | 0.42              |
| 30:N:318:LYS:HB3  | 30:N:318:LYS:HE2  | 1.76                     | 0.42              |
| 31:T:32:ILE:H     | 31:T:32:ILE:HG13  | 1.66                     | 0.42              |
| 1:1:113:THR:HG22  | 1:1:134:LEU:HD22  | 2.00                     | 0.42              |
| 5:5:172:MET:N     | 5:5:192:SER:HB3   | 2.34                     | 0.42              |
| 6:6:199:VAL:O     | 6:6:203:VAL:HG23  | 2.20                     | 0.42              |
| 8:A:225:VAL:HG13  | 8:A:236:LEU:HB2   | 2.02                     | 0.42              |
| 11:D:28:LYS:HE3   | 11:D:28:LYS:HB2   | 1.78                     | 0.42              |
| 18:O:20:PRO:HA    | 18:O:23:HIS:CG    | 2.55                     | 0.42              |
| 19:P:197:THR:O    | 19:P:200:SER:OG   | 2.31                     | 0.42              |
| 21:S:436:ILE:HD13 | 21:S:443:ILE:HG12 | 2.00                     | 0.42              |
| 7:a:93:MET:HA     | 7:a:96:ILE:HG12   | 2.01                     | 0.42              |
| 7:a:170:TYR:CZ    | 6:e:55:ASN:HB3    | 2.54                     | 0.42              |
| 1:b:165:MET:HG2   | 1:b:169:GLU:HB3   | 2.02                     | 0.42              |
| 6:e:46:THR:HB     | 6:e:58:TYR:HA     | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:H:146:VAL:HG22 | 26:H:156:VAL:HG22 | 2.01                     | 0.42              |
| 26:H:465:GLN:NE2  | 26:H:465:GLN:HA   | 2.35                     | 0.42              |
| 27:M:281:ASP:OD1  | 27:M:282:GLU:N    | 2.53                     | 0.42              |
| 28:Q:70:ALA:HB3   | 28:Q:73:LYS:HB2   | 2.02                     | 0.42              |
| 32:o:729:GLU:N    | 32:o:729:GLU:OE1  | 2.52                     | 0.42              |
| 1:1:50:THR:HG23   | 1:1:52:LYS:HZ1    | 1.85                     | 0.42              |
| 2:2:124:GLY:HA2   | 2:2:144:ALA:HB1   | 2.02                     | 0.42              |
| 10:C:94:HIS:CG    | 10:C:114:ARG:HG2  | 2.55                     | 0.42              |
| 15:I:130:VAL:HG22 | 15:I:154:MET:O    | 2.19                     | 0.42              |
| 16:K:265:ALA:HB1  | 16:K:311:ASN:OD1  | 2.20                     | 0.42              |
| 16:K:369:ASP:HA   | 16:K:372:ILE:HG12 | 2.01                     | 0.42              |
| 17:L:263:ILE:HD12 | 17:L:304:THR:HG23 | 2.00                     | 0.42              |
| 18:O:273:GLN:HA   | 18:O:276:LYS:HD3  | 2.00                     | 0.42              |
| 7:a:193:ASP:CG    | 6:e:57:ARG:HH22   | 2.28                     | 0.42              |
| 32:o:117:ASP:OD1  | 32:o:138:ARG:NH2  | 2.53                     | 0.42              |
| 32:o:568:LEU:HD21 | 32:o:883:THR:HA   | 2.02                     | 0.42              |
| 32:o:893:PHE:HA   | 32:o:896:LYS:HE2  | 2.02                     | 0.42              |
| 32:o:911:LYS:HE2  | 32:o:911:LYS:HB3  | 1.68                     | 0.42              |
| 32:o:919:GLU:HB2  | 32:o:921:GLU:OE1  | 2.19                     | 0.42              |
| 2:2:48:ARG:HD3    | 2:2:199:GLY:C     | 2.44                     | 0.42              |
| 6:6:84:VAL:HG12   | 6:6:88:LYS:HD2    | 2.02                     | 0.42              |
| 8:A:123:ASN:OD1   | 9:B:83:ARG:NH2    | 2.52                     | 0.42              |
| 12:E:88:MET:HE3   | 12:E:138:PHE:CD1  | 2.55                     | 0.42              |
| 13:F:61:LYS:HB2   | 13:F:61:LYS:HE2   | 1.84                     | 0.42              |
| 14:G:53:LEU:HD12  | 14:G:53:LEU:HA    | 1.80                     | 0.42              |
| 19:P:9:ALA:C      | 19:P:11:LYS:H     | 2.28                     | 0.42              |
| 19:P:58:VAL:O     | 19:P:62:ILE:HG23  | 2.20                     | 0.42              |
| 22:V:254:ARG:HH22 | 22:V:277:LYS:HD3  | 1.84                     | 0.42              |
| 4:g:139:TYR:CE2   | 4:g:171:ARG:HB2   | 2.54                     | 0.42              |
| 4:g:166:GLN:NE2   | 4:g:198:GLN:OE1   | 2.53                     | 0.42              |
| 25:J:155:LYS:O    | 25:J:158:LYS:HB3  | 2.19                     | 0.42              |
| 26:H:150:LYS:HD3  | 26:H:150:LYS:HA   | 1.87                     | 0.42              |
| 26:H:379:LEU:HA   | 26:H:380:PRO:HD3  | 1.95                     | 0.42              |
| 27:M:76:PRO:HG2   | 27:M:150:LYS:HZ1  | 1.84                     | 0.42              |
| 28:Q:361:HIS:O    | 28:Q:365:ILE:HG12 | 2.19                     | 0.42              |
| 29:U:301:ILE:HD13 | 29:U:301:ILE:HA   | 1.90                     | 0.42              |
| 32:o:948:TRP:CD1  | 32:o:948:TRP:H    | 2.37                     | 0.42              |
| 1:1:38:ARG:NH1    | 1:1:186:GLY:O     | 2.39                     | 0.42              |
| 3:3:135:ASP:OD1   | 3:3:136:PHE:N     | 2.50                     | 0.42              |
| 5:5:242:ARG:HH21  | 4:g:145:ASP:CG    | 2.27                     | 0.42              |
| 7:7:46:SER:HB3    | 7:7:55:ILE:HG13   | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:A:217:GLU:OE2   | 8:A:218:PHE:N     | 2.53                     | 0.42              |
| 12:E:19:GLY:HA3   | 13:F:27:GLU:OE1   | 2.20                     | 0.42              |
| 15:I:213:ILE:HD13 | 26:H:427:GLY:HA3  | 2.01                     | 0.42              |
| 15:I:246:ARG:HG2  | 15:I:247:ILE:N    | 2.34                     | 0.42              |
| 16:K:322:ASP:OD2  | 16:K:323:THR:HG23 | 2.20                     | 0.42              |
| 16:K:333:ARG:NH1  | 25:J:139:VAL:O    | 2.37                     | 0.42              |
| 19:P:30:ASN:OD1   | 19:P:30:ASN:N     | 2.52                     | 0.42              |
| 22:V:25:GLU:HA    | 22:V:61:TYR:O     | 2.20                     | 0.42              |
| 23:W:134:LYS:HD3  | 23:W:134:LYS:HA   | 1.76                     | 0.42              |
| 23:W:143:ASN:HD21 | 23:W:150:ASN:HB2  | 1.84                     | 0.42              |
| 1:b:40:THR:HG21   | 1:b:187:SER:HA    | 2.02                     | 0.42              |
| 5:f:201:ILE:HD11  | 5:f:219:TYR:CD1   | 2.54                     | 0.42              |
| 25:J:246:PHE:HA   | 25:J:291:ILE:O    | 2.19                     | 0.42              |
| 26:H:191:ILE:HD12 | 26:H:191:ILE:HA   | 1.79                     | 0.42              |
| 27:M:290:ARG:HD3  | 27:M:306:LEU:HD21 | 2.01                     | 0.42              |
| 27:M:327:THR:OG1  | 27:M:328:ASN:N    | 2.53                     | 0.42              |
| 27:M:400:MET:HE3  | 27:M:400:MET:O    | 2.18                     | 0.42              |
| 28:Q:267:LEU:HD22 | 28:Q:331:THR:HG22 | 2.02                     | 0.42              |
| 29:U:110:PHE:O    | 29:U:114:THR:OG1  | 2.32                     | 0.42              |
| 30:N:17:GLN:O     | 30:N:20:VAL:HG12  | 2.20                     | 0.42              |
| 31:T:25:LYS:HA    | 31:T:25:LYS:HD3   | 1.67                     | 0.42              |
| 31:T:139:ASP:HB3  | 31:T:142:LEU:HD12 | 2.01                     | 0.42              |
| 32:o:327:GLN:HA   | 32:o:330:ILE:HG12 | 2.01                     | 0.42              |
| 32:o:595:MET:O    | 32:o:599:ILE:HG12 | 2.20                     | 0.42              |
| 3:3:29:LEU:HD13   | 3:3:40:PHE:CD1    | 2.55                     | 0.42              |
| 4:4:158:LEU:HD13  | 4:4:198:GLN:HE22  | 1.85                     | 0.42              |
| 8:A:96:ARG:HH11   | 8:A:124:LEU:HD22  | 1.85                     | 0.42              |
| 10:C:27:GLU:OE2   | 15:I:431:ASN:ND2  | 2.52                     | 0.42              |
| 10:C:69:LEU:HD22  | 10:C:111:LEU:HD11 | 2.02                     | 0.42              |
| 11:D:176:GLU:OE2  | 12:E:56:SER:OG    | 2.32                     | 0.42              |
| 14:G:38:ILE:HD11  | 14:G:196:ALA:HA   | 2.02                     | 0.42              |
| 15:I:193:GLU:HB3  | 15:I:346:ARG:NH1  | 2.35                     | 0.42              |
| 26:H:281:GLN:NE2  | 26:H:290:MET:HE3  | 2.35                     | 0.42              |
| 26:H:307:PHE:O    | 26:H:307:PHE:CG   | 2.72                     | 0.42              |
| 28:Q:263:LYS:HZ3  | 28:Q:324:GLU:HB3  | 1.85                     | 0.42              |
| 29:U:102:SER:O    | 29:U:106:ILE:HG13 | 2.20                     | 0.42              |
| 30:N:194:ILE:HD13 | 30:N:203:ARG:NH1  | 2.35                     | 0.42              |
| 32:o:201:LEU:HA   | 32:o:204:CYS:SG   | 2.59                     | 0.42              |
| 32:o:754:LYS:HD2  | 32:o:783:VAL:O    | 2.19                     | 0.42              |
| 3:3:203:ARG:H     | 3:3:203:ARG:HD3   | 1.85                     | 0.42              |
| 7:7:53:VAL:HG11   | 7:7:160:LEU:HD13  | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:A:167:LYS:HB3   | 8:A:186:PHE:HE2   | 1.84                     | 0.42              |
| 11:D:84:ILE:O     | 11:D:88:LYS:HG3   | 2.20                     | 0.42              |
| 13:F:82:ARG:HD2   | 13:F:82:ARG:HA    | 1.96                     | 0.42              |
| 13:F:155:GLU:HG2  | 14:G:60:VAL:HG11  | 2.00                     | 0.42              |
| 15:I:89:GLN:CG    | 15:I:90:GLU:N     | 2.83                     | 0.42              |
| 16:K:119:VAL:HG21 | 25:J:114:CYS:SG   | 2.59                     | 0.42              |
| 17:L:333:LEU:HD23 | 17:L:333:LEU:HA   | 1.87                     | 0.42              |
| 17:L:367:LYS:HA   | 17:L:367:LYS:HD3  | 1.92                     | 0.42              |
| 19:P:28:ALA:O     | 19:P:69:ARG:NH2   | 2.46                     | 0.42              |
| 19:P:198:VAL:HA   | 19:P:201:ARG:NH2  | 2.34                     | 0.42              |
| 20:R:127:GLU:O    | 20:R:130:GLN:HG2  | 2.19                     | 0.42              |
| 20:R:358:GLY:C    | 24:Y:78:LYS:HG2   | 2.45                     | 0.42              |
| 22:V:90:LYS:HG2   | 22:V:94:MET:HE2   | 2.02                     | 0.42              |
| 7:a:181:ALA:O     | 7:a:185:ASN:ND2   | 2.52                     | 0.42              |
| 4:g:136:SER:O     | 4:g:140:THR:HG23  | 2.19                     | 0.42              |
| 4:g:147:HIS:HB2   | 4:g:160:LEU:HD13  | 2.02                     | 0.42              |
| 3:h:59:ASP:HA     | 3:h:62:THR:HG22   | 2.01                     | 0.42              |
| 27:M:351:LEU:HD22 | 27:M:387:ASN:HB3  | 2.02                     | 0.42              |
| 28:Q:142:ALA:HB2  | 28:Q:157:LEU:HD22 | 2.02                     | 0.42              |
| 29:U:22:TYR:CD1   | 29:U:125:VAL:HG11 | 2.55                     | 0.42              |
| 30:N:171:LYS:HE2  | 30:N:171:LYS:HB2  | 1.85                     | 0.42              |
| 32:o:265:LEU:HB3  | 32:o:288:LEU:HD11 | 2.02                     | 0.42              |
| 32:o:525:MET:HE2  | 32:o:562:TRP:CZ3  | 2.55                     | 0.42              |
| 32:o:864:MET:HE2  | 32:o:864:MET:HA   | 2.02                     | 0.42              |
| 32:o:969:GLU:OE2  | 32:o:989:TYR:HB3  | 2.19                     | 0.42              |
| 3:3:39:LYS:HZ1    | 5:f:284:ASN:HB3   | 1.85                     | 0.41              |
| 8:A:145:SER:OG    | 8:A:146:VAL:N     | 2.53                     | 0.41              |
| 9:B:44:VAL:HG23   | 9:B:211:LEU:HD11  | 2.02                     | 0.41              |
| 9:B:197:LYS:HD3   | 9:B:204:PHE:CE2   | 2.55                     | 0.41              |
| 14:G:32:GLU:HB2   | 14:G:169:ARG:HH21 | 1.85                     | 0.41              |
| 16:K:211:LEU:O    | 16:K:317:ALA:HA   | 2.20                     | 0.41              |
| 17:L:92:GLU:O     | 17:L:96:LYS:HG3   | 2.20                     | 0.41              |
| 20:R:105:LYS:HE2  | 20:R:109:LYS:HE2  | 2.02                     | 0.41              |
| 22:V:54:LEU:HD21  | 22:V:69:PHE:HE1   | 1.85                     | 0.41              |
| 23:W:96:LEU:HD23  | 23:W:96:LEU:HA    | 1.90                     | 0.41              |
| 3:h:97:GLU:OE1    | 3:h:98:ARG:NH1    | 2.53                     | 0.41              |
| 29:U:170:GLY:O    | 29:U:174:LEU:HD23 | 2.20                     | 0.41              |
| 30:N:640:VAL:O    | 30:N:643:PRO:HD2  | 2.20                     | 0.41              |
| 30:N:672:ASN:HB3  | 30:N:675:VAL:HG23 | 2.02                     | 0.41              |
| 32:o:235:GLN:OE1  | 32:o:235:GLN:N    | 2.52                     | 0.41              |
| 1:1:22:ILE:HG22   | 1:1:35:ALA:HB2    | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:A:75:ILE:HB     | 8:A:79:ILE:HG22   | 2.02                     | 0.41              |
| 10:C:66:LEU:HD13  | 10:C:214:ALA:HB2  | 2.01                     | 0.41              |
| 10:C:135:PHE:H    | 10:C:151:SER:HG   | 1.65                     | 0.41              |
| 11:D:96:HIS:NE2   | 11:D:100:LEU:HD12 | 2.35                     | 0.41              |
| 16:K:344:ARG:O    | 16:K:349:ARG:NH2  | 2.44                     | 0.41              |
| 18:O:226:LYS:C    | 18:O:227:ILE:HD12 | 2.45                     | 0.41              |
| 21:S:82:TYR:HB3   | 21:S:89:LYS:HB2   | 2.03                     | 0.41              |
| 23:W:99:LYS:HG2   | 23:W:100:HIS:CD2  | 2.54                     | 0.41              |
| 7:a:189:ARG:NH2   | 6:e:54:ILE:O      | 2.43                     | 0.41              |
| 7:a:203:VAL:O     | 7:a:206:ALA:HB3   | 2.20                     | 0.41              |
| 1:b:33:LEU:HD11   | 1:b:119:ALA:HB3   | 2.01                     | 0.41              |
| 6:e:84:VAL:HG12   | 6:e:88:LYS:NZ     | 2.35                     | 0.41              |
| 5:f:273:TRP:O     | 5:f:276:LYS:HG2   | 2.19                     | 0.41              |
| 2:i:51:GLN:OE1    | 2:i:51:GLN:N      | 2.53                     | 0.41              |
| 26:H:205:ASP:OD1  | 32:o:362:LEU:HD13 | 2.21                     | 0.41              |
| 29:U:79:MET:O     | 29:U:83:ILE:HG12  | 2.21                     | 0.41              |
| 30:N:340:HIS:HB2  | 30:N:374:ILE:HG12 | 2.00                     | 0.41              |
| 30:N:504:TYR:HD2  | 30:N:517:LEU:HD11 | 1.85                     | 0.41              |
| 5:5:125:ALA:HB3   | 6:6:147:VAL:HG22  | 2.01                     | 0.41              |
| 6:6:128:THR:HG22  | 6:6:144:PHE:HB2   | 2.01                     | 0.41              |
| 7:7:47:MET:HE1    | 7:7:206:ALA:HA    | 2.03                     | 0.41              |
| 12:E:21:LEU:H     | 12:E:21:LEU:HD12  | 1.84                     | 0.41              |
| 16:K:86:VAL:HG23  | 25:J:62:LEU:HB2   | 2.02                     | 0.41              |
| 18:O:186:ASN:ND2  | 18:O:225:ASP:H    | 2.17                     | 0.41              |
| 18:O:248:TYR:O    | 18:O:251:LEU:HG   | 2.20                     | 0.41              |
| 19:P:24:ILE:HD12  | 19:P:24:ILE:HA    | 1.81                     | 0.41              |
| 19:P:96:MET:O     | 19:P:100:VAL:HG23 | 2.21                     | 0.41              |
| 21:S:330:LEU:H    | 24:Y:64:TRP:HZ3   | 1.67                     | 0.41              |
| 23:W:158:ILE:HG13 | 23:W:169:SER:OG   | 2.20                     | 0.41              |
| 7:a:197:ASP:O     | 7:a:201:THR:HG22  | 2.21                     | 0.41              |
| 3:h:29:LEU:HB3    | 3:h:37:SER:HB3    | 2.03                     | 0.41              |
| 2:i:133:ASP:OD1   | 2:i:136:GLY:N     | 2.53                     | 0.41              |
| 27:M:428:LYS:HD2  | 27:M:428:LYS:HA   | 1.71                     | 0.41              |
| 29:U:92:TRP:CH2   | 29:U:106:ILE:HB   | 2.55                     | 0.41              |
| 30:N:15:GLU:HG2   | 30:N:16:ASN:H     | 1.85                     | 0.41              |
| 30:N:256:GLN:OE1  | 30:N:904:VAL:N    | 2.47                     | 0.41              |
| 3:3:183:TRP:HZ2   | 5:f:242:ARG:HA    | 1.85                     | 0.41              |
| 4:4:23:ARG:NH2    | 5:5:191:ASP:OD2   | 2.51                     | 0.41              |
| 5:5:187:ILE:H     | 5:5:198:LYS:NZ    | 2.18                     | 0.41              |
| 5:5:270:GLU:H     | 5:5:270:GLU:HG3   | 1.73                     | 0.41              |
| 9:B:41:ASN:ND2    | 9:B:41:ASN:H      | 2.17                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:F:44:ALA:HB3   | 13:F:216:VAL:HG12 | 2.03                     | 0.41              |
| 16:K:158:ILE:HD11 | 16:K:253:MET:HE1  | 2.02                     | 0.41              |
| 17:L:247:PRO:HB3  | 27:M:310:ASN:ND2  | 2.36                     | 0.41              |
| 17:L:312:MET:HE3  | 17:L:342:ARG:HD3  | 2.01                     | 0.41              |
| 18:O:194:LEU:O    | 18:O:198:THR:OG1  | 2.26                     | 0.41              |
| 19:P:72:TRP:NE1   | 19:P:110:LEU:HD11 | 2.35                     | 0.41              |
| 19:P:111:ASP:O    | 19:P:115:ARG:HG3  | 2.19                     | 0.41              |
| 20:R:29:LYS:HG3   | 20:R:49:PHE:CD2   | 2.56                     | 0.41              |
| 7:a:265:LYS:HD3   | 7:a:266:ILE:N     | 2.35                     | 0.41              |
| 6:e:170:ASP:HA    | 6:e:174:ASN:HB2   | 2.02                     | 0.41              |
| 4:g:140:THR:O     | 4:g:144:LEU:HG    | 2.20                     | 0.41              |
| 2:i:163:ALA:HB1   | 2:i:187:ALA:HB1   | 2.02                     | 0.41              |
| 32:o:575:MET:HB3  | 32:o:606:CYS:SG   | 2.61                     | 0.41              |
| 3:3:110:ALA:HB2   | 3:3:121:ILE:HD13  | 2.02                     | 0.41              |
| 4:4:132:ALA:HB3   | 4:4:137:GLY:HA2   | 2.02                     | 0.41              |
| 7:7:152:VAL:HG23  | 7:7:233:ILE:HD12  | 2.03                     | 0.41              |
| 9:B:12:PHE:HE1    | 10:C:129:ARG:HH11 | 1.69                     | 0.41              |
| 9:B:143:ASN:OD1   | 9:B:143:ASN:N     | 2.54                     | 0.41              |
| 11:D:138:PHE:CE1  | 11:D:217:PRO:HG3  | 2.55                     | 0.41              |
| 12:E:21:LEU:HD11  | 13:F:77:LEU:HD21  | 2.02                     | 0.41              |
| 12:E:106:ASP:OD1  | 12:E:107:ILE:N    | 2.53                     | 0.41              |
| 13:F:50:LYS:HD2   | 13:F:59:TYR:HB3   | 2.01                     | 0.41              |
| 13:F:121:GLN:OE1  | 13:F:121:GLN:HA   | 2.21                     | 0.41              |
| 14:G:44:ASP:OD2   | 14:G:220:SER:HB2  | 2.20                     | 0.41              |
| 17:L:353:ASN:OD1  | 17:L:353:ASN:N    | 2.50                     | 0.41              |
| 18:O:137:TYR:HA   | 18:O:140:LYS:HB2  | 2.02                     | 0.41              |
| 18:O:329:MET:HE3  | 19:P:308:LEU:HD22 | 2.01                     | 0.41              |
| 20:R:351:LYS:HE2  | 20:R:351:LYS:HB2  | 1.89                     | 0.41              |
| 22:V:20:ARG:C     | 22:V:172:GLN:HE21 | 2.28                     | 0.41              |
| 23:W:72:ILE:O     | 23:W:76:LEU:HG    | 2.20                     | 0.41              |
| 3:h:191:LYS:HB2   | 3:h:194:GLU:O     | 2.21                     | 0.41              |
| 2:i:128:ILE:HA    | 2:i:141:SER:HA    | 2.02                     | 0.41              |
| 25:J:230:VAL:HG13 | 25:J:272:MET:HE1  | 2.02                     | 0.41              |
| 26:H:450:VAL:HG12 | 26:H:451:ILE:HD13 | 2.02                     | 0.41              |
| 28:Q:148:LYS:HE2  | 28:Q:148:LYS:HB2  | 1.81                     | 0.41              |
| 29:U:102:SER:HA   | 29:U:105:LYS:HG3  | 2.02                     | 0.41              |
| 29:U:143:VAL:HA   | 29:U:150:THR:HA   | 2.03                     | 0.41              |
| 30:N:116:GLN:O    | 30:N:120:ASP:N    | 2.54                     | 0.41              |
| 32:o:44:LYS:NZ    | 32:o:48:ASP:OD1   | 2.40                     | 0.41              |
| 32:o:835:ALA:HB2  | 32:o:848:THR:HG21 | 2.02                     | 0.41              |
| 32:o:932:ALA:HB1  | 32:o:962:ARG:HE   | 1.85                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:107:SER:HB2   | 8:A:108:TYR:HD2   | 1.86                     | 0.41              |
| 2:2:217:ARG:HD2   | 2:2:217:ARG:HA    | 1.87                     | 0.41              |
| 4:4:101:ASN:HB3   | 4:4:133:HIS:HD2   | 1.85                     | 0.41              |
| 6:6:30:THR:HB     | 6:6:161:ALA:HB3   | 2.02                     | 0.41              |
| 11:D:12:SER:OG    | 11:D:14:ASP:OD1   | 2.24                     | 0.41              |
| 12:E:10:ARG:NH2   | 13:F:3:ARG:HD3    | 2.35                     | 0.41              |
| 12:E:109:VAL:HB   | 12:E:154:GLN:OE1  | 2.21                     | 0.41              |
| 12:E:122:ARG:HD2  | 12:E:122:ARG:HA   | 1.79                     | 0.41              |
| 12:E:211:LYS:HD3  | 12:E:211:LYS:HA   | 1.88                     | 0.41              |
| 13:F:71:GLY:HA3   | 13:F:222:PHE:CE1  | 2.56                     | 0.41              |
| 15:I:207:LEU:H    | 15:I:207:LEU:HD12 | 1.86                     | 0.41              |
| 15:I:336:PRO:O    | 26:H:459:SER:OG   | 2.30                     | 0.41              |
| 16:K:330:ARG:NH1  | 25:J:140:GLU:OE1  | 2.52                     | 0.41              |
| 17:L:103:GLN:O    | 27:M:128:PHE:N    | 2.53                     | 0.41              |
| 17:L:345:ARG:H    | 17:L:345:ARG:HG2  | 1.66                     | 0.41              |
| 18:O:383:LYS:HE2  | 18:O:383:LYS:HB3  | 1.79                     | 0.41              |
| 19:P:198:VAL:HA   | 19:P:201:ARG:HH12 | 1.85                     | 0.41              |
| 22:V:256:GLU:HA   | 22:V:256:GLU:OE1  | 2.21                     | 0.41              |
| 24:Y:33:ASP:OD2   | 24:Y:34:GLU:N     | 2.53                     | 0.41              |
| 7:a:214:MET:SD    | 7:a:214:MET:C     | 3.03                     | 0.41              |
| 7:a:242:LYS:HB2   | 7:a:242:LYS:HE2   | 1.72                     | 0.41              |
| 2:i:32:ILE:HD12   | 2:i:128:ILE:HG22  | 2.01                     | 0.41              |
| 25:J:186:ILE:HG13 | 25:J:310:ILE:HG21 | 2.02                     | 0.41              |
| 27:M:221:TYR:CD1  | 27:M:221:TYR:C    | 2.97                     | 0.41              |
| 27:M:385:GLU:OE2  | 27:M:385:GLU:N    | 2.54                     | 0.41              |
| 30:N:28:ILE:HG22  | 30:N:64:ILE:HD11  | 2.02                     | 0.41              |
| 32:o:542:ILE:O    | 32:o:546:ILE:HG12 | 2.20                     | 0.41              |
| 32:o:774:ARG:HB2  | 32:o:810:ASN:HD22 | 1.85                     | 0.41              |
| 5:5:240:ALA:HB1   | 5:5:247:GLY:HA2   | 2.03                     | 0.41              |
| 7:7:230:LEU:HB3   | 7:7:242:LYS:HE2   | 2.01                     | 0.41              |
| 8:A:135:ARG:HH11  | 14:G:125:LEU:HA   | 1.85                     | 0.41              |
| 10:C:209:ASP:OD1  | 10:C:209:ASP:N    | 2.51                     | 0.41              |
| 14:G:113:ALA:HA   | 14:G:138:PHE:HZ   | 1.86                     | 0.41              |
| 14:G:179:LEU:HD11 | 14:G:187:LEU:HD22 | 2.03                     | 0.41              |
| 15:I:229:LYS:HG2  | 15:I:350:PHE:CD2  | 2.56                     | 0.41              |
| 15:I:330:LYS:HE3  | 15:I:330:LYS:HB3  | 1.88                     | 0.41              |
| 16:K:350:ARG:O    | 16:K:350:ARG:HD3  | 2.21                     | 0.41              |
| 20:R:141:TYR:HB3  | 20:R:150:ALA:HB2  | 2.01                     | 0.41              |
| 21:S:475:TYR:HE2  | 29:U:288:PHE:HB2  | 1.86                     | 0.41              |
| 22:V:254:ARG:HD2  | 22:V:254:ARG:C    | 2.46                     | 0.41              |
| 4:g:99:GLN:HA     | 4:g:121:TYR:HB2   | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:J:159:GLU:O    | 25:J:163:VAL:HG23 | 2.21                     | 0.41              |
| 31:T:185:ILE:O    | 31:T:189:ILE:HG13 | 2.21                     | 0.41              |
| 32:o:332:ASN:ND2  | 32:o:335:LEU:HD22 | 2.35                     | 0.41              |
| 32:o:406:TRP:HA   | 32:o:409:LYS:HD3  | 2.03                     | 0.41              |
| 8:A:115:ASP:OD1   | 8:A:115:ASP:N     | 2.51                     | 0.41              |
| 9:B:200:VAL:HG11  | 9:B:204:PHE:CD1   | 2.56                     | 0.41              |
| 10:C:65:LYS:HE2   | 10:C:77:VAL:O     | 2.21                     | 0.41              |
| 10:C:240:VAL:HG12 | 10:C:245:THR:HG23 | 2.03                     | 0.41              |
| 12:E:59:LEU:HD12  | 12:E:59:LEU:HA    | 1.88                     | 0.41              |
| 12:E:134:MET:HB2  | 12:E:134:MET:HE2  | 1.76                     | 0.41              |
| 13:F:66:CYS:HB2   | 13:F:89:ARG:HG3   | 2.02                     | 0.41              |
| 15:I:334:LEU:HD23 | 15:I:334:LEU:HA   | 1.85                     | 0.41              |
| 15:I:341:PRO:HG2  | 26:H:418:GLU:HG3  | 2.01                     | 0.41              |
| 15:I:342:GLY:HA2  | 26:H:420:ARG:HH22 | 1.85                     | 0.41              |
| 17:L:207:PHE:HE2  | 17:L:215:PRO:HD2  | 1.86                     | 0.41              |
| 18:O:95:SER:O     | 18:O:99:LEU:HG    | 2.21                     | 0.41              |
| 18:O:137:TYR:HB3  | 18:O:142:ASP:HB2  | 2.03                     | 0.41              |
| 18:O:392:TRP:CE3  | 18:O:392:TRP:HA   | 2.55                     | 0.41              |
| 21:S:377:TYR:O    | 21:S:381:VAL:HG23 | 2.21                     | 0.41              |
| 22:V:227:MET:CE   | 22:V:301:ASN:HD22 | 2.34                     | 0.41              |
| 1:b:36:ASP:C      | 1:b:52:LYS:HZ1    | 2.29                     | 0.41              |
| 1:b:86:THR:HA     | 1:b:90:GLY:O      | 2.20                     | 0.41              |
| 4:g:168:LEU:HB3   | 4:g:176:PHE:HE2   | 1.85                     | 0.41              |
| 27:M:221:TYR:HE1  | 27:M:348:GLU:HG2  | 1.85                     | 0.41              |
| 28:Q:63:GLN:HB2   | 28:Q:103:LYS:NZ   | 2.36                     | 0.41              |
| 32:o:618:GLN:O    | 32:o:622:HIS:ND1  | 2.53                     | 0.41              |
| 1:1:158:ASP:HB3   | 1:b:180:GLN:NE2   | 2.31                     | 0.41              |
| 2:2:189:GLN:HA    | 2:2:192:ILE:HG12  | 2.03                     | 0.41              |
| 3:3:39:LYS:NZ     | 5:f:284:ASN:HB3   | 2.35                     | 0.41              |
| 3:3:202:MET:HB3   | 3:3:203:ARG:NH1   | 2.35                     | 0.41              |
| 5:5:163:TYR:O     | 5:5:166:LYS:HG2   | 2.21                     | 0.41              |
| 6:6:92:LYS:HB3    | 6:6:92:LYS:HE2    | 1.93                     | 0.41              |
| 6:6:96:PHE:HE1    | 13:F:65:LYS:HE2   | 1.86                     | 0.41              |
| 7:7:103:LEU:HD22  | 7:7:128:TYR:CD2   | 2.55                     | 0.41              |
| 9:B:21:ILE:O      | 9:B:25:LEU:HD23   | 2.21                     | 0.41              |
| 10:C:26:LEU:HD23  | 10:C:26:LEU:HA    | 1.94                     | 0.41              |
| 10:C:226:TYR:HB2  | 10:C:228:LYS:NZ   | 2.35                     | 0.41              |
| 12:E:45:GLY:HA2   | 12:E:153:TYR:CD1  | 2.56                     | 0.41              |
| 12:E:205:LYS:HZ1  | 12:E:212:LEU:H    | 1.68                     | 0.41              |
| 13:F:201:LEU:HD13 | 13:F:205:SER:HA   | 2.03                     | 0.41              |
| 14:G:86:ARG:O     | 14:G:89:VAL:HG12  | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:I:248:VAL:N    | 15:I:251:GLU:OE2  | 2.37                     | 0.41              |
| 17:L:199:LEU:HB3  | 17:L:200:PRO:HD3  | 2.02                     | 0.41              |
| 18:O:343:GLN:NE2  | 19:P:364:ARG:HG2  | 2.35                     | 0.41              |
| 18:O:367:LYS:HE2  | 18:O:367:LYS:HB3  | 1.91                     | 0.41              |
| 19:P:147:LYS:HB3  | 19:P:156:ALA:HB2  | 2.02                     | 0.41              |
| 20:R:70:TYR:HB3   | 20:R:71:LEU:H     | 1.71                     | 0.41              |
| 20:R:374:ASN:HB2  | 20:R:376:GLN:HG3  | 2.02                     | 0.41              |
| 21:S:223:LEU:HD11 | 30:N:70:TYR:CE1   | 2.56                     | 0.41              |
| 21:S:278:LYS:HG2  | 21:S:316:LEU:CD1  | 2.51                     | 0.41              |
| 22:V:149:GLY:O    | 29:U:176:ARG:NH1  | 2.52                     | 0.41              |
| 23:W:108:GLN:CD   | 23:W:108:GLN:H    | 2.29                     | 0.41              |
| 7:a:44:VAL:HG13   | 7:a:57:ALA:HB2    | 2.02                     | 0.41              |
| 4:g:105:GLY:HA2   | 4:g:116:LEU:HA    | 2.03                     | 0.41              |
| 2:i:217:ARG:HE    | 2:i:218:ASN:ND2   | 2.18                     | 0.41              |
| 26:H:169:GLU:N    | 26:H:169:GLU:OE1  | 2.54                     | 0.41              |
| 28:Q:174:LEU:HA   | 28:Q:177:VAL:CG1  | 2.51                     | 0.41              |
| 29:U:213:LYS:HA   | 29:U:213:LYS:HD3  | 1.81                     | 0.41              |
| 30:N:141:ILE:HD12 | 30:N:165:ILE:HG21 | 2.03                     | 0.41              |
| 30:N:163:LEU:O    | 30:N:167:GLU:HG3  | 2.21                     | 0.41              |
| 30:N:389:TYR:CB   | 30:N:404:SER:HB2  | 2.50                     | 0.41              |
| 30:N:642:ASP:OD1  | 30:N:642:ASP:C    | 2.63                     | 0.41              |
| 31:T:103:SER:HB2  | 31:T:141:LEU:HD12 | 2.02                     | 0.41              |
| 31:T:112:ASN:O    | 31:T:115:SER:OG   | 2.38                     | 0.41              |
| 32:o:76:LYS:HG3   | 32:o:149:TRP:CZ3  | 2.55                     | 0.41              |
| 32:o:223:LEU:HA   | 32:o:226:GLU:HG3  | 2.01                     | 0.41              |
| 32:o:273:LEU:HD23 | 32:o:273:LEU:HA   | 1.83                     | 0.41              |
| 2:2:38:ASN:OD1    | 2:2:39:ASN:N      | 2.50                     | 0.41              |
| 4:4:109:LYS:HA    | 4:4:109:LYS:HD3   | 1.79                     | 0.41              |
| 4:4:150:PRO:HD3   | 5:f:283:ASN:OD1   | 2.21                     | 0.41              |
| 10:C:4:ARG:NH1    | 12:E:10:ARG:HA    | 2.37                     | 0.41              |
| 10:C:66:LEU:HD11  | 10:C:212:GLU:HB3  | 2.02                     | 0.41              |
| 14:G:36:THR:HA    | 14:G:165:THR:O    | 2.19                     | 0.41              |
| 14:G:211:ASP:OD1  | 14:G:212:PHE:N    | 2.51                     | 0.41              |
| 14:G:216:ILE:HG13 | 14:G:231:VAL:HB   | 2.03                     | 0.41              |
| 15:I:280:PHE:O    | 15:I:280:PHE:CG   | 2.74                     | 0.41              |
| 18:O:242:ILE:HG23 | 18:O:245:ASP:HB3  | 2.03                     | 0.41              |
| 19:P:61:LYS:NZ    | 19:P:65:LEU:HG    | 2.36                     | 0.41              |
| 21:S:242:LEU:HD23 | 21:S:242:LEU:HA   | 1.86                     | 0.41              |
| 22:V:110:SER:HA   | 22:V:141:VAL:HG23 | 2.03                     | 0.41              |
| 1:b:47:ASN:OD1    | 1:b:48:ARG:N      | 2.54                     | 0.41              |
| 3:h:3:ASP:OD2     | 3:h:6:SER:OG      | 2.34                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:H:223:GLU:HA   | 26:H:227:LEU:HD12 | 2.03                     | 0.41              |
| 27:M:166:ARG:HH11 | 27:M:253:GLN:NE2  | 2.19                     | 0.41              |
| 30:N:17:GLN:HE22  | 31:T:32:ILE:HD11  | 1.86                     | 0.41              |
| 30:N:622:ALA:HB2  | 30:N:644:LEU:HD13 | 2.01                     | 0.41              |
| 31:T:93:ASN:HB3   | 31:T:96:LEU:HB3   | 2.03                     | 0.41              |
| 32:o:224:LEU:HD13 | 32:o:233:LEU:HB2  | 2.03                     | 0.41              |
| 32:o:560:THR:O    | 32:o:563:VAL:HG22 | 2.21                     | 0.41              |
| 32:o:948:TRP:CD1  | 32:o:948:TRP:N    | 2.89                     | 0.41              |
| 1:1:74:ILE:HG23   | 1:1:101:PHE:HE1   | 1.86                     | 0.40              |
| 2:2:233:LYS:HE3   | 3:3:162:ASP:HB3   | 2.03                     | 0.40              |
| 3:3:25:CYS:SG     | 3:3:42:LYS:HB2    | 2.61                     | 0.40              |
| 3:3:107:PRO:HG2   | 3:3:124:PHE:HD2   | 1.86                     | 0.40              |
| 3:3:194:GLU:HG3   | 3:3:195:VAL:H     | 1.86                     | 0.40              |
| 5:5:233:LYS:HE2   | 5:5:233:LYS:HB2   | 1.72                     | 0.40              |
| 6:6:50:THR:O      | 6:6:52:TYR:N      | 2.54                     | 0.40              |
| 6:6:221:LEU:HB2   | 6:6:238:LEU:HD11  | 2.03                     | 0.40              |
| 8:A:88:PRO:HB3    | 14:G:155:GLY:C    | 2.46                     | 0.40              |
| 10:C:160:TRP:CG   | 10:C:163:ILE:HD13 | 2.56                     | 0.40              |
| 12:E:200:VAL:O    | 12:E:203:ILE:HG22 | 2.22                     | 0.40              |
| 14:G:137:ILE:HG22 | 14:G:148:LEU:HD11 | 2.02                     | 0.40              |
| 15:I:108:THR:OG1  | 15:I:121:THR:O    | 2.39                     | 0.40              |
| 16:K:367:ASP:OD2  | 16:K:370:SER:N    | 2.53                     | 0.40              |
| 16:K:374:ARG:HD2  | 16:K:411:TYR:HE2  | 1.86                     | 0.40              |
| 17:L:133:ASN:HA   | 17:L:137:ARG:HH21 | 1.85                     | 0.40              |
| 18:O:297:ILE:HD11 | 18:O:336:LEU:HB3  | 2.03                     | 0.40              |
| 19:P:270:LEU:HD23 | 19:P:270:LEU:HA   | 1.78                     | 0.40              |
| 19:P:395:ARG:HG3  | 28:Q:354:PHE:CE1  | 2.56                     | 0.40              |
| 21:S:121:VAL:HG12 | 21:S:128:ILE:HG22 | 2.03                     | 0.40              |
| 21:S:223:LEU:HD23 | 21:S:223:LEU:HA   | 1.85                     | 0.40              |
| 22:V:22:ASP:O     | 22:V:171:ARG:NH2  | 2.54                     | 0.40              |
| 22:V:293:VAL:HG21 | 29:U:189:ARG:NE   | 2.35                     | 0.40              |
| 1:b:59:LYS:HA     | 1:b:59:LYS:HD2    | 1.69                     | 0.40              |
| 6:e:30:THR:H      | 6:e:45:ASP:CG     | 2.29                     | 0.40              |
| 5:f:134:LEU:HD12  | 5:f:134:LEU:HA    | 1.95                     | 0.40              |
| 4:g:38:LEU:HD12   | 4:g:64:ILE:HG13   | 2.03                     | 0.40              |
| 25:J:48:ARG:NH2   | 30:N:608:LEU:O    | 2.54                     | 0.40              |
| 25:J:160:ILE:CG2  | 25:J:202:VAL:HG21 | 2.51                     | 0.40              |
| 26:H:308:PHE:O    | 26:H:353:PHE:HA   | 2.21                     | 0.40              |
| 28:Q:174:LEU:HA   | 28:Q:177:VAL:HG12 | 2.03                     | 0.40              |
| 30:N:90:ASP:OD1   | 30:N:92:ASP:N     | 2.54                     | 0.40              |
| 30:N:395:ALA:HB3  | 30:N:401:LYS:HE3  | 2.02                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:N:498:ILE:HG12 | 30:N:524:ILE:HG21 | 2.02                     | 0.40              |
| 30:N:774:ASN:N    | 30:N:883:SER:O    | 2.51                     | 0.40              |
| 31:T:38:ASN:O     | 31:T:51:TYR:OH    | 2.37                     | 0.40              |
| 31:T:157:TYR:HA   | 31:T:160:ALA:HB3  | 2.03                     | 0.40              |
| 32:o:115:LEU:HD12 | 32:o:115:LEU:HA   | 1.89                     | 0.40              |
| 32:o:474:LEU:HD23 | 32:o:474:LEU:HA   | 1.90                     | 0.40              |
| 1:1:204:ARG:HD2   | 1:1:204:ARG:HA    | 1.95                     | 0.40              |
| 4:4:173:PRO:HG3   | 4:g:22:THR:HG21   | 2.03                     | 0.40              |
| 5:5:110:ILE:N     | 5:5:110:ILE:HD12  | 2.36                     | 0.40              |
| 5:5:148:ARG:NH2   | 5:5:180:THR:HA    | 2.35                     | 0.40              |
| 5:5:265:ASN:OD1   | 5:5:265:ASN:C     | 2.64                     | 0.40              |
| 5:5:285:VAL:HA    | 3:h:38:ASN:ND2    | 2.36                     | 0.40              |
| 7:7:78:VAL:HG11   | 7:7:100:LEU:HG    | 2.02                     | 0.40              |
| 7:7:97:GLU:HG2    | 7:7:101:LYS:HE2   | 2.03                     | 0.40              |
| 10:C:194:LEU:HD12 | 10:C:242:THR:HG21 | 2.02                     | 0.40              |
| 15:I:57:LEU:HD21  | 32:o:252:CYS:HA   | 2.02                     | 0.40              |
| 34:K:501:ATP:O3B  | 17:L:339:ARG:NH1  | 2.52                     | 0.40              |
| 17:L:98:LEU:HD12  | 17:L:98:LEU:HA    | 1.89                     | 0.40              |
| 18:O:296:LEU:HD13 | 18:O:313:ILE:HG23 | 2.03                     | 0.40              |
| 21:S:223:LEU:HD11 | 30:N:70:TYR:HE1   | 1.86                     | 0.40              |
| 22:V:57:PHE:CE1   | 22:V:105:VAL:HG13 | 2.56                     | 0.40              |
| 22:V:80:VAL:HG11  | 22:V:107:TRP:HZ3  | 1.86                     | 0.40              |
| 7:a:222:ALA:HB3   | 7:a:223:ARG:NH1   | 2.36                     | 0.40              |
| 3:h:149:MET:HE1   | 3:h:170:ALA:HA    | 2.03                     | 0.40              |
| 2:i:81:THR:HB     | 2:i:127:LEU:HD21  | 2.03                     | 0.40              |
| 27:M:228:LYS:HB2  | 34:M:501:ATP:O2B  | 2.21                     | 0.40              |
| 28:Q:133:LEU:HD12 | 28:Q:133:LEU:HA   | 1.86                     | 0.40              |
| 29:U:236:LEU:HD12 | 29:U:237:PRO:HD2  | 2.02                     | 0.40              |
| 30:N:545:SER:HB2  | 30:N:580:ASN:HD22 | 1.87                     | 0.40              |
| 30:N:555:ILE:HG21 | 30:N:571:LEU:HG   | 2.03                     | 0.40              |
| 31:T:69:SER:HB2   | 31:T:74:ASN:HB3   | 2.03                     | 0.40              |
| 31:T:164:LEU:HD11 | 31:T:181:LEU:HB3  | 2.02                     | 0.40              |
| 32:o:93:ARG:NH1   | 32:o:125:THR:O    | 2.54                     | 0.40              |
| 32:o:352:LYS:HB2  | 32:o:390:LEU:HD13 | 2.02                     | 0.40              |
| 1:1:152:PHE:HE2   | 1:1:185:ASP:HB2   | 1.86                     | 0.40              |
| 1:1:209:PRO:HA    | 1:1:212:TYR:CE2   | 2.55                     | 0.40              |
| 4:4:135:TYR:HD2   | 4:g:25:ILE:HD12   | 1.87                     | 0.40              |
| 7:7:42:THR:HG22   | 7:7:74:ARG:NH1    | 2.36                     | 0.40              |
| 7:7:80:ASP:O      | 7:7:239:LEU:HB2   | 2.21                     | 0.40              |
| 8:A:112:MET:HE2   | 8:A:117:LEU:HB2   | 2.03                     | 0.40              |
| 8:A:121:MET:HE3   | 8:A:121:MET:HB3   | 1.81                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:B:65:SER:OG     | 9:B:66:LEU:N      | 2.54                     | 0.40              |
| 9:B:71:ILE:HG12   | 9:B:138:GLY:HA3   | 2.02                     | 0.40              |
| 9:B:149:GLN:NE2   | 9:B:151:ASP:OD1   | 2.54                     | 0.40              |
| 13:F:132:LEU:HB2  | 13:F:147:PHE:HB3  | 2.03                     | 0.40              |
| 15:I:297:GLY:HA3  | 15:I:301:GLU:HB2  | 2.04                     | 0.40              |
| 16:K:365:GLU:OE1  | 16:K:365:GLU:N    | 2.54                     | 0.40              |
| 17:L:344:ASP:O    | 17:L:345:ARG:C    | 2.64                     | 0.40              |
| 20:R:130:GLN:HG3  | 20:R:160:LYS:HE3  | 2.03                     | 0.40              |
| 21:S:316:LEU:HD23 | 21:S:320:ILE:HG12 | 2.03                     | 0.40              |
| 22:V:274:GLN:HB3  | 22:V:279:HIS:CD2  | 2.56                     | 0.40              |
| 7:a:51:ASN:HB3    | 7:a:234:ASP:OD1   | 2.21                     | 0.40              |
| 7:a:122:PRO:HB2   | 7:a:159:PHE:CD2   | 2.56                     | 0.40              |
| 4:g:9:VAL:HG23    | 4:g:12:SER:H      | 1.86                     | 0.40              |
| 4:g:95:ARG:NH1    | 4:g:96:ARG:HB2    | 2.36                     | 0.40              |
| 4:g:113:LYS:HB3   | 4:g:113:LYS:HE3   | 1.91                     | 0.40              |
| 2:i:79:ALA:O      | 2:i:82:GLU:HG3    | 2.22                     | 0.40              |
| 26:H:224:VAL:HG22 | 26:H:243:PRO:HG2  | 2.03                     | 0.40              |
| 30:N:193:ALA:HA   | 30:N:197:VAL:HG23 | 2.03                     | 0.40              |
| 30:N:302:PHE:HE2  | 30:N:712:ASN:HB3  | 1.85                     | 0.40              |
| 30:N:350:LYS:HD3  | 30:N:350:LYS:HA   | 1.91                     | 0.40              |
| 30:N:547:LEU:HD23 | 30:N:547:LEU:HA   | 1.88                     | 0.40              |
| 32:o:452:LEU:HD21 | 32:o:489:ALA:HB2  | 2.02                     | 0.40              |
| 1:1:93:SER:OG     | 1:1:95:GLU:OE2    | 2.26                     | 0.40              |
| 1:1:133:PRO:HD2   | 1:1:137:SER:O     | 2.20                     | 0.40              |
| 4:4:7:ILE:HG23    | 4:4:14:ILE:HB     | 2.04                     | 0.40              |
| 5:5:156:LYS:NZ    | 11:D:98:LEU:O     | 2.54                     | 0.40              |
| 7:7:100:LEU:O     | 7:7:104:VAL:HG23  | 2.21                     | 0.40              |
| 8:A:174:LYS:HD3   | 8:A:214:LEU:HD22  | 2.04                     | 0.40              |
| 8:A:199:TRP:HZ3   | 8:A:236:LEU:HD11  | 1.85                     | 0.40              |
| 11:D:61:PRO:O     | 11:D:63:LYS:NZ    | 2.43                     | 0.40              |
| 12:E:78:MET:HB2   | 12:E:78:MET:HE2   | 1.86                     | 0.40              |
| 12:E:164:PHE:C    | 12:E:165:TYR:HD1  | 2.29                     | 0.40              |
| 13:F:66:CYS:HA    | 13:F:89:ARG:HE    | 1.86                     | 0.40              |
| 15:I:361:ILE:HA   | 15:I:364:ILE:HG22 | 2.04                     | 0.40              |
| 15:I:380:LEU:HD21 | 15:I:416:PHE:HD2  | 1.86                     | 0.40              |
| 17:L:238:THR:CG2  | 17:L:239:ILE:N    | 2.84                     | 0.40              |
| 17:L:364:HIS:CE1  | 17:L:392:ARG:HB2  | 2.56                     | 0.40              |
| 20:R:53:LYS:HE2   | 20:R:53:LYS:HB2   | 1.94                     | 0.40              |
| 21:S:402:ILE:HG21 | 21:S:407:ILE:HD11 | 2.04                     | 0.40              |
| 21:S:411:LEU:HD23 | 21:S:411:LEU:HA   | 1.88                     | 0.40              |
| 24:Y:65:ASP:CG    | 24:Y:66:ASP:H     | 2.29                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:Y:66:ASP:OD1   | 24:Y:66:ASP:N     | 2.54                     | 0.40              |
| 7:a:219:TYR:CZ    | 7:a:250:MET:HE2   | 2.57                     | 0.40              |
| 5:f:188:TYR:CE1   | 5:f:198:LYS:HD3   | 2.56                     | 0.40              |
| 26:H:98:GLN:N     | 26:H:176:VAL:O    | 2.54                     | 0.40              |
| 27:M:167:VAL:O    | 27:M:170:MET:HG2  | 2.21                     | 0.40              |
| 30:N:42:GLU:OE1   | 30:N:42:GLU:N     | 2.52                     | 0.40              |
| 30:N:233:ASN:HD21 | 30:N:266:SER:HB3  | 1.87                     | 0.40              |
| 30:N:270:LEU:HD23 | 30:N:270:LEU:HA   | 1.80                     | 0.40              |
| 30:N:816:LYS:HB2  | 30:N:816:LYS:HE3  | 1.90                     | 0.40              |
| 31:T:100:ASP:OD1  | 31:T:101:LYS:HG3  | 2.21                     | 0.40              |
| 32:o:232:LYS:HD3  | 32:o:235:GLN:NE2  | 2.36                     | 0.40              |
| 1:1:134:LEU:HD23  | 1:1:134:LEU:HA    | 1.91                     | 0.40              |
| 2:2:54:ILE:HD11   | 3:3:147:PHE:CD2   | 2.55                     | 0.40              |
| 14:G:157:TYR:CD1  | 14:G:157:TYR:C    | 2.99                     | 0.40              |
| 16:K:334:LEU:H    | 16:K:334:LEU:HD12 | 1.86                     | 0.40              |
| 17:L:88:TYR:OH    | 27:M:58:MET:O     | 2.38                     | 0.40              |
| 18:O:337:LEU:HD22 | 18:O:350:ILE:HD12 | 2.02                     | 0.40              |
| 20:R:338:TYR:HB3  | 20:R:377:LEU:HD21 | 2.03                     | 0.40              |
| 21:S:47:THR:HG21  | 21:S:52:TYR:CE1   | 2.57                     | 0.40              |
| 21:S:482:PRO:HB2  | 29:U:294:ASN:OD1  | 2.21                     | 0.40              |
| 23:W:185:ILE:O    | 23:W:189:PRO:HD2  | 2.22                     | 0.40              |
| 4:g:162:LYS:HD2   | 4:g:198:GLN:CD    | 2.46                     | 0.40              |
| 3:h:161:GLU:O     | 2:i:236:ARG:NH2   | 2.54                     | 0.40              |
| 25:J:186:ILE:HG12 | 25:J:310:ILE:HG12 | 2.04                     | 0.40              |
| 26:H:333:MET:SD   | 26:H:334:LEU:HD23 | 2.61                     | 0.40              |
| 28:Q:350:ILE:O    | 28:Q:353:PRO:HD2  | 2.22                     | 0.40              |
| 30:N:6:ALA:O      | 30:N:10:LEU:HB2   | 2.21                     | 0.40              |
| 30:N:310:ASP:HA   | 30:N:787:MET:HE1  | 2.02                     | 0.40              |
| 30:N:882:ILE:HD13 | 30:N:882:ILE:HA   | 1.88                     | 0.40              |
| 30:N:886:LYS:H    | 30:N:886:LYS:HG2  | 1.57                     | 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   | 1     | 203/215 (94%) | 195 (96%) | 8 (4%)   | 0        | 100         | 100 |
| 1   | b     | 203/215 (94%) | 197 (97%) | 6 (3%)   | 0        | 100         | 100 |
| 2   | 2     | 220/261 (84%) | 217 (99%) | 3 (1%)   | 0        | 100         | 100 |
| 2   | i     | 220/261 (84%) | 217 (99%) | 3 (1%)   | 0        | 100         | 100 |
| 3   | 3     | 202/205 (98%) | 192 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 3   | h     | 202/205 (98%) | 196 (97%) | 6 (3%)   | 0        | 100         | 100 |
| 4   | 4     | 196/198 (99%) | 191 (97%) | 5 (3%)   | 0        | 100         | 100 |
| 4   | g     | 196/198 (99%) | 192 (98%) | 4 (2%)   | 0        | 100         | 100 |
| 5   | 5     | 210/287 (73%) | 207 (99%) | 3 (1%)   | 0        | 100         | 100 |
| 5   | f     | 210/287 (73%) | 206 (98%) | 4 (2%)   | 0        | 100         | 100 |
| 6   | 6     | 220/241 (91%) | 214 (97%) | 5 (2%)   | 1 (0%)   | 24          | 55  |
| 6   | e     | 220/241 (91%) | 217 (99%) | 3 (1%)   | 0        | 100         | 100 |
| 7   | 7     | 231/266 (87%) | 223 (96%) | 8 (4%)   | 0        | 100         | 100 |
| 7   | a     | 231/266 (87%) | 224 (97%) | 7 (3%)   | 0        | 100         | 100 |
| 8   | A     | 241/252 (96%) | 236 (98%) | 5 (2%)   | 0        | 100         | 100 |
| 9   | B     | 248/250 (99%) | 242 (98%) | 6 (2%)   | 0        | 100         | 100 |
| 10  | C     | 242/258 (94%) | 234 (97%) | 7 (3%)   | 1 (0%)   | 30          | 59  |
| 11  | D     | 239/254 (94%) | 231 (97%) | 8 (3%)   | 0        | 100         | 100 |
| 12  | E     | 240/260 (92%) | 232 (97%) | 8 (3%)   | 0        | 100         | 100 |
| 13  | F     | 231/234 (99%) | 223 (96%) | 8 (4%)   | 0        | 100         | 100 |
| 14  | G     | 241/288 (84%) | 233 (97%) | 8 (3%)   | 0        | 100         | 100 |
| 15  | I     | 390/437 (89%) | 345 (88%) | 43 (11%) | 2 (0%)   | 24          | 55  |
| 16  | K     | 381/428 (89%) | 336 (88%) | 43 (11%) | 2 (0%)   | 24          | 55  |
| 17  | L     | 357/437 (82%) | 320 (90%) | 36 (10%) | 1 (0%)   | 36          | 64  |
| 18  | O     | 384/393 (98%) | 356 (93%) | 25 (6%)  | 3 (1%)   | 16          | 46  |
| 19  | P     | 434/445 (98%) | 415 (96%) | 18 (4%)  | 1 (0%)   | 43          | 71  |
| 20  | R     | 393/429 (92%) | 373 (95%) | 19 (5%)  | 1 (0%)   | 36          | 64  |
| 21  | S     | 459/523 (88%) | 430 (94%) | 28 (6%)  | 1 (0%)   | 43          | 71  |
| 22  | V     | 286/306 (94%) | 265 (93%) | 20 (7%)  | 1 (0%)   | 36          | 64  |
| 23  | W     | 188/268 (70%) | 172 (92%) | 16 (8%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 24  | Y     | 29/89 (33%)       | 26 (90%)    | 2 (7%)   | 1 (3%)   | 3           | 21  |
| 25  | J     | 364/405 (90%)     | 345 (95%)   | 19 (5%)  | 0        | 100         | 100 |
| 26  | H     | 379/467 (81%)     | 333 (88%)   | 46 (12%) | 0        | 100         | 100 |
| 27  | M     | 359/434 (83%)     | 330 (92%)   | 28 (8%)  | 1 (0%)   | 36          | 64  |
| 28  | Q     | 407/434 (94%)     | 385 (95%)   | 22 (5%)  | 0        | 100         | 100 |
| 29  | U     | 288/338 (85%)     | 270 (94%)   | 17 (6%)  | 1 (0%)   | 36          | 64  |
| 30  | N     | 863/945 (91%)     | 816 (95%)   | 47 (5%)  | 0        | 100         | 100 |
| 31  | T     | 253/274 (92%)     | 237 (94%)   | 15 (6%)  | 1 (0%)   | 30          | 59  |
| 32  | o     | 811/993 (82%)     | 756 (93%)   | 55 (7%)  | 0        | 100         | 100 |
| All | All   | 11671/13187 (88%) | 11029 (94%) | 624 (5%) | 18 (0%)  | 44          | 71  |

All (18) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | K     | 143 | SER  |
| 18  | O     | 205 | ILE  |
| 22  | V     | 161 | THR  |
| 15  | I     | 178 | THR  |
| 17  | L     | 175 | GLN  |
| 18  | O     | 166 | ARG  |
| 24  | Y     | 74  | THR  |
| 6   | 6     | 51  | ASP  |
| 19  | P     | 108 | LYS  |
| 16  | K     | 419 | ASN  |
| 18  | O     | 305 | ILE  |
| 15  | I     | 386 | ASP  |
| 20  | R     | 70  | TYR  |
| 29  | U     | 183 | ALA  |
| 27  | M     | 430 | VAL  |
| 31  | T     | 259 | ILE  |
| 10  | C     | 52  | VAL  |
| 21  | S     | 432 | ILE  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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   | 1     | 169/178 (95%)  | 162 (96%)  | 7 (4%)   | 27          | 50  |
| 1   | b     | 169/178 (95%)  | 168 (99%)  | 1 (1%)   | 78          | 77  |
| 2   | 2     | 181/214 (85%)  | 177 (98%)  | 4 (2%)   | 45          | 62  |
| 2   | i     | 181/214 (85%)  | 178 (98%)  | 3 (2%)   | 53          | 65  |
| 3   | 3     | 172/173 (99%)  | 167 (97%)  | 5 (3%)   | 37          | 56  |
| 3   | h     | 172/173 (99%)  | 170 (99%)  | 2 (1%)   | 63          | 70  |
| 4   | 4     | 175/175 (100%) | 172 (98%)  | 3 (2%)   | 53          | 65  |
| 4   | g     | 175/175 (100%) | 172 (98%)  | 3 (2%)   | 53          | 65  |
| 5   | 5     | 169/235 (72%)  | 164 (97%)  | 5 (3%)   | 36          | 56  |
| 5   | f     | 169/235 (72%)  | 164 (97%)  | 5 (3%)   | 36          | 56  |
| 6   | 6     | 185/201 (92%)  | 185 (100%) | 0        | 100         | 100 |
| 6   | e     | 185/201 (92%)  | 183 (99%)  | 2 (1%)   | 65          | 71  |
| 7   | 7     | 199/224 (89%)  | 196 (98%)  | 3 (2%)   | 57          | 66  |
| 7   | a     | 199/224 (89%)  | 193 (97%)  | 6 (3%)   | 36          | 56  |
| 8   | A     | 207/210 (99%)  | 200 (97%)  | 7 (3%)   | 32          | 53  |
| 9   | B     | 209/209 (100%) | 204 (98%)  | 5 (2%)   | 43          | 60  |
| 10  | C     | 203/216 (94%)  | 195 (96%)  | 8 (4%)   | 28          | 51  |
| 11  | D     | 213/226 (94%)  | 205 (96%)  | 8 (4%)   | 29          | 51  |
| 12  | E     | 198/215 (92%)  | 189 (96%)  | 9 (4%)   | 24          | 48  |
| 13  | F     | 192/193 (100%) | 184 (96%)  | 8 (4%)   | 26          | 49  |
| 14  | G     | 200/239 (84%)  | 191 (96%)  | 9 (4%)   | 24          | 48  |
| 15  | I     | 349/385 (91%)  | 333 (95%)  | 16 (5%)  | 24          | 47  |
| 16  | K     | 336/374 (90%)  | 319 (95%)  | 17 (5%)  | 21          | 46  |
| 17  | L     | 305/377 (81%)  | 296 (97%)  | 9 (3%)   | 36          | 56  |
| 18  | O     | 361/368 (98%)  | 348 (96%)  | 13 (4%)  | 31          | 53  |
| 19  | P     | 408/415 (98%)  | 399 (98%)  | 9 (2%)   | 45          | 62  |
| 20  | R     | 349/379 (92%)  | 332 (95%)  | 17 (5%)  | 22          | 47  |
| 21  | S     | 433/489 (88%)  | 414 (96%)  | 19 (4%)  | 25          | 49  |
| 22  | V     | 252/268 (94%)  | 237 (94%)  | 15 (6%)  | 17          | 42  |
| 23  | W     | 165/230 (72%)  | 161 (98%)  | 4 (2%)   | 43          | 60  |

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| Mol | Chain | Analysed          | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-------------------|------------|----------|-------------|-----|
| 24  | Y     | 31/82 (38%)       | 31 (100%)  | 0        | 100         | 100 |
| 25  | J     | 322/352 (92%)     | 310 (96%)  | 12 (4%)  | 30          | 52  |
| 26  | H     | 326/399 (82%)     | 318 (98%)  | 8 (2%)   | 42          | 59  |
| 27  | M     | 311/375 (83%)     | 294 (94%)  | 17 (6%)  | 19          | 44  |
| 28  | Q     | 374/391 (96%)     | 363 (97%)  | 11 (3%)  | 37          | 56  |
| 29  | U     | 265/308 (86%)     | 255 (96%)  | 10 (4%)  | 29          | 51  |
| 30  | N     | 729/797 (92%)     | 701 (96%)  | 28 (4%)  | 29          | 51  |
| 31  | T     | 240/256 (94%)     | 237 (99%)  | 3 (1%)   | 61          | 69  |
| 32  | o     | 697/850 (82%)     | 677 (97%)  | 20 (3%)  | 37          | 56  |
| All | All   | 10175/11403 (89%) | 9844 (97%) | 331 (3%) | 34          | 54  |

All (331) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 50  | THR  |
| 1   | 1     | 62  | CYS  |
| 1   | 1     | 82  | LEU  |
| 1   | 1     | 104 | LEU  |
| 1   | 1     | 153 | ILE  |
| 1   | 1     | 165 | MET  |
| 1   | 1     | 191 | VAL  |
| 2   | 2     | 59  | ASN  |
| 2   | 2     | 112 | LEU  |
| 2   | 2     | 149 | ASP  |
| 2   | 2     | 249 | ILE  |
| 3   | 3     | 16  | THR  |
| 3   | 3     | 23  | ILE  |
| 3   | 3     | 25  | CYS  |
| 3   | 3     | 64  | ASN  |
| 3   | 3     | 82  | ILE  |
| 4   | 4     | 5   | LEU  |
| 4   | 4     | 102 | VAL  |
| 4   | 4     | 146 | HIS  |
| 5   | 5     | 78  | THR  |
| 5   | 5     | 117 | LEU  |
| 5   | 5     | 134 | LEU  |
| 5   | 5     | 172 | MET  |
| 5   | 5     | 215 | LEU  |
| 7   | 7     | 100 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | 7     | 133 | MET  |
| 7   | 7     | 149 | VAL  |
| 8   | A     | 20  | SER  |
| 8   | A     | 42  | SER  |
| 8   | A     | 69  | VAL  |
| 8   | A     | 89  | ASP  |
| 8   | A     | 114 | CYS  |
| 8   | A     | 157 | THR  |
| 8   | A     | 222 | ASP  |
| 9   | B     | 21  | ILE  |
| 9   | B     | 41  | ASN  |
| 9   | B     | 113 | GLU  |
| 9   | B     | 177 | LYS  |
| 9   | B     | 193 | LEU  |
| 10  | C     | 3   | SER  |
| 10  | C     | 12  | ILE  |
| 10  | C     | 45  | VAL  |
| 10  | C     | 111 | LEU  |
| 10  | C     | 115 | LEU  |
| 10  | C     | 169 | THR  |
| 10  | C     | 197 | LEU  |
| 10  | C     | 226 | TYR  |
| 11  | D     | 8   | LEU  |
| 11  | D     | 71  | VAL  |
| 11  | D     | 72  | VAL  |
| 11  | D     | 81  | ASP  |
| 11  | D     | 98  | LEU  |
| 11  | D     | 126 | VAL  |
| 11  | D     | 131 | VAL  |
| 11  | D     | 151 | GLU  |
| 12  | E     | 21  | LEU  |
| 12  | E     | 28  | LEU  |
| 12  | E     | 64  | ILE  |
| 12  | E     | 78  | MET  |
| 12  | E     | 88  | MET  |
| 12  | E     | 121 | LEU  |
| 12  | E     | 122 | ARG  |
| 12  | E     | 192 | THR  |
| 12  | E     | 226 | ASP  |
| 13  | F     | 2   | PHE  |
| 13  | F     | 9   | ASP  |
| 13  | F     | 21  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | F     | 34  | VAL  |
| 13  | F     | 56  | LEU  |
| 13  | F     | 112 | LEU  |
| 13  | F     | 166 | GLN  |
| 13  | F     | 187 | ASP  |
| 14  | G     | 6   | THR  |
| 14  | G     | 36  | THR  |
| 14  | G     | 53  | LEU  |
| 14  | G     | 68  | GLN  |
| 14  | G     | 78  | TYR  |
| 14  | G     | 134 | VAL  |
| 14  | G     | 143 | LYS  |
| 14  | G     | 181 | ASP  |
| 14  | G     | 200 | ILE  |
| 15  | I     | 55  | CYS  |
| 15  | I     | 111 | GLU  |
| 15  | I     | 121 | THR  |
| 15  | I     | 132 | ILE  |
| 15  | I     | 170 | VAL  |
| 15  | I     | 194 | ILE  |
| 15  | I     | 214 | LYS  |
| 15  | I     | 227 | THR  |
| 15  | I     | 321 | ASP  |
| 15  | I     | 328 | THR  |
| 15  | I     | 329 | ASN  |
| 15  | I     | 333 | THR  |
| 15  | I     | 344 | ILE  |
| 15  | I     | 345 | ASP  |
| 15  | I     | 365 | HIS  |
| 15  | I     | 391 | ASP  |
| 16  | K     | 49  | PHE  |
| 16  | K     | 60  | LEU  |
| 16  | K     | 63  | LEU  |
| 16  | K     | 75  | LEU  |
| 16  | K     | 86  | VAL  |
| 16  | K     | 96  | ILE  |
| 16  | K     | 159 | SER  |
| 16  | K     | 168 | ASP  |
| 16  | K     | 197 | LEU  |
| 16  | K     | 217 | THR  |
| 16  | K     | 221 | MET  |
| 16  | K     | 253 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | K     | 289 | ASP  |
| 16  | K     | 318 | THR  |
| 16  | K     | 374 | ARG  |
| 16  | K     | 408 | GLU  |
| 16  | K     | 428 | LYS  |
| 17  | L     | 123 | SER  |
| 17  | L     | 141 | LYS  |
| 17  | L     | 152 | THR  |
| 17  | L     | 190 | ILE  |
| 17  | L     | 276 | CYS  |
| 17  | L     | 284 | ASP  |
| 17  | L     | 332 | THR  |
| 17  | L     | 382 | MET  |
| 17  | L     | 425 | VAL  |
| 18  | O     | 38  | TRP  |
| 18  | O     | 41  | LEU  |
| 18  | O     | 55  | THR  |
| 18  | O     | 70  | TYR  |
| 18  | O     | 82  | LEU  |
| 18  | O     | 98  | TYR  |
| 18  | O     | 153 | LEU  |
| 18  | O     | 198 | THR  |
| 18  | O     | 206 | THR  |
| 18  | O     | 263 | PHE  |
| 18  | O     | 322 | ASP  |
| 18  | O     | 347 | LEU  |
| 18  | O     | 393 | VAL  |
| 19  | P     | 21  | PHE  |
| 19  | P     | 167 | THR  |
| 19  | P     | 178 | GLN  |
| 19  | P     | 247 | THR  |
| 19  | P     | 261 | LEU  |
| 19  | P     | 269 | VAL  |
| 19  | P     | 305 | THR  |
| 19  | P     | 419 | VAL  |
| 19  | P     | 434 | THR  |
| 20  | R     | 203 | ASP  |
| 20  | R     | 218 | CYS  |
| 20  | R     | 233 | ASP  |
| 20  | R     | 237 | THR  |
| 20  | R     | 239 | THR  |
| 20  | R     | 265 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | R     | 286 | LEU  |
| 20  | R     | 317 | ILE  |
| 20  | R     | 324 | ARG  |
| 20  | R     | 327 | ASP  |
| 20  | R     | 337 | VAL  |
| 20  | R     | 340 | GLN  |
| 20  | R     | 353 | MET  |
| 20  | R     | 368 | LEU  |
| 20  | R     | 385 | ASN  |
| 20  | R     | 395 | ASN  |
| 20  | R     | 406 | GLN  |
| 21  | S     | 39  | ASN  |
| 21  | S     | 41  | ILE  |
| 21  | S     | 73  | THR  |
| 21  | S     | 131 | THR  |
| 21  | S     | 159 | ASN  |
| 21  | S     | 204 | ASP  |
| 21  | S     | 234 | ILE  |
| 21  | S     | 269 | GLU  |
| 21  | S     | 288 | THR  |
| 21  | S     | 297 | ILE  |
| 21  | S     | 303 | ASN  |
| 21  | S     | 322 | LEU  |
| 21  | S     | 324 | MET  |
| 21  | S     | 332 | PHE  |
| 21  | S     | 337 | ASN  |
| 21  | S     | 386 | ASN  |
| 21  | S     | 408 | CYS  |
| 21  | S     | 446 | THR  |
| 21  | S     | 471 | LEU  |
| 22  | V     | 22  | ASP  |
| 22  | V     | 25  | GLU  |
| 22  | V     | 53  | MET  |
| 22  | V     | 83  | VAL  |
| 22  | V     | 103 | MET  |
| 22  | V     | 104 | VAL  |
| 22  | V     | 114 | PHE  |
| 22  | V     | 153 | ILE  |
| 22  | V     | 161 | THR  |
| 22  | V     | 185 | ILE  |
| 22  | V     | 204 | HIS  |
| 22  | V     | 249 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | V     | 266 | LEU  |
| 22  | V     | 281 | SER  |
| 22  | V     | 302 | SER  |
| 23  | W     | 34  | GLU  |
| 23  | W     | 72  | ILE  |
| 23  | W     | 79  | THR  |
| 23  | W     | 151 | THR  |
| 7   | a     | 100 | LEU  |
| 7   | a     | 133 | MET  |
| 7   | a     | 162 | TYR  |
| 7   | a     | 216 | VAL  |
| 7   | a     | 250 | MET  |
| 7   | a     | 253 | ASP  |
| 1   | b     | 165 | MET  |
| 6   | e     | 126 | VAL  |
| 6   | e     | 152 | ARG  |
| 5   | f     | 108 | LYS  |
| 5   | f     | 161 | LEU  |
| 5   | f     | 192 | SER  |
| 5   | f     | 204 | VAL  |
| 5   | f     | 245 | TYR  |
| 4   | g     | 25  | ILE  |
| 4   | g     | 41  | HIS  |
| 4   | g     | 161 | LEU  |
| 3   | h     | 88  | THR  |
| 3   | h     | 105 | VAL  |
| 2   | i     | 64  | HIS  |
| 2   | i     | 95  | HIS  |
| 2   | i     | 128 | ILE  |
| 25  | J     | 72  | VAL  |
| 25  | J     | 103 | ASN  |
| 25  | J     | 107 | LEU  |
| 25  | J     | 142 | VAL  |
| 25  | J     | 148 | ASP  |
| 25  | J     | 160 | ILE  |
| 25  | J     | 165 | GLU  |
| 25  | J     | 193 | THR  |
| 25  | J     | 235 | VAL  |
| 25  | J     | 248 | ASP  |
| 25  | J     | 311 | ASP  |
| 25  | J     | 328 | LEU  |
| 26  | H     | 83  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | H     | 99  | VAL  |
| 26  | H     | 198 | MET  |
| 26  | H     | 199 | THR  |
| 26  | H     | 200 | VAL  |
| 26  | H     | 216 | ASP  |
| 26  | H     | 356 | ASN  |
| 26  | H     | 414 | SER  |
| 27  | M     | 78  | LEU  |
| 27  | M     | 81  | ASN  |
| 27  | M     | 136 | ASP  |
| 27  | M     | 138 | ASP  |
| 27  | M     | 177 | THR  |
| 27  | M     | 179 | THR  |
| 27  | M     | 183 | VAL  |
| 27  | M     | 256 | ILE  |
| 27  | M     | 276 | THR  |
| 27  | M     | 284 | ASP  |
| 27  | M     | 306 | LEU  |
| 27  | M     | 331 | ASP  |
| 27  | M     | 343 | LEU  |
| 27  | M     | 383 | THR  |
| 27  | M     | 394 | VAL  |
| 27  | M     | 417 | GLU  |
| 27  | M     | 421 | GLU  |
| 28  | Q     | 59  | LEU  |
| 28  | Q     | 80  | HIS  |
| 28  | Q     | 94  | VAL  |
| 28  | Q     | 102 | GLU  |
| 28  | Q     | 158 | ILE  |
| 28  | Q     | 219 | ASP  |
| 28  | Q     | 240 | PHE  |
| 28  | Q     | 277 | ASP  |
| 28  | Q     | 280 | ASN  |
| 28  | Q     | 328 | ASP  |
| 28  | Q     | 404 | ASN  |
| 29  | U     | 5   | HIS  |
| 29  | U     | 66  | TRP  |
| 29  | U     | 76  | MET  |
| 29  | U     | 109 | LEU  |
| 29  | U     | 146 | ASP  |
| 29  | U     | 156 | HIS  |
| 29  | U     | 180 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | U     | 204 | LEU  |
| 29  | U     | 229 | LEU  |
| 29  | U     | 267 | VAL  |
| 30  | N     | 5   | THR  |
| 30  | N     | 10  | LEU  |
| 30  | N     | 36  | TRP  |
| 30  | N     | 101 | ILE  |
| 30  | N     | 123 | PHE  |
| 30  | N     | 164 | ASP  |
| 30  | N     | 260 | ASP  |
| 30  | N     | 343 | THR  |
| 30  | N     | 373 | VAL  |
| 30  | N     | 415 | PHE  |
| 30  | N     | 438 | ASP  |
| 30  | N     | 455 | MET  |
| 30  | N     | 572 | LEU  |
| 30  | N     | 593 | PHE  |
| 30  | N     | 660 | LEU  |
| 30  | N     | 668 | THR  |
| 30  | N     | 677 | ASP  |
| 30  | N     | 681 | ASN  |
| 30  | N     | 689 | LYS  |
| 30  | N     | 722 | THR  |
| 30  | N     | 724 | THR  |
| 30  | N     | 725 | LEU  |
| 30  | N     | 734 | VAL  |
| 30  | N     | 756 | THR  |
| 30  | N     | 858 | LYS  |
| 30  | N     | 891 | VAL  |
| 30  | N     | 903 | VAL  |
| 30  | N     | 919 | THR  |
| 31  | T     | 40  | LEU  |
| 31  | T     | 76  | ASP  |
| 31  | T     | 119 | THR  |
| 32  | o     | 68  | LEU  |
| 32  | o     | 108 | ASP  |
| 32  | o     | 146 | PHE  |
| 32  | o     | 225 | LEU  |
| 32  | o     | 279 | THR  |
| 32  | o     | 280 | ASP  |
| 32  | o     | 293 | MET  |
| 32  | o     | 342 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | o     | 398 | LYS  |
| 32  | o     | 430 | LEU  |
| 32  | o     | 431 | ASP  |
| 32  | o     | 467 | VAL  |
| 32  | o     | 510 | LEU  |
| 32  | o     | 551 | LEU  |
| 32  | o     | 752 | ILE  |
| 32  | o     | 797 | THR  |
| 32  | o     | 818 | CYS  |
| 32  | o     | 843 | ASP  |
| 32  | o     | 850 | LEU  |
| 32  | o     | 868 | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 88  | GLN  |
| 2   | 2     | 201 | ASN  |
| 2   | 2     | 229 | GLN  |
| 4   | 4     | 10  | GLN  |
| 4   | 4     | 65  | GLN  |
| 4   | 4     | 118 | GLN  |
| 4   | 4     | 133 | HIS  |
| 4   | 4     | 198 | GLN  |
| 5   | 5     | 99  | ASN  |
| 5   | 5     | 104 | GLN  |
| 5   | 5     | 254 | HIS  |
| 5   | 5     | 283 | ASN  |
| 6   | 6     | 214 | HIS  |
| 8   | A     | 15  | HIS  |
| 8   | A     | 181 | ASN  |
| 8   | A     | 240 | ASN  |
| 9   | B     | 20  | GLN  |
| 9   | B     | 149 | GLN  |
| 9   | B     | 244 | ASN  |
| 10  | C     | 96  | GLN  |
| 11  | D     | 118 | GLN  |
| 11  | D     | 167 | ASN  |
| 12  | E     | 114 | GLN  |
| 12  | E     | 147 | HIS  |
| 12  | E     | 157 | HIS  |
| 13  | F     | 60  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | F     | 86  | ASN  |
| 13  | F     | 100 | ASN  |
| 13  | F     | 166 | GLN  |
| 13  | F     | 210 | ASN  |
| 14  | G     | 68  | GLN  |
| 14  | G     | 183 | HIS  |
| 16  | K     | 64  | GLN  |
| 16  | K     | 200 | GLN  |
| 16  | K     | 319 | ASN  |
| 16  | K     | 414 | GLN  |
| 16  | K     | 419 | ASN  |
| 17  | L     | 273 | HIS  |
| 17  | L     | 302 | GLN  |
| 18  | O     | 122 | HIS  |
| 18  | O     | 175 | ASN  |
| 18  | O     | 304 | ASN  |
| 18  | O     | 343 | GLN  |
| 19  | P     | 178 | GLN  |
| 19  | P     | 183 | GLN  |
| 19  | P     | 230 | HIS  |
| 19  | P     | 246 | GLN  |
| 20  | R     | 19  | ASN  |
| 20  | R     | 114 | ASN  |
| 20  | R     | 132 | GLN  |
| 20  | R     | 136 | ASN  |
| 20  | R     | 184 | GLN  |
| 20  | R     | 406 | GLN  |
| 21  | S     | 32  | GLN  |
| 21  | S     | 39  | ASN  |
| 21  | S     | 70  | ASN  |
| 21  | S     | 191 | HIS  |
| 21  | S     | 205 | ASN  |
| 21  | S     | 227 | ASN  |
| 21  | S     | 450 | ASN  |
| 22  | V     | 97  | GLN  |
| 22  | V     | 111 | HIS  |
| 22  | V     | 172 | GLN  |
| 22  | V     | 193 | ASN  |
| 22  | V     | 200 | ASN  |
| 22  | V     | 291 | ASN  |
| 23  | W     | 12  | ASN  |
| 23  | W     | 80  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | W     | 102 | GLN  |
| 23  | W     | 108 | GLN  |
| 7   | a     | 35  | GLN  |
| 7   | a     | 185 | ASN  |
| 7   | a     | 246 | GLN  |
| 1   | b     | 180 | GLN  |
| 4   | g     | 41  | HIS  |
| 4   | g     | 63  | ASN  |
| 4   | g     | 166 | GLN  |
| 3   | h     | 169 | GLN  |
| 2   | i     | 189 | GLN  |
| 25  | J     | 52  | ASN  |
| 25  | J     | 220 | GLN  |
| 25  | J     | 376 | HIS  |
| 26  | H     | 467 | ASN  |
| 27  | M     | 72  | ASN  |
| 27  | M     | 238 | GLN  |
| 27  | M     | 253 | GLN  |
| 28  | Q     | 19  | GLN  |
| 28  | Q     | 150 | GLN  |
| 28  | Q     | 418 | GLN  |
| 28  | Q     | 425 | GLN  |
| 29  | U     | 127 | GLN  |
| 29  | U     | 128 | GLN  |
| 29  | U     | 173 | HIS  |
| 29  | U     | 181 | GLN  |
| 29  | U     | 223 | HIS  |
| 29  | U     | 298 | ASN  |
| 30  | N     | 176 | GLN  |
| 30  | N     | 231 | ASN  |
| 30  | N     | 336 | ASN  |
| 30  | N     | 361 | ASN  |
| 30  | N     | 459 | ASN  |
| 30  | N     | 580 | ASN  |
| 30  | N     | 613 | HIS  |
| 31  | T     | 47  | GLN  |
| 31  | T     | 83  | ASN  |
| 31  | T     | 112 | ASN  |
| 31  | T     | 132 | HIS  |
| 32  | o     | 166 | ASN  |
| 32  | o     | 347 | ASN  |
| 32  | o     | 391 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | o     | 403 | ASN  |
| 32  | o     | 801 | HIS  |
| 32  | o     | 810 | ASN  |
| 32  | o     | 842 | GLN  |
| 32  | o     | 874 | ASN  |
| 32  | o     | 926 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 34  | ATP  | L     | 501 | 33   | 32,33,33     | 0.42 | 0           | 48,52,52    | 0.35 | 0           |
| 36  | ADP  | J     | 502 | -    | 28,29,29     | 1.41 | 4 (14%)     | 43,45,45    | 1.89 | 8 (18%)     |
| 34  | ATP  | M     | 501 | 33   | 32,33,33     | 0.35 | 0           | 48,52,52    | 0.37 | 0           |
| 34  | ATP  | K     | 501 | 33   | 32,33,33     | 0.39 | 0           | 48,52,52    | 0.40 | 0           |
| 34  | ATP  | J     | 501 | 33   | 32,33,33     | 0.33 | 0           | 48,52,52    | 0.38 | 0           |
| 34  | ATP  | H     | 501 | 33   | 32,33,33     | 0.33 | 0           | 48,52,52    | 0.37 | 0           |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 34  | ATP  | L     | 501 | 33   | -       | 3/22/38/38 | 0/3/3/3 |
| 36  | ADP  | J     | 502 | -    | -       | 2/16/32/32 | 0/3/3/3 |
| 34  | ATP  | M     | 501 | 33   | -       | 3/22/38/38 | 0/3/3/3 |
| 34  | ATP  | K     | 501 | 33   | -       | 1/22/38/38 | 0/3/3/3 |
| 34  | ATP  | J     | 501 | 33   | -       | 4/22/38/38 | 0/3/3/3 |
| 34  | ATP  | H     | 501 | 33   | -       | 4/22/38/38 | 0/3/3/3 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 36  | J     | 502 | ADP  | C5-C4 | 4.76  | 1.47        | 1.39     |
| 36  | J     | 502 | ADP  | C5-C6 | 2.66  | 1.48        | 1.41     |
| 36  | J     | 502 | ADP  | C5-N7 | -2.42 | 1.34        | 1.39     |
| 36  | J     | 502 | ADP  | C8-N7 | 2.22  | 1.35        | 1.31     |

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 36  | J     | 502 | ADP  | C5-C4-N3    | -6.25 | 118.11      | 126.72   |
| 36  | J     | 502 | ADP  | N3-C4-N9    | 5.05  | 135.75      | 127.17   |
| 36  | J     | 502 | ADP  | C2-N3-C4    | 3.79  | 121.09      | 111.83   |
| 36  | J     | 502 | ADP  | C4-C5-N7    | -3.23 | 106.89      | 110.58   |
| 36  | J     | 502 | ADP  | N3-C2-N1    | -3.15 | 123.82      | 128.58   |
| 36  | J     | 502 | ADP  | C3'-C2'-C1' | 2.83  | 106.82      | 101.46   |
| 36  | J     | 502 | ADP  | C5-N7-C8    | 2.38  | 107.19      | 103.45   |
| 36  | J     | 502 | ADP  | C4-N9-C8    | 2.33  | 108.19      | 105.74   |

There are no chirality outliers.

All (17) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | L     | 501 | ATP  | C5'-O5'-PA-O2A  |
| 34  | L     | 501 | ATP  | C5'-O5'-PA-O3A  |
| 34  | J     | 501 | ATP  | C5'-O5'-PA-O2A  |
| 34  | J     | 501 | ATP  | C5'-O5'-PA-O3A  |
| 34  | H     | 501 | ATP  | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 34  | H     | 501 | ATP  | C3'-C4'-C5'-O5' |
| 36  | J     | 502 | ADP  | C5'-O5'-PA-O3A  |
| 34  | L     | 501 | ATP  | C4'-C5'-O5'-PA  |
| 34  | H     | 501 | ATP  | C4'-C5'-O5'-PA  |
| 34  | M     | 501 | ATP  | C3'-C4'-C5'-O5' |
| 34  | M     | 501 | ATP  | O4'-C4'-C5'-O5' |
| 36  | J     | 502 | ADP  | C5'-O5'-PA-O1A  |
| 34  | K     | 501 | ATP  | C4'-C5'-O5'-PA  |
| 34  | J     | 501 | ATP  | C4'-C5'-O5'-PA  |
| 34  | H     | 501 | ATP  | PB-O3A-PA-O5'   |
| 34  | M     | 501 | ATP  | PB-O3B-PG-O1G   |
| 34  | J     | 501 | ATP  | O4'-C4'-C5'-O5' |

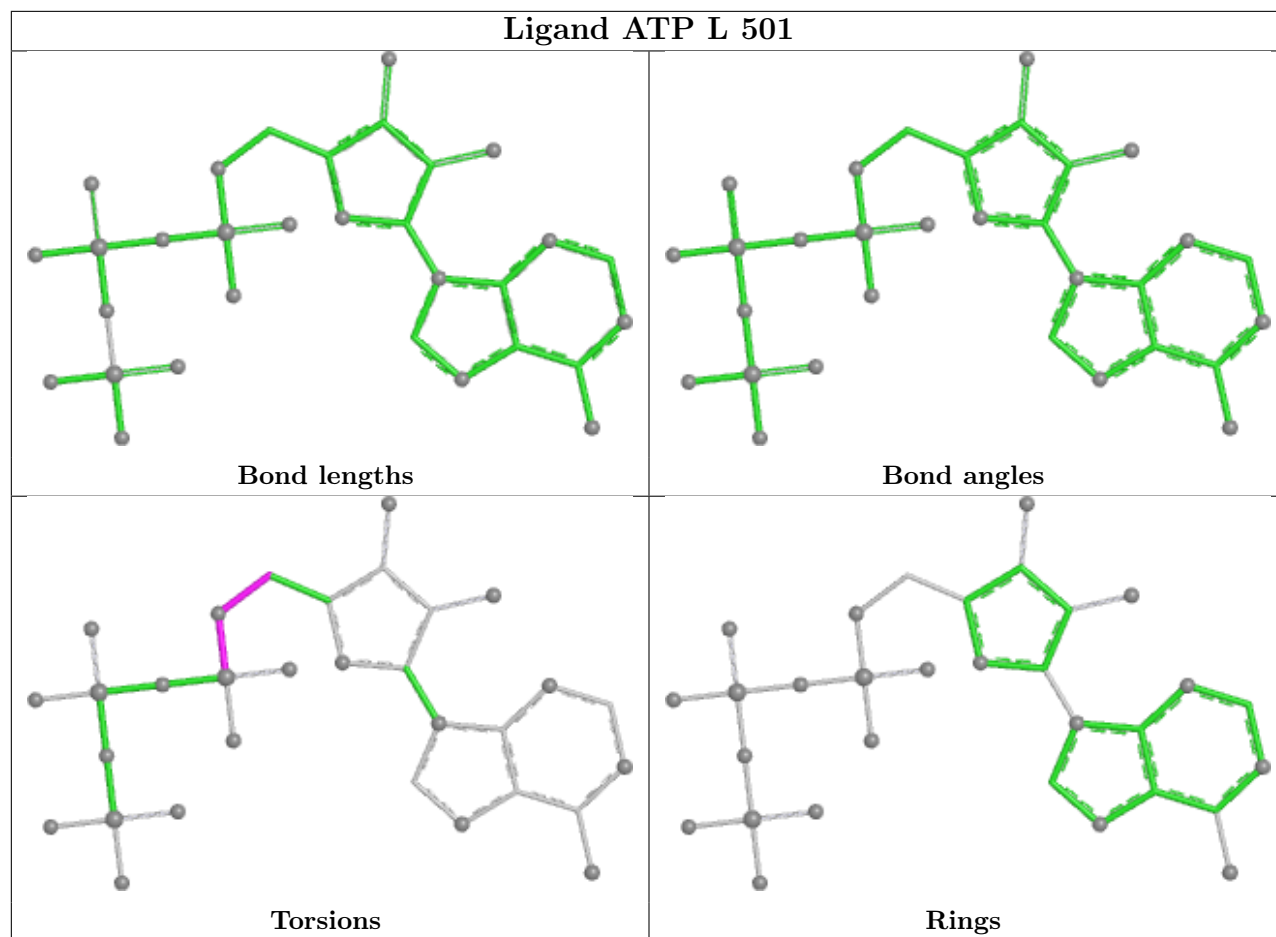
There are no ring outliers.

5 monomers are involved in 20 short contacts:

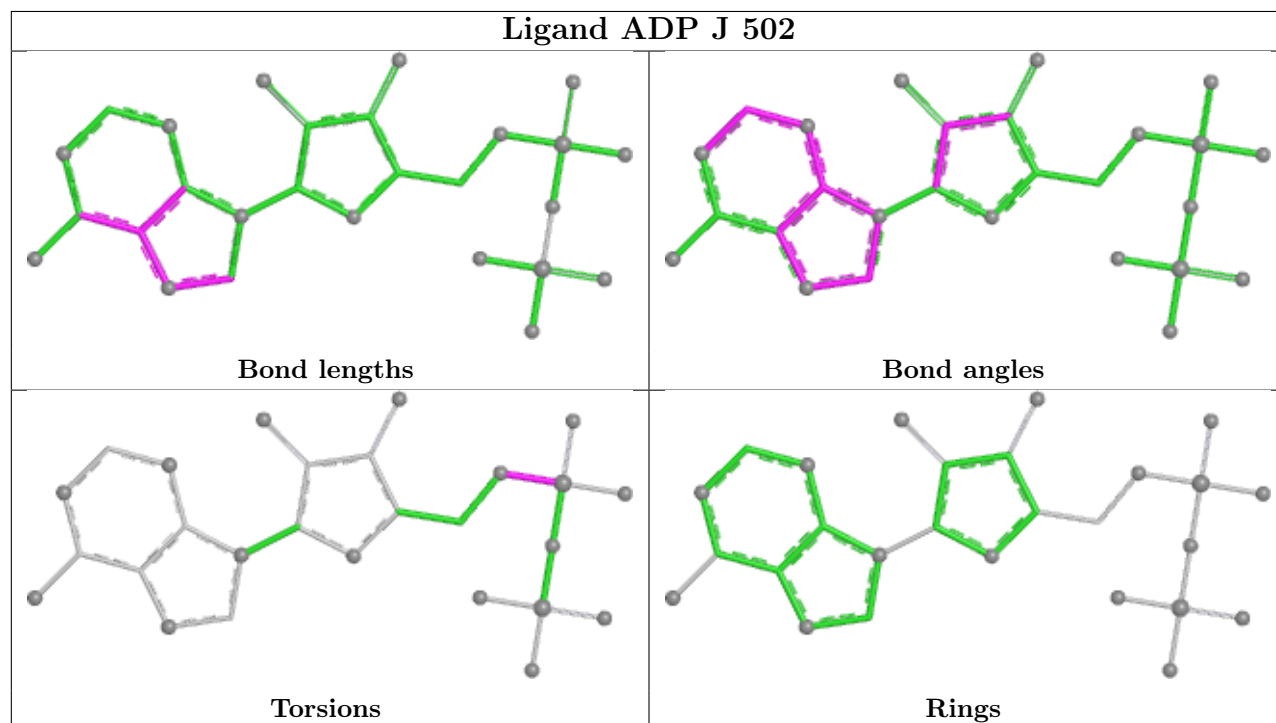
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 36  | J     | 502 | ADP  | 4       | 0            |
| 34  | M     | 501 | ATP  | 4       | 0            |
| 34  | K     | 501 | ATP  | 6       | 0            |
| 34  | J     | 501 | ATP  | 3       | 0            |
| 34  | H     | 501 | ATP  | 3       | 0            |

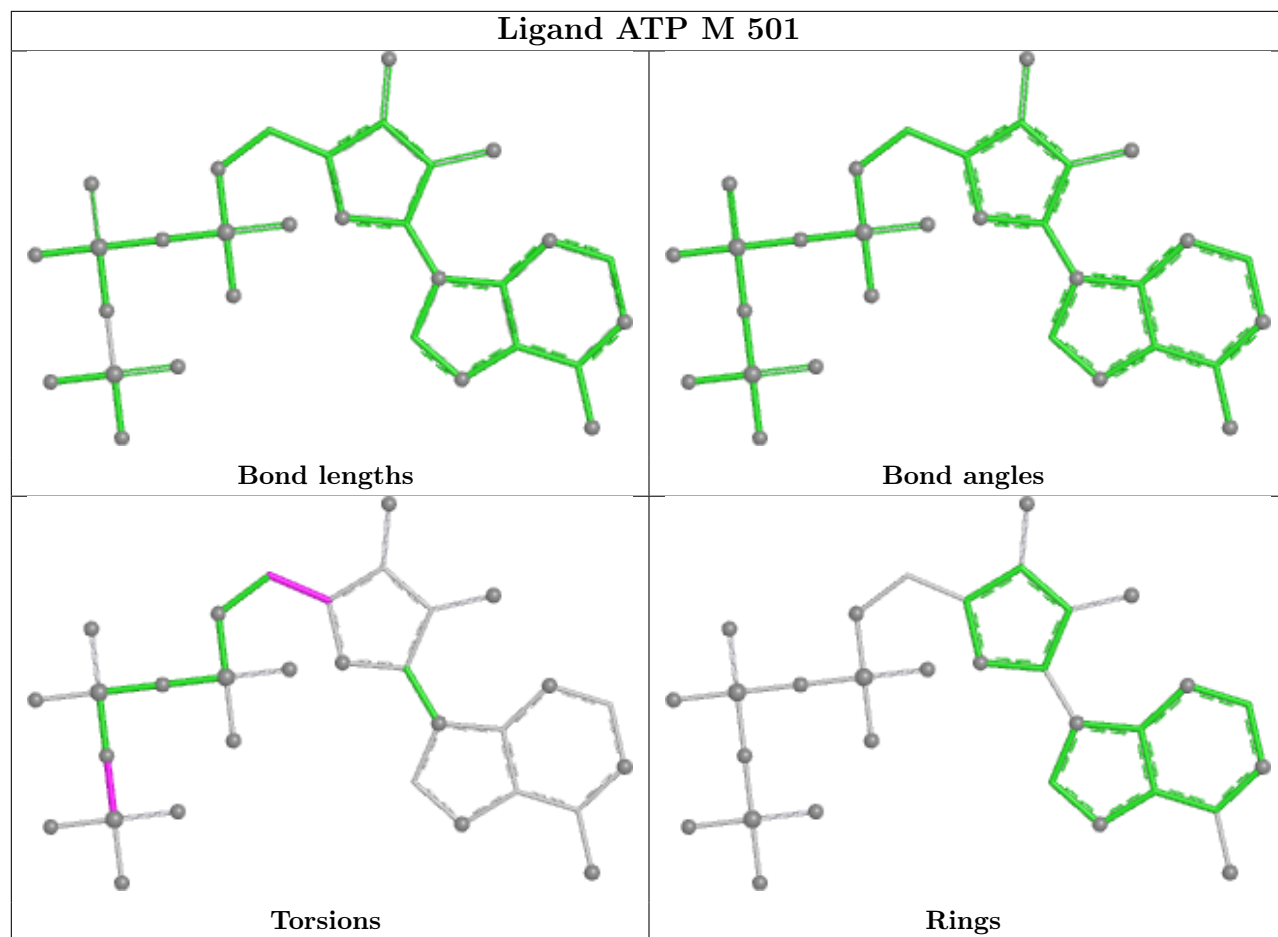
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

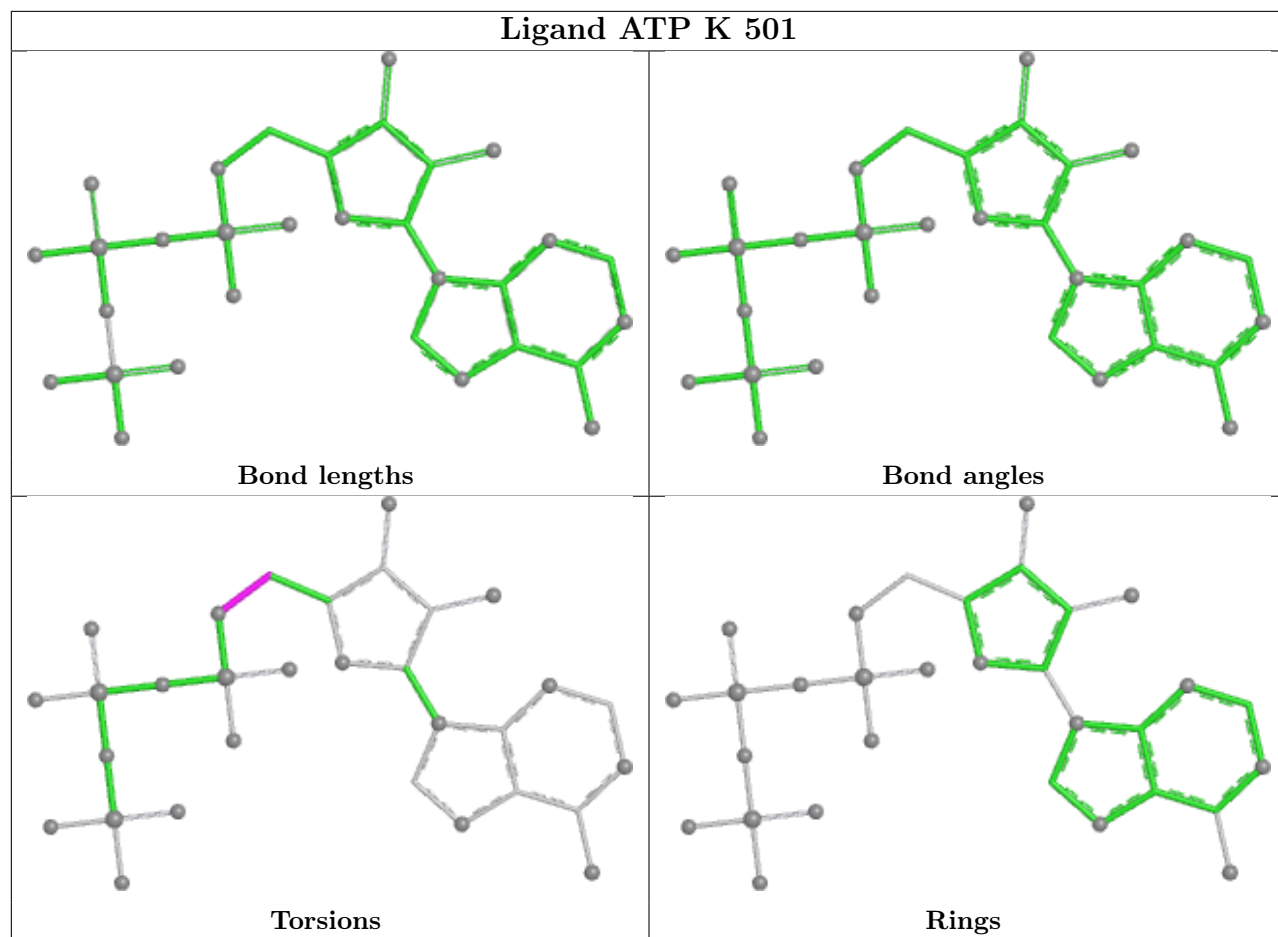
## Ligand ATP L 501



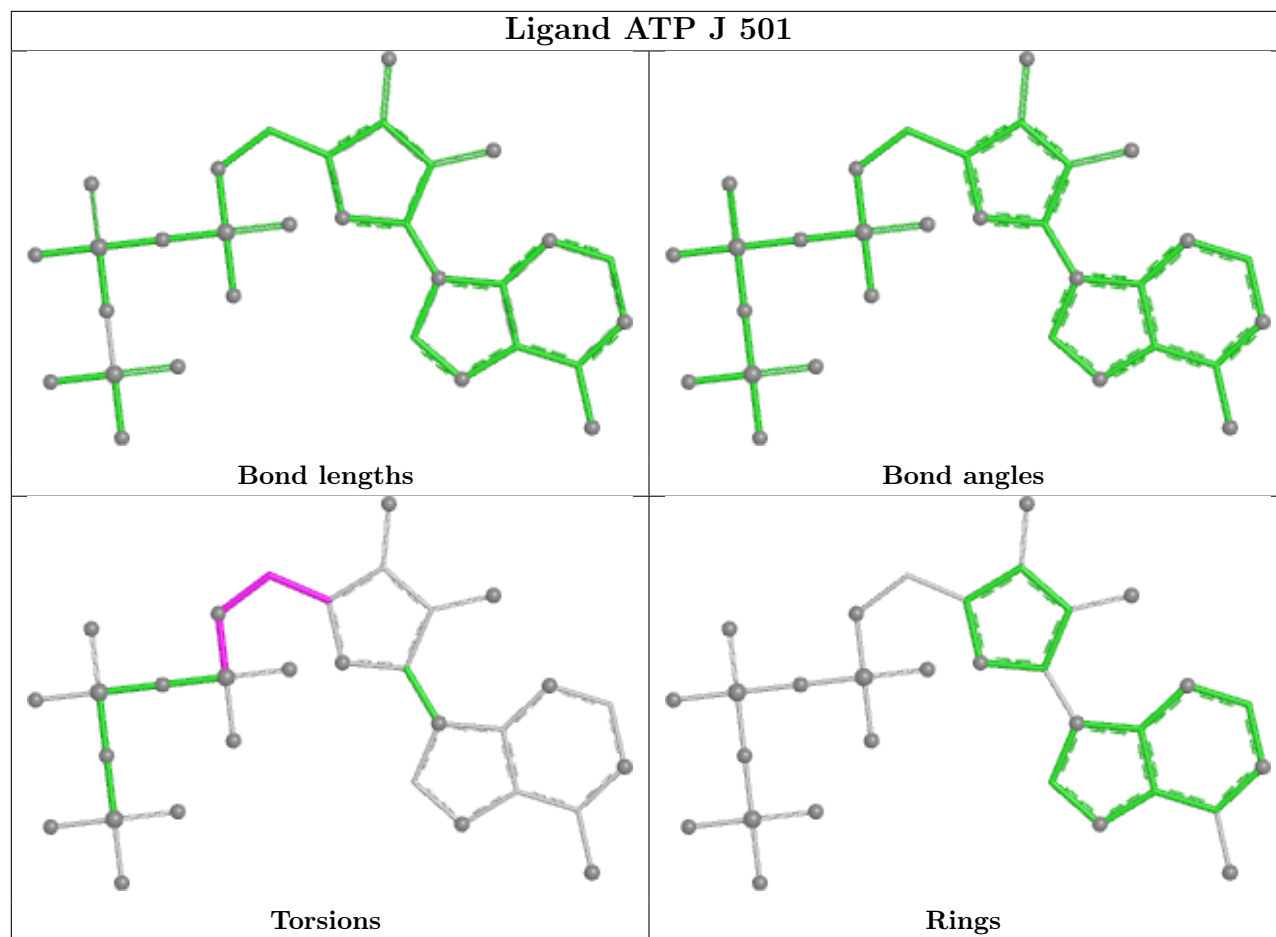
## Ligand ADP J 502

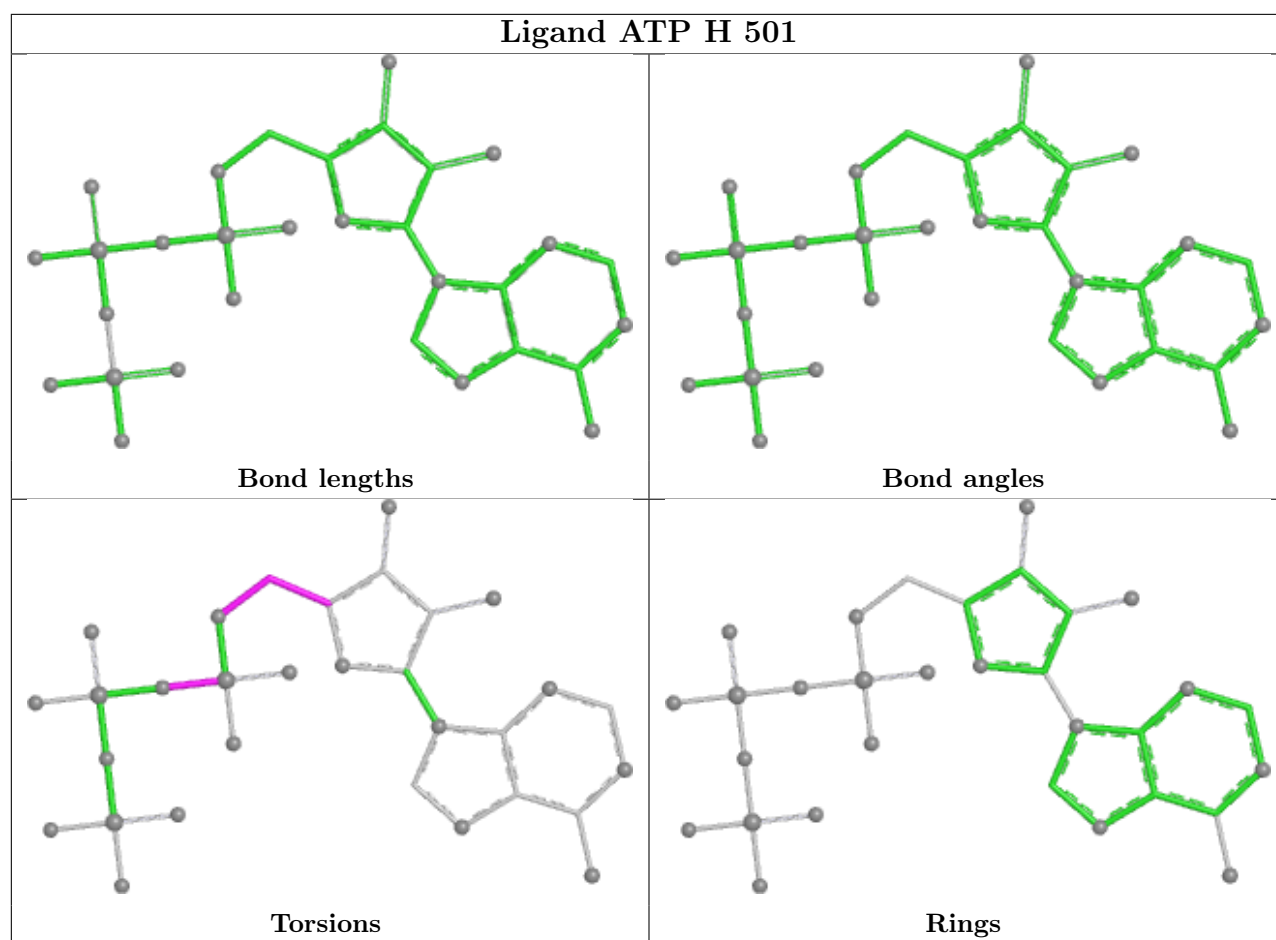






## Ligand ATP J 501





## 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.

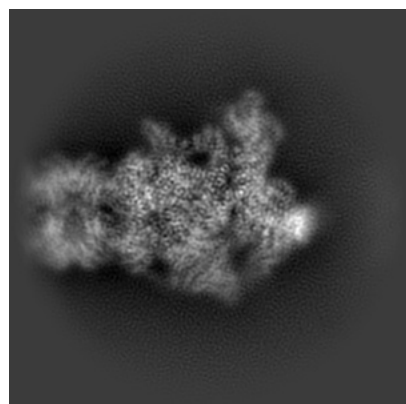
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45579. These allow visual inspection of the internal detail of the map and identification of artifacts.

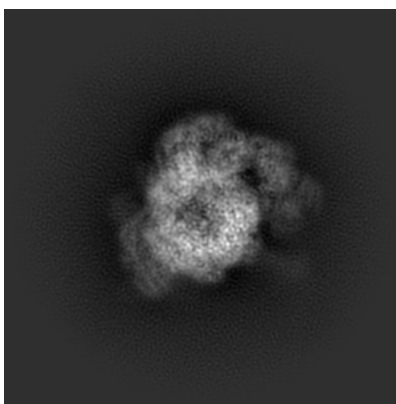
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

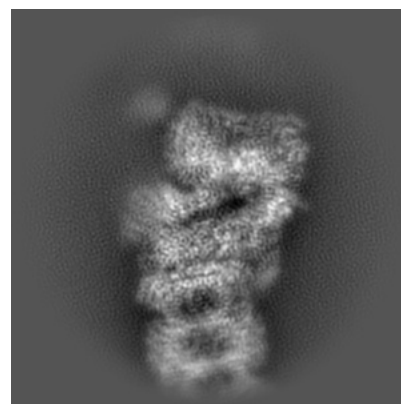
#### 6.1.1 Primary map



X

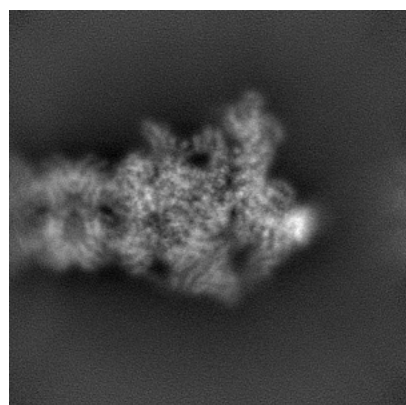


Y

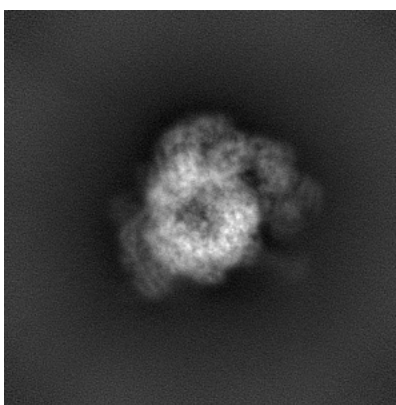


Z

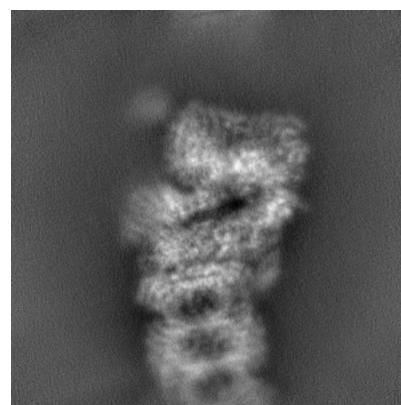
#### 6.1.2 Raw map



X



Y

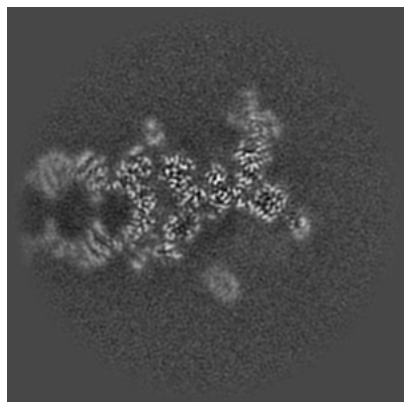


Z

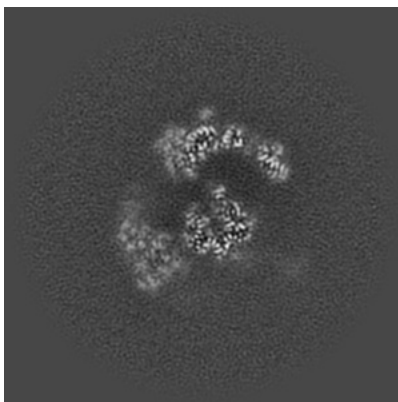
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

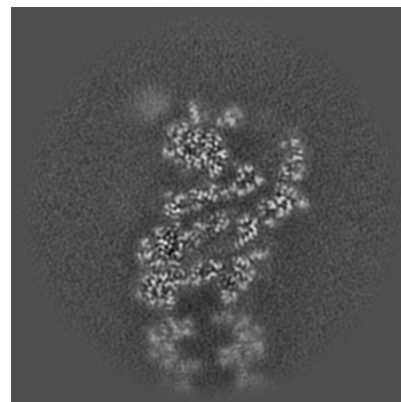
### 6.2.1 Primary map



X Index: 170

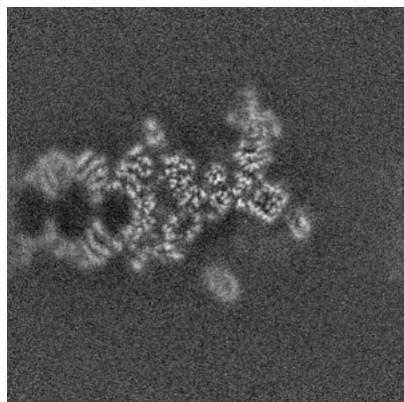


Y Index: 170

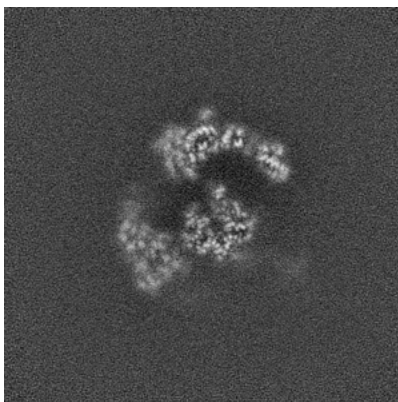


Z Index: 170

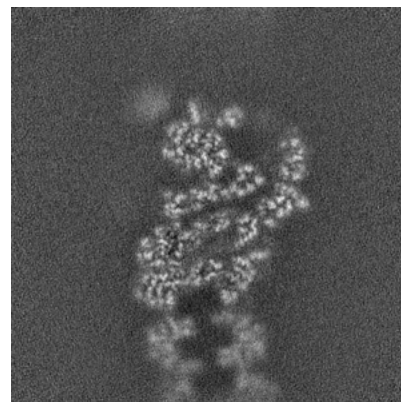
### 6.2.2 Raw map



X Index: 170



Y Index: 170

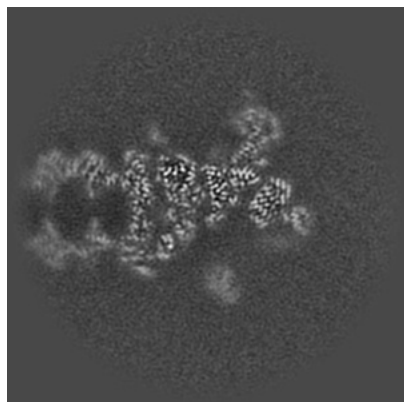


Z Index: 170

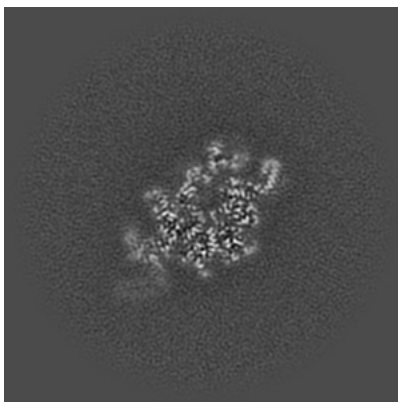
The images above show central slices of the map in three orthogonal directions.

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

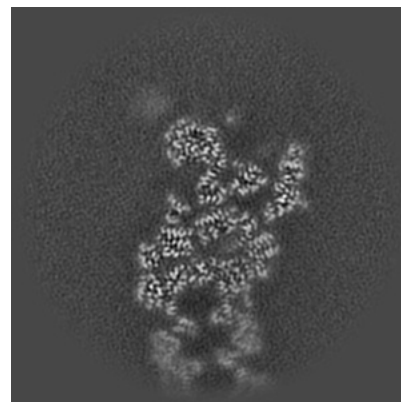
### 6.3.1 Primary map



X Index: 164

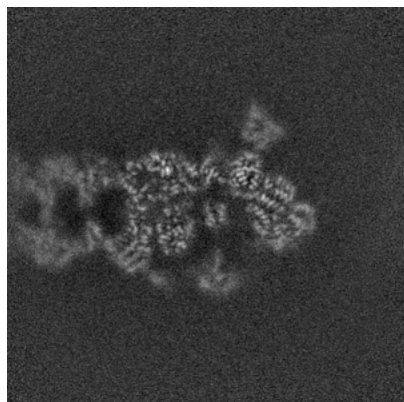


Y Index: 139

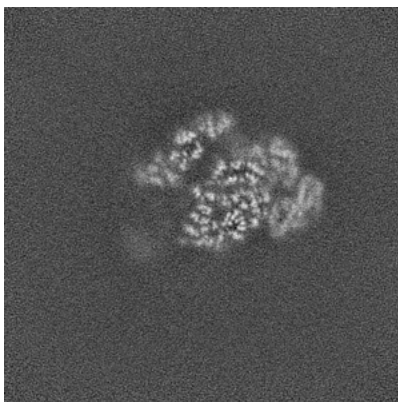


Z Index: 175

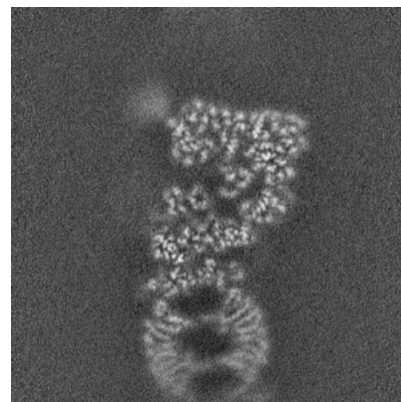
### 6.3.2 Raw map



X Index: 155



Y Index: 208

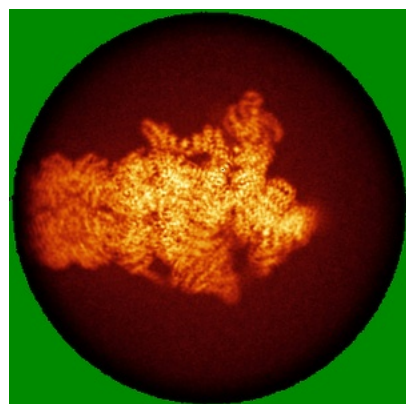


Z Index: 158

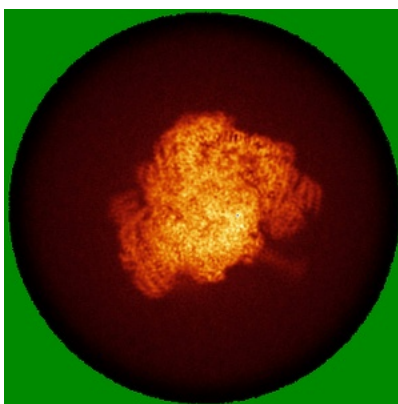
The images above show the largest variance slices of the map in three orthogonal directions.

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

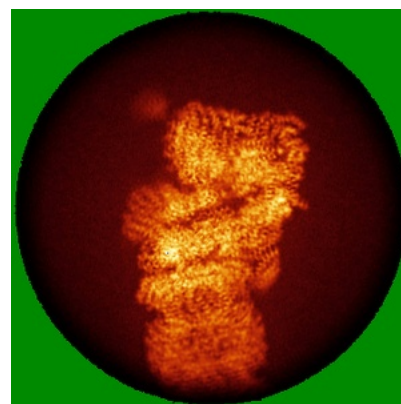
### 6.4.1 Primary map



X

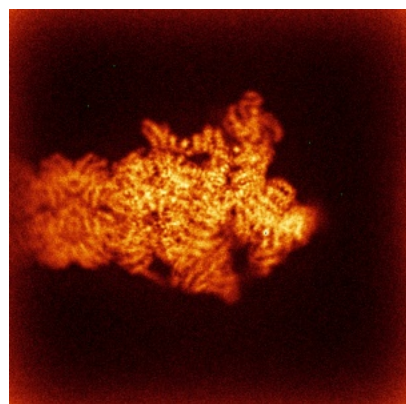


Y

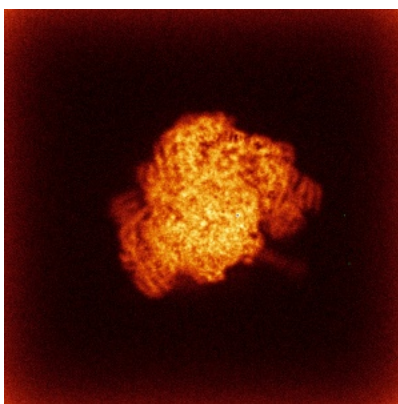


Z

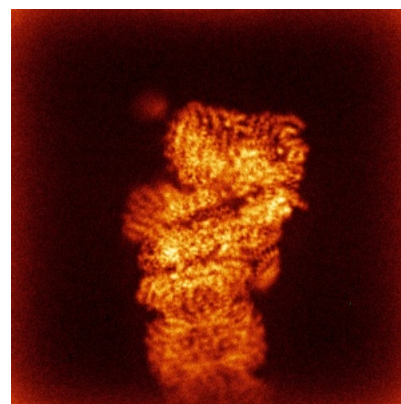
### 6.4.2 Raw map



X



Y

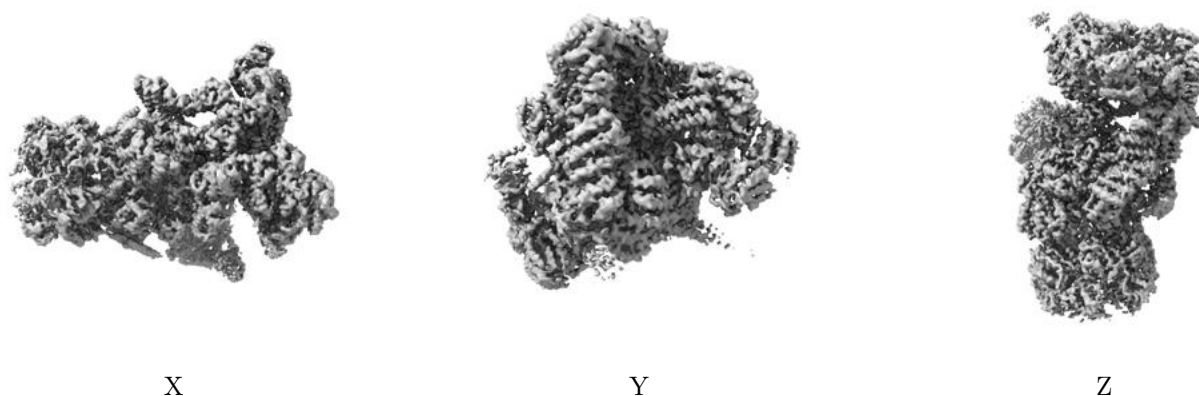


Z

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.

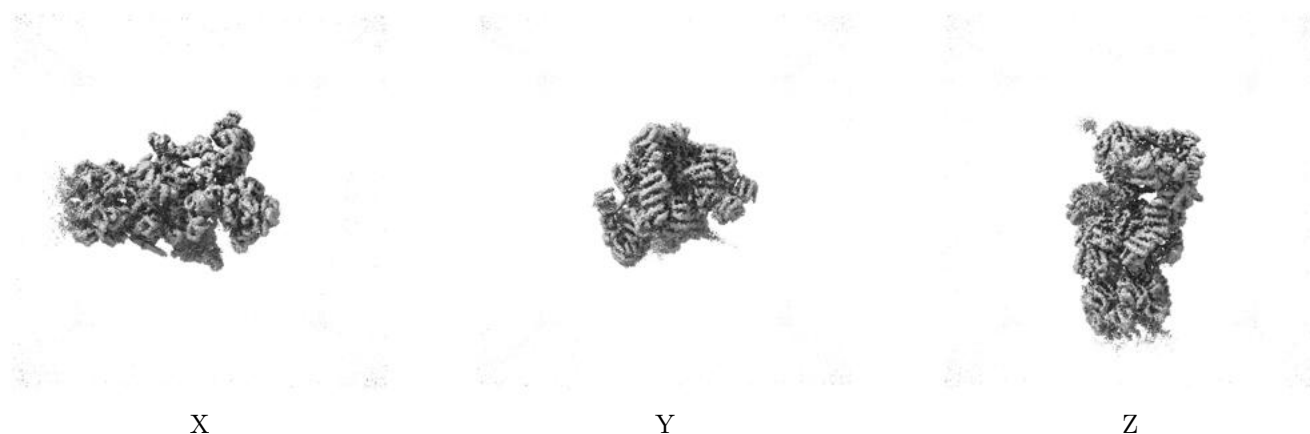
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.33. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

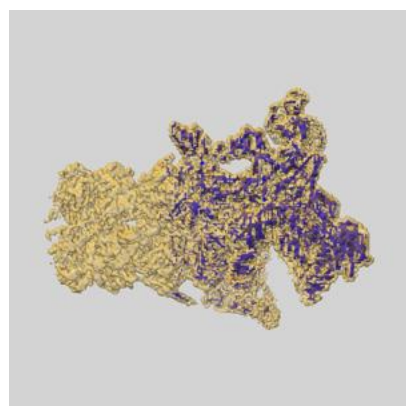
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

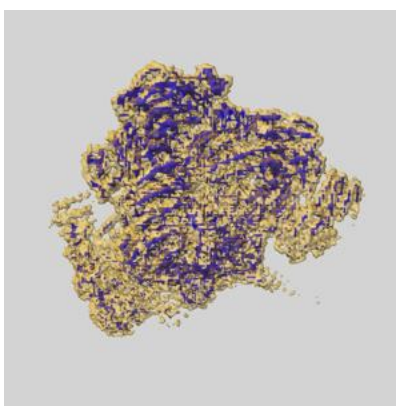
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

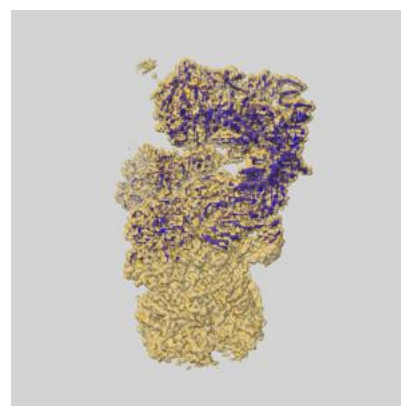
### 6.6.1 emd\_45579\_msk\_1.map [i](#)



X



Y

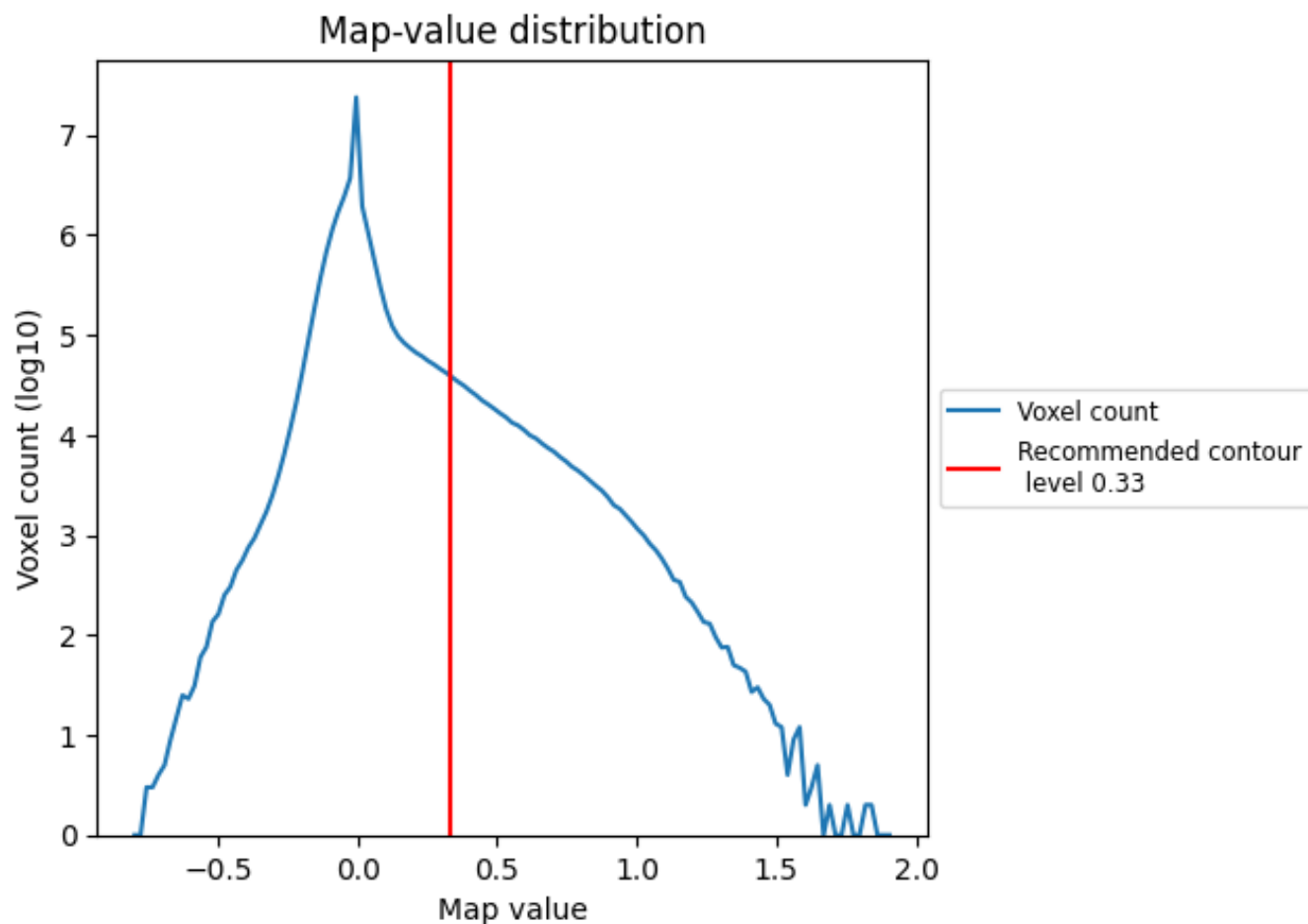


Z

## 7 Map analysis [i](#)

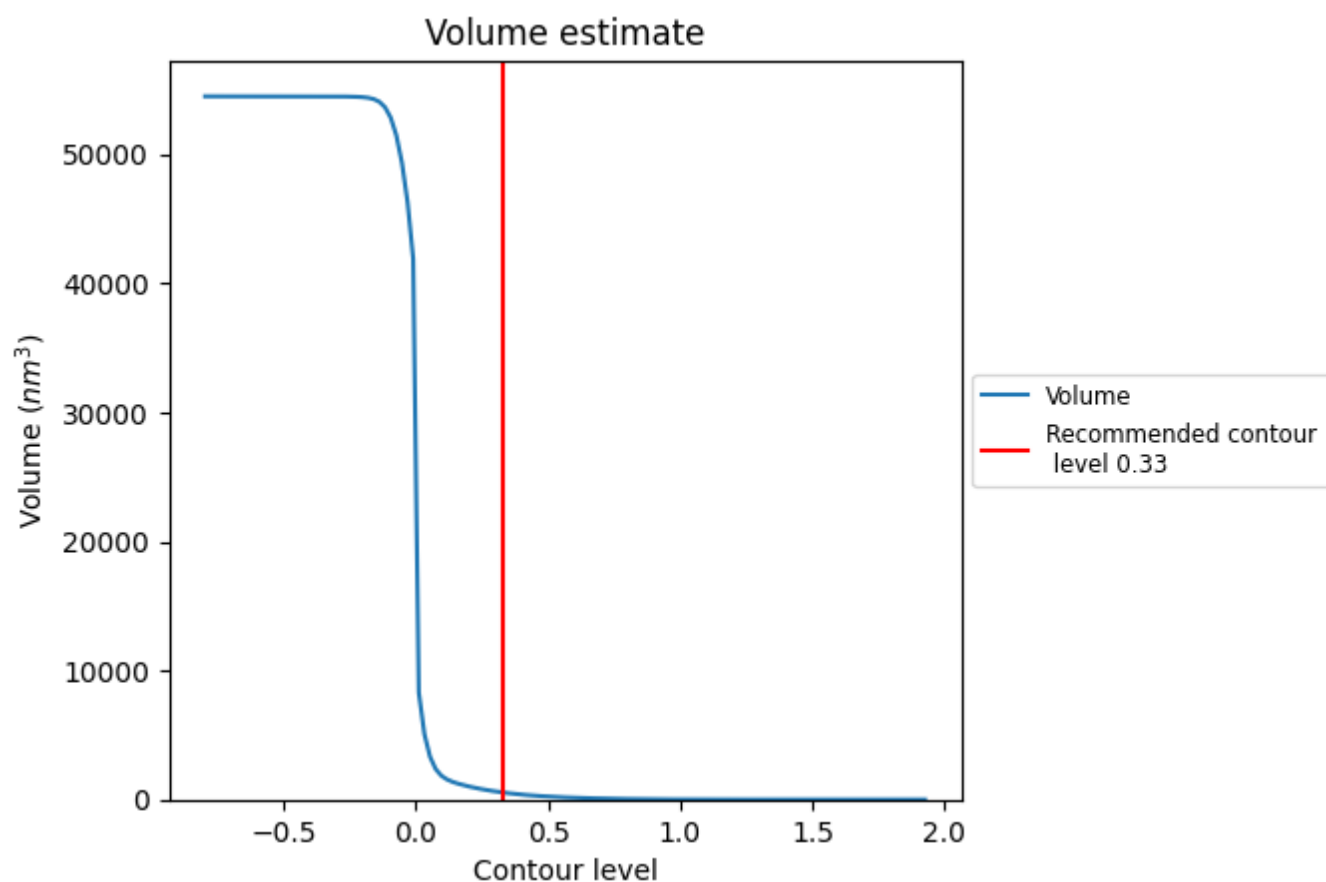
This section contains the results of statistical analysis of the map.

### 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.

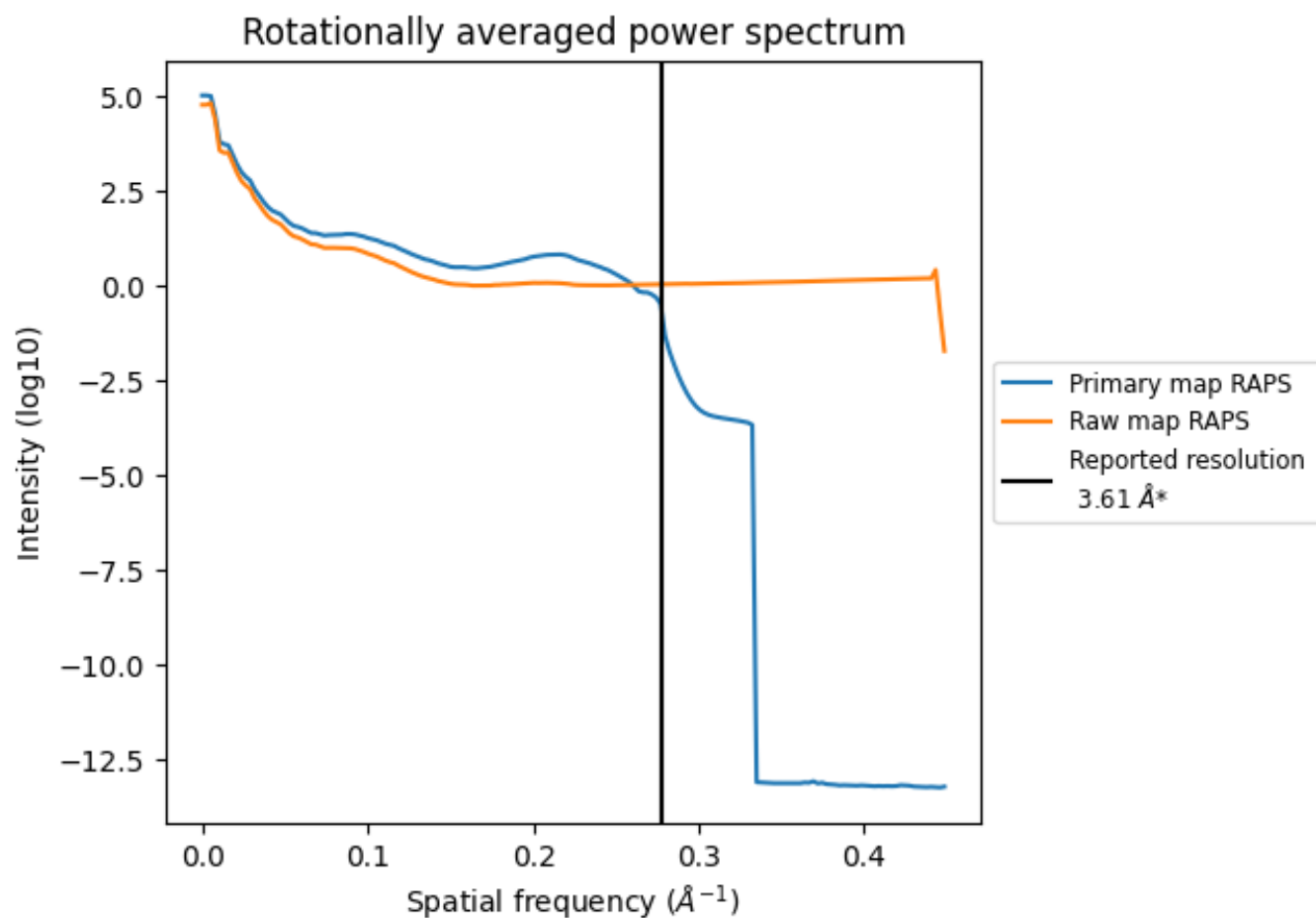
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 547 nm<sup>3</sup>; this corresponds to an approximate mass of 494 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 ⓘ

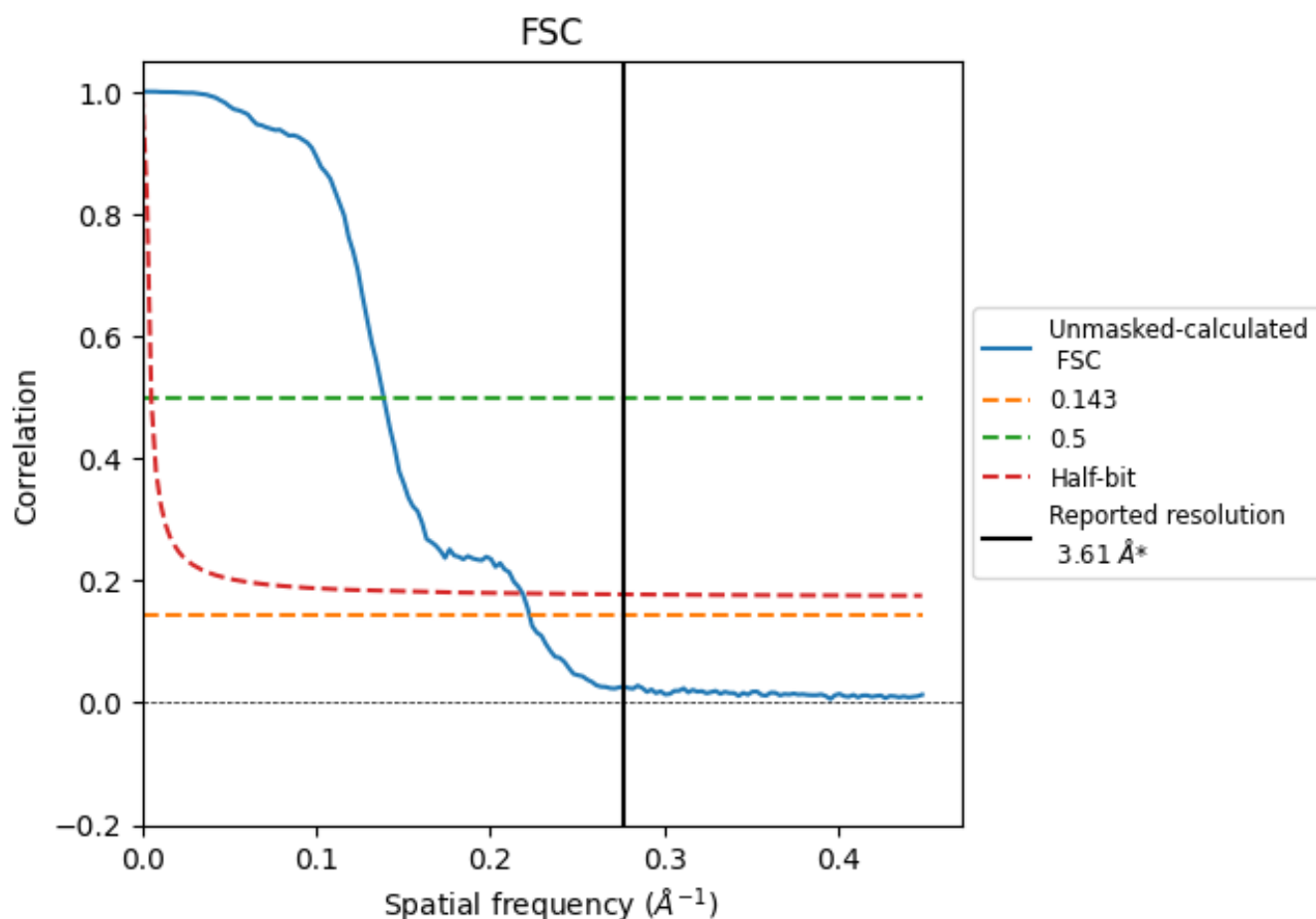


\*Reported resolution corresponds to spatial frequency of 0.277 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.277 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

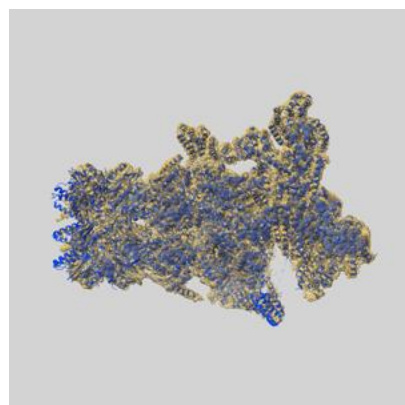
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.61                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 4.49                               | 7.20 | 4.57     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.49 differs from the reported value 3.61 by more than 10 %

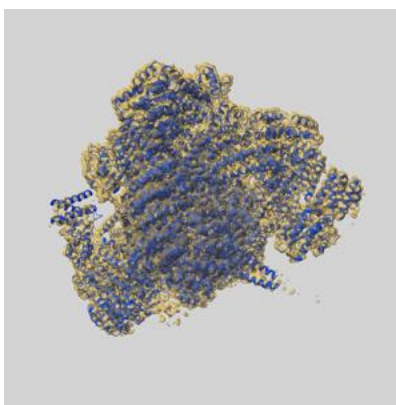
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45579 and PDB model 9CGC. Per-residue inclusion information can be found in section [3](#) on page [12](#).

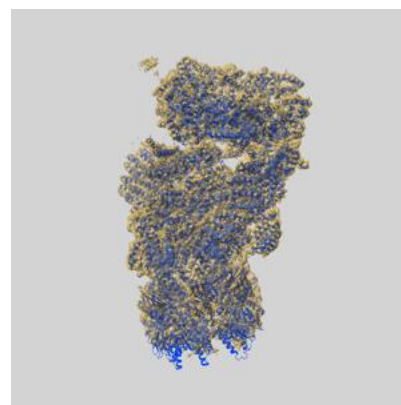
### 9.1 Map-model overlay [i](#)



X



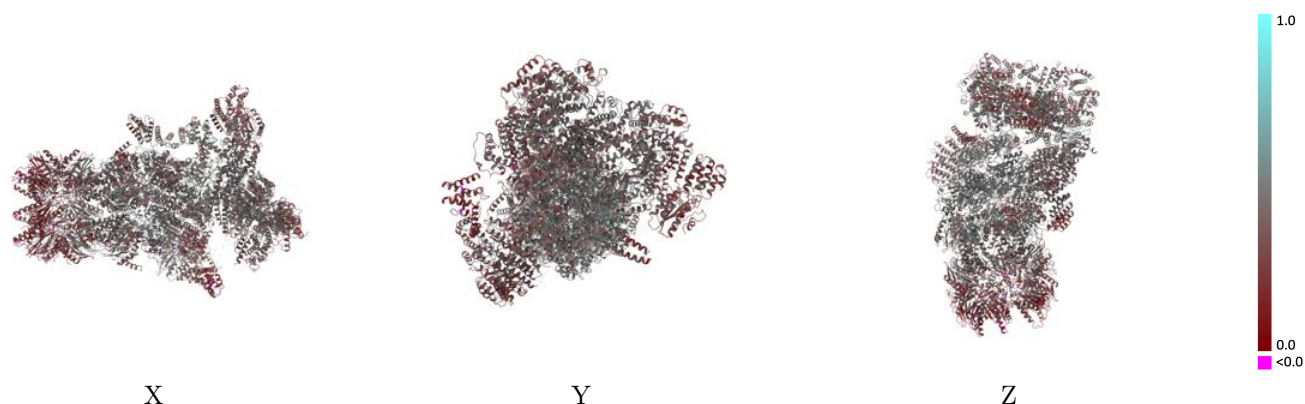
Y



Z

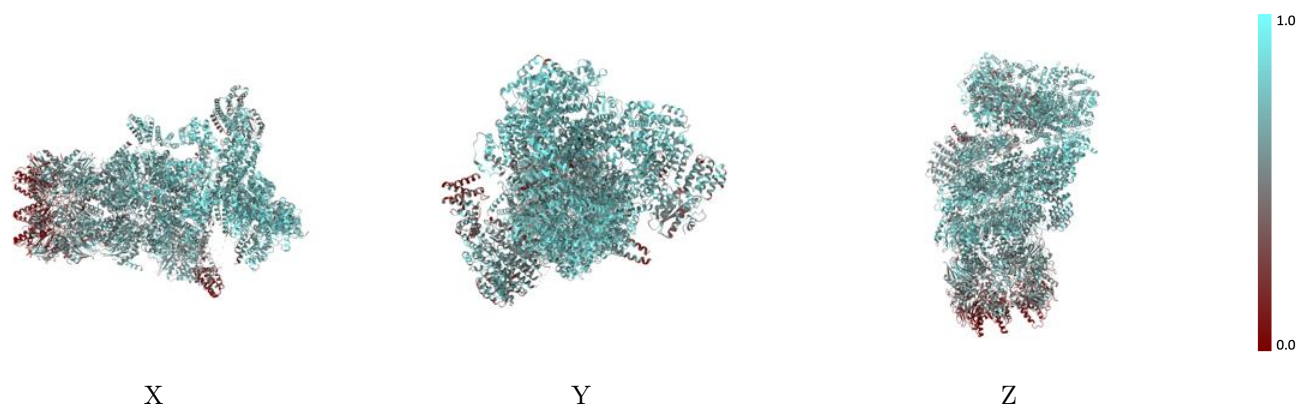
The images above show the 3D surface view of the map at the recommended contour level 0.33 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



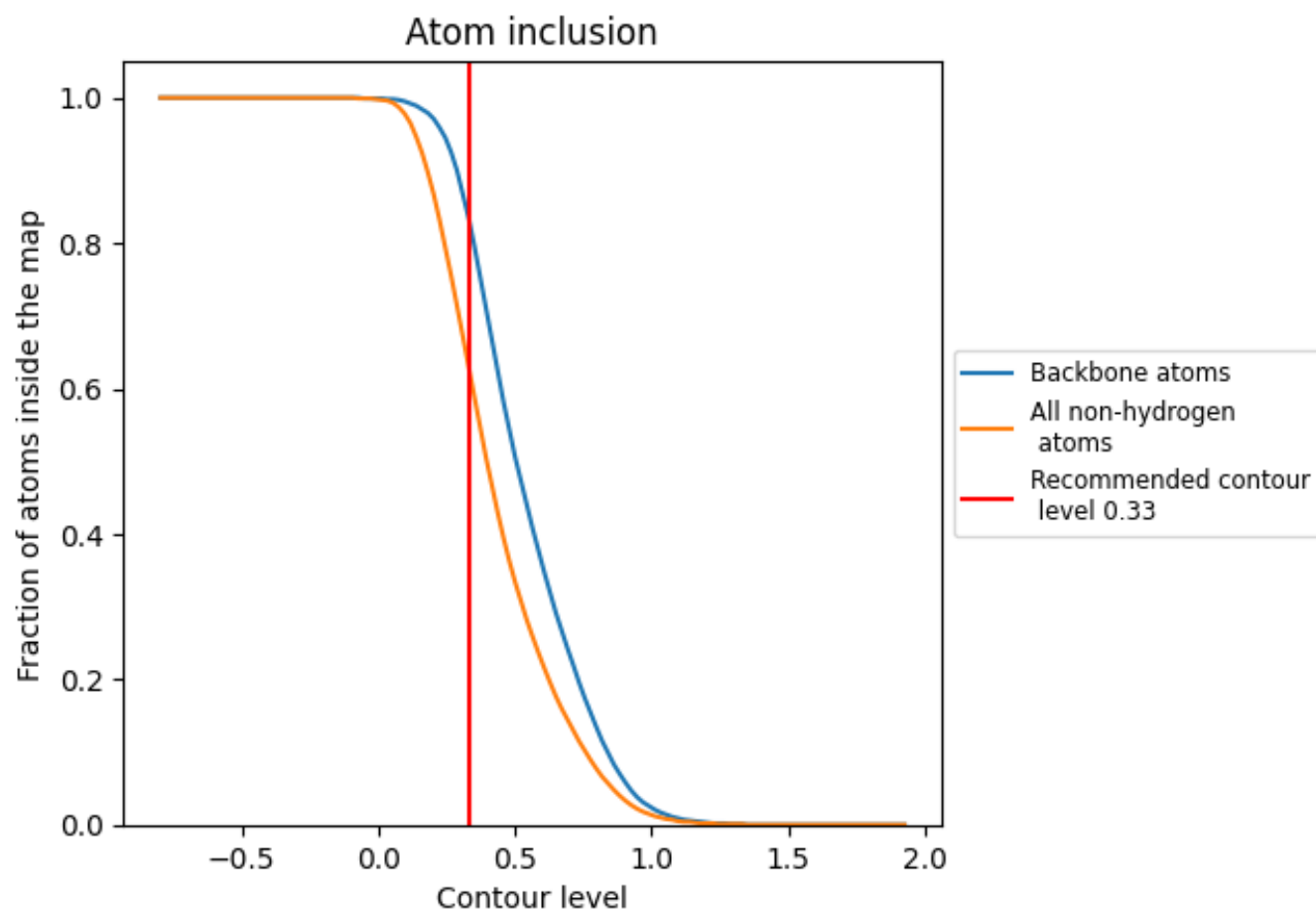
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.33).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 63% 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 (0.33) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.6310   |  0.3860   |
| 1     |  0.5810   |  0.3460   |
| 2     |  0.5730   |  0.3760   |
| 3     |  0.5370   |  0.3600   |
| 4     |  0.5320   |  0.3400   |
| 5     |  0.5870   |  0.3450   |
| 6     |  0.5460   |  0.3530   |
| 7     |  0.5670   |  0.3600   |
| A     |  0.7200   |  0.4420   |
| B     |  0.6540   |  0.4290   |
| C     |  0.6240   |  0.4010   |
| D     |  0.6700   |  0.4070   |
| E     |  0.6730   |  0.4150   |
| F     |  0.7210   |  0.4440   |
| G     |  0.7370  |  0.4490  |
| H     |  0.7320 |  0.4600 |
| I     |  0.6590 |  0.4290 |
| J     |  0.6980 |  0.4520 |
| K     |  0.7140 |  0.4660 |
| L     |  0.7360 |  0.4620 |
| M     |  0.7200 |  0.4600 |
| N     |  0.7610 |  0.4190 |
| O     |  0.6520 |  0.3500 |
| P     |  0.7600 |  0.4130 |
| Q     |  0.7200 |  0.3870 |
| R     |  0.7190 |  0.3880 |
| S     |  0.7450 |  0.4140 |
| T     |  0.7320 |  0.3810 |
| U     |  0.7020 |  0.4300 |
| V     |  0.7380 |  0.4550 |
| W     |  0.5530 |  0.3320 |
| Y     |  0.7960 |  0.4220 |
| a     |  0.3820 |  0.2730 |
| b     |  0.3350 |  0.2400 |
| e     |  0.3590 |  0.2640 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| f     |  0.3290 |  0.2720 |
| g     |  0.2470 |  0.2470 |
| h     |  0.2230 |  0.2400 |
| i     |  0.2750 |  0.2500 |
| o     |  0.5520 |  0.3300 |