



## Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 01:39 AM UTC

PDB ID : 6J30 / pdb\_00006j30  
EMDB ID : EMD-9773  
Title : yeast proteasome in Ub-engaged state (C2)  
Authors : Cong, Y.  
Deposited on : 2019-01-03  
Resolution : 4.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

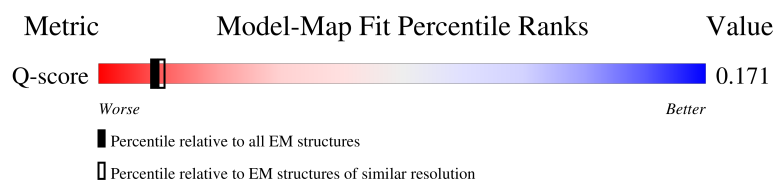
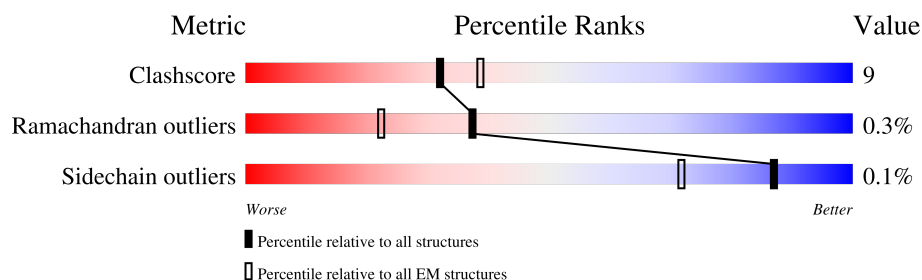
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.50 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                       | 2937 ( 4.00 - 5.00 )                                     |

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    | <div> <div>11%</div> <div>73%</div> <div>18%</div> <div>9%</div> </div>  |
| 1   | b     | 215    | <div> <div>10%</div> <div>71%</div> <div>20%</div> <div>9%</div> </div>  |
| 2   | 2     | 261    | <div> <div>13%</div> <div>70%</div> <div>16%</div> <div>13%</div> </div> |
| 2   | i     | 261    | <div> <div>9%</div> <div>69%</div> <div>18%</div> <div>13%</div> </div>  |

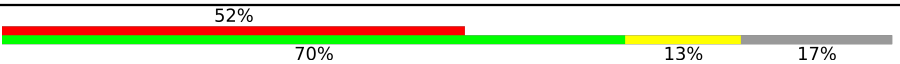
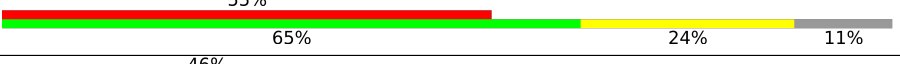
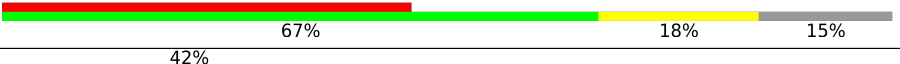
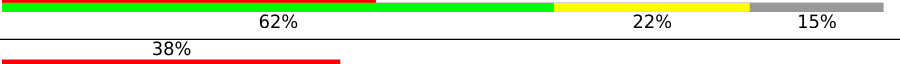
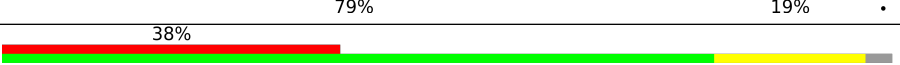
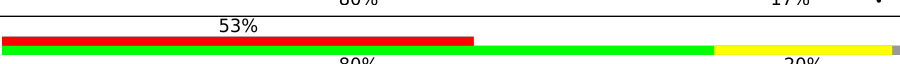
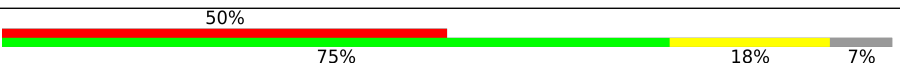
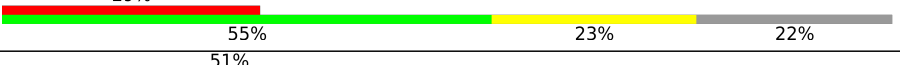
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | 3     | 205    |                  |
| 3   | h     | 205    |                  |
| 4   | 4     | 198    |                  |
| 4   | g     | 198    |                  |
| 5   | 5     | 287    |                  |
| 5   | f     | 287    |                  |
| 6   | 6     | 241    |                  |
| 6   | e     | 241    |                  |
| 7   | 7     | 266    |                  |
| 7   | a     | 266    |                  |
| 8   | A     | 252    |                  |
| 8   | c     | 252    |                  |
| 9   | B     | 250    |                  |
| 9   | j     | 250    |                  |
| 10  | C     | 258    |                  |
| 10  | d     | 258    |                  |
| 11  | D     | 254    |                  |
| 11  | n     | 254    |                  |
| 12  | E     | 260    |                  |
| 12  | m     | 260    |                  |
| 13  | F     | 234    |                  |
| 13  | l     | 234    |                  |
| 14  | G     | 288    |                  |
| 14  | k     | 288    |                  |
| 15  | H     | 467    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 16  | I     | 437    |    |
| 17  | J     | 405    |    |
| 18  | K     | 428    |    |
| 19  | L     | 437    |    |
| 20  | M     | 434    |    |
| 21  | N     | 945    |    |
| 22  | O     | 393    |    |
| 23  | P     | 445    |    |
| 24  | Q     | 434    |    |
| 25  | R     | 429    |    |
| 26  | S     | 523    |   |
| 27  | T     | 274    |  |
| 28  | U     | 338    |  |
| 29  | V     | 306    |  |
| 30  | W     | 268    |  |
| 31  | X     | 156    |  |
| 32  | Y     | 89     |  |
| 33  | Z     | 993    |  |

## 2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 106227 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     | 196      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1512  | 955 | 250 | 300 | 7 |         |       |
| 1   | b     | 196      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1512  | 955 | 250 | 300 | 7 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | 2     | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1719  | 1082 | 298 | 332 | 7 |         |       |
| 2   | i     | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1719  | 1082 | 298 | 332 | 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     | 195      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1561  | 992 | 264 | 299 | 6 |         |       |
| 4   | g     | 195      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1561  | 992 | 264 | 299 | 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     | 229      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1790  | 1133 | 306 | 344 | 7 |         |       |
| 7   | a     | 232      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1815  | 1148 | 311 | 349 | 7 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8   | A     | 241      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1907  | 1214 | 320 | 365 | 8 |         |       |
| 8   | c     | 241      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1907  | 1214 | 320 | 365 | 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 |         |       |
| 9   | j     | 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 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10  | d     | 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     | 240      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1881  | 1176 | 329 | 372 | 4 |         |       |
| 11  | n     | 240      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1881  | 1176 | 329 | 372 | 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 |         |       |
| 12  | m     | 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 |         |       |
| 13  | l     | 231      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1773  | 1114 | 307 | 348 | 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     |
|     |       |          | 1892  | 1203 | 329 | 356 | 4 |         |       |
| 14  | k     | 243      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1892  | 1203 | 329 | 356 | 4 |         |       |

- Molecule 15 is a protein called 26S proteasome regulatory subunit 7 homolog.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 15  | H     | 355      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2787  | 1755 | 500 | 515 | 17 |         |       |

- Molecule 16 is a protein called 26S proteasome regulatory subunit 4 homolog.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 16  | I     | 362      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2822  | 1773 | 471 | 563 | 15 |         |       |

- Molecule 17 is a protein called 26S proteasome regulatory subunit 8 homolog.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 17  | J     | 373      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2928  | 1837 | 527 | 547 | 17 |         |       |

- Molecule 18 is a protein called 26S proteasome regulatory subunit 6B homolog.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 18  | K     | 381      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3019  | 1898 | 530 | 581 | 10 |         |       |

- Molecule 19 is a protein called 26S proteasome subunit RPT4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 19  | L     | 371      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2937  | 1852 | 519 | 554 | 12 |         |       |

- Molecule 20 is a protein called 26S proteasome regulatory subunit 6A.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 20  | M     | 367      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2866  | 1799 | 503 | 553 | 11 |         |       |

- Molecule 21 is a protein called 26S proteasome regulatory subunit RPN2.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 21  | N     | 849      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6562  | 4174 | 1099 | 1261 | 28 |         |       |

- Molecule 22 is a protein called 26S proteasome regulatory subunit RPN9.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 22  | O     | 387      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3182  | 2047 | 520 | 606 | 9 |         |       |

- Molecule 23 is a protein called 26S proteasome regulatory subunit RPN5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 23  | P     | 432      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3545  | 2260 | 592 | 684 | 9 |         |       |

- Molecule 24 is a protein called 26S proteasome regulatory subunit RPN6.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 24  | Q     | 431      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3471  | 2205 | 574 | 676 | 16 |         |       |

- Molecule 25 is a protein called 26S proteasome regulatory subunit RPN7.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 25  | R     | 400      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3218  | 2051 | 527 | 630 | 10 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 26  | S     | 475      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3894  | 2488 | 653 | 738 | 15 |         |       |

- Molecule 27 is a protein called 26S proteasome regulatory subunit RPN12.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 27  | T     | 272      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2235  | 1432 | 355 | 441 | 7 |         |       |

- Molecule 28 is a protein called 26S proteasome regulatory subunit RPN8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 28  | U     | 262      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2118  | 1348 | 362 | 402 | 6 |         |       |

- Molecule 29 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 29  | V     | 284      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2236  | 1405 | 381 | 436 | 14 |         |       |

- Molecule 30 is a protein called 26S proteasome regulatory subunit RPN10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | W     | 197      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1534  | 962 | 269 | 300 | 3 |         |       |

- Molecule 31 is a protein called 26S proteasome regulatory subunit RPN13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | X     | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 906   | 586 | 148 | 169 | 3 |         |       |

- Molecule 32 is a protein called 26S proteasome complex subunit SEM1.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 32  | Y     | 27       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 236   | 143 | 39 | 54 |         |       |

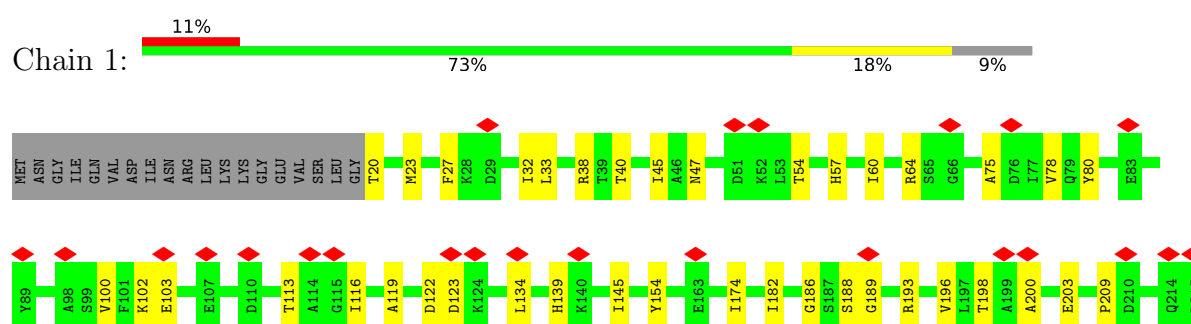
- Molecule 33 is a protein called 26S proteasome regulatory subunit RPN1.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 33  | Z     | 813      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6290  | 3995 | 1029 | 1237 | 29 |         |       |

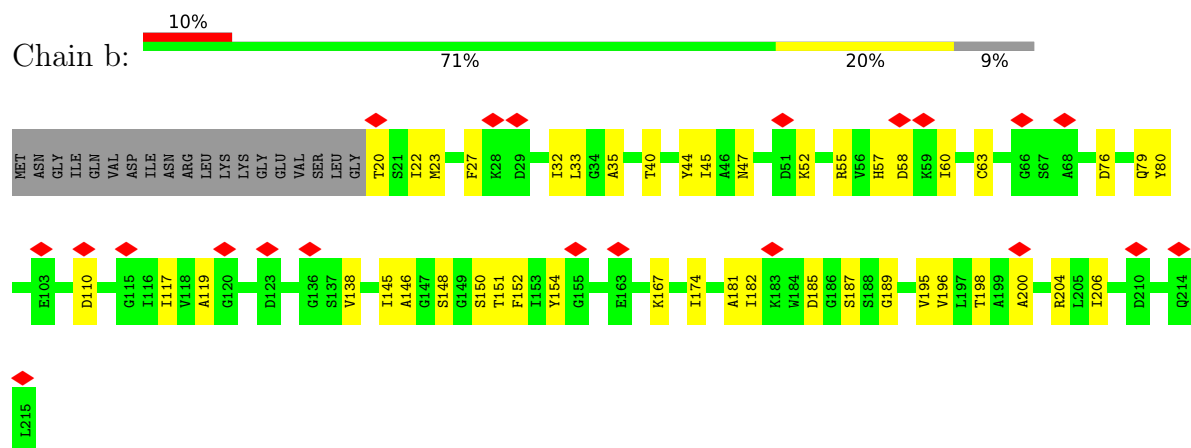
### 3 Residue-property plots

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.

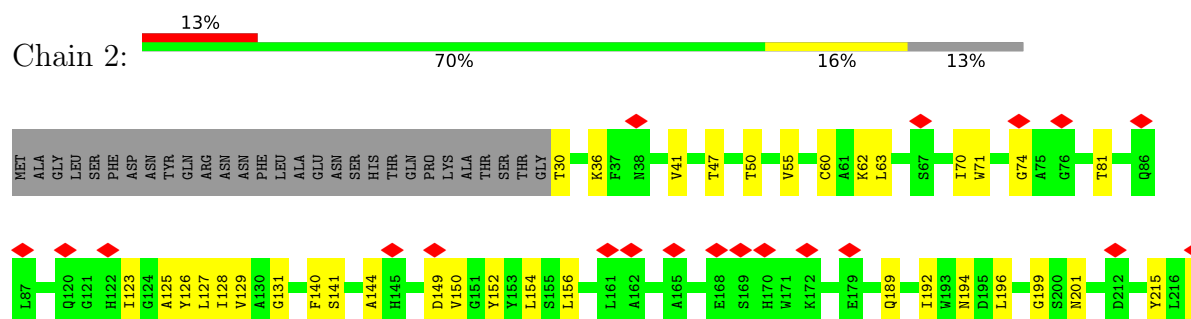
- Molecule 1: Proteasome subunit beta type-1

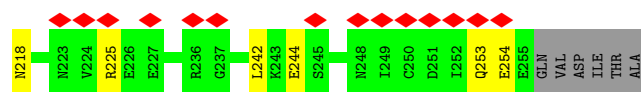


- Molecule 1: Proteasome subunit beta type-1

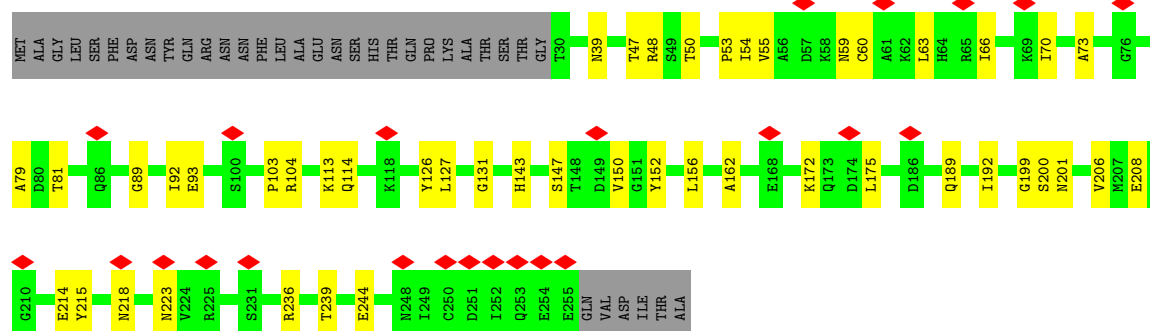


- Molecule 2: Proteasome subunit beta type-2

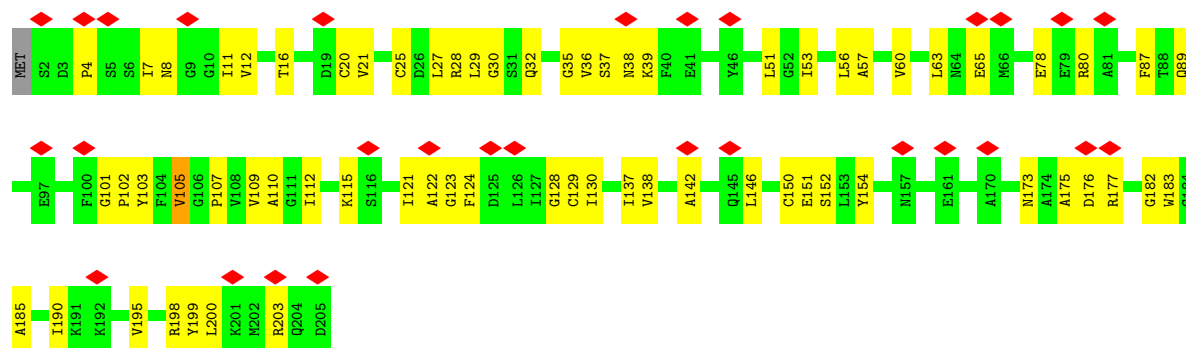




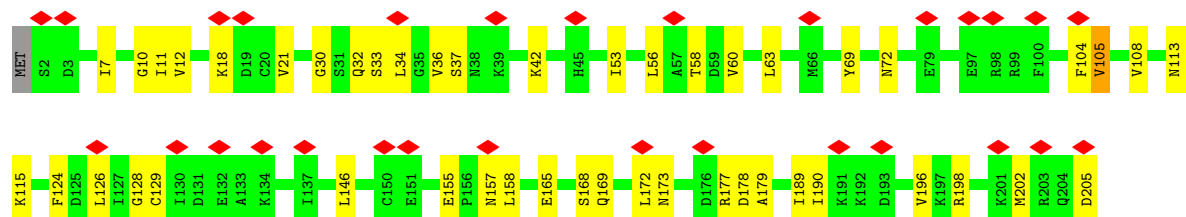
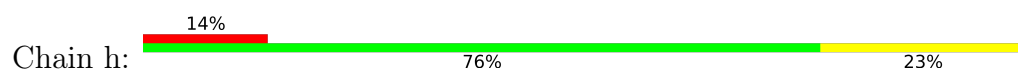
• Molecule 2: Proteasome subunit beta type-2



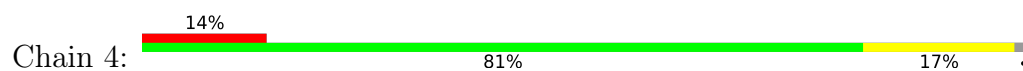
• Molecule 3: Proteasome subunit beta type-3

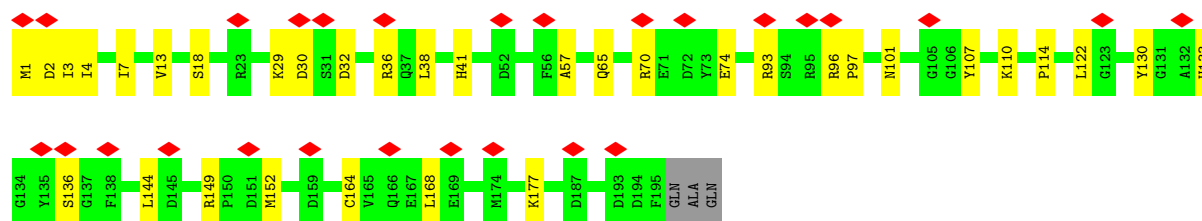


• Molecule 3: Proteasome subunit beta type-3

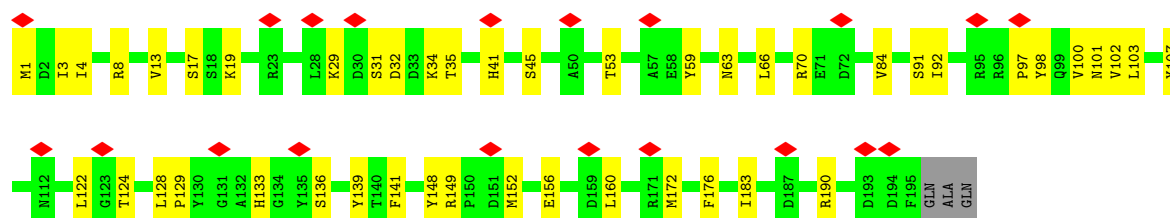
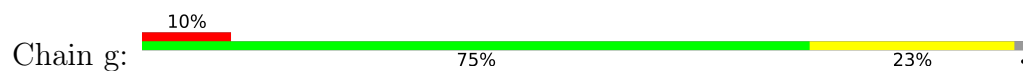


• Molecule 4: Proteasome subunit beta type-4

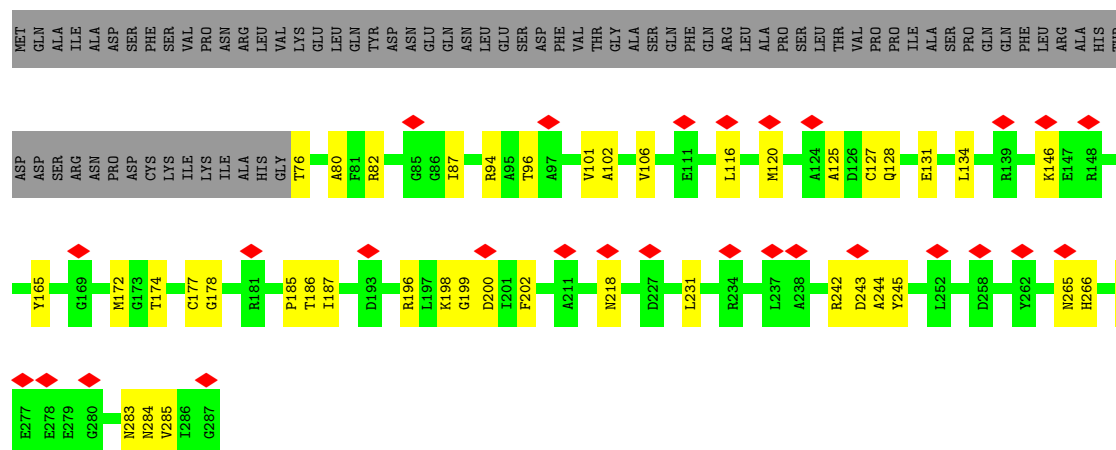




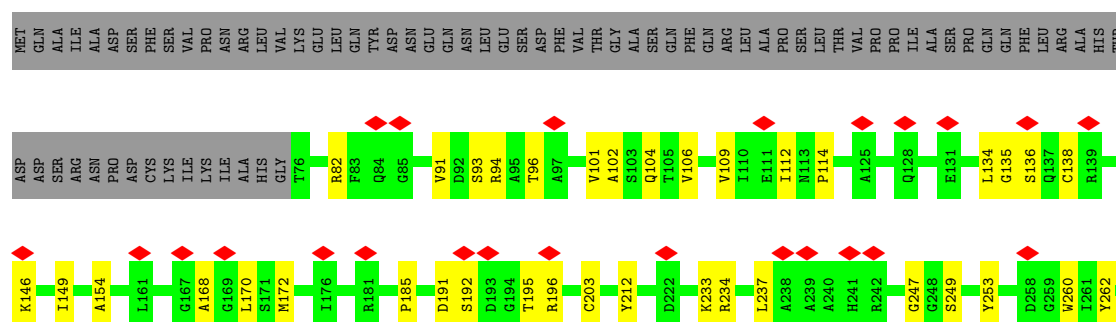
• Molecule 4: Proteasome subunit beta type-4

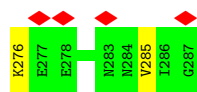


• Molecule 5: Proteasome subunit beta type-5

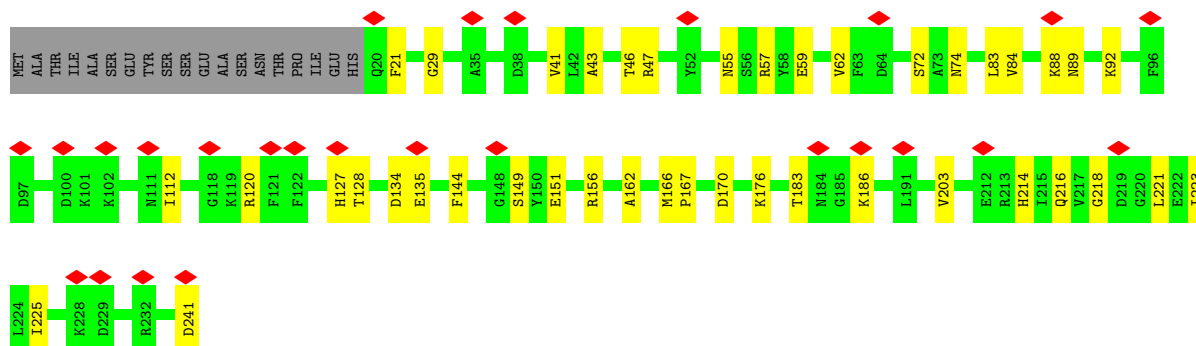
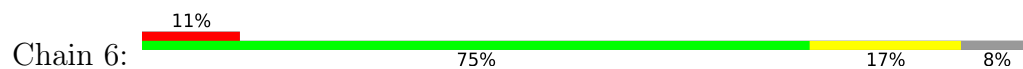


• Molecule 5: Proteasome subunit beta type-5

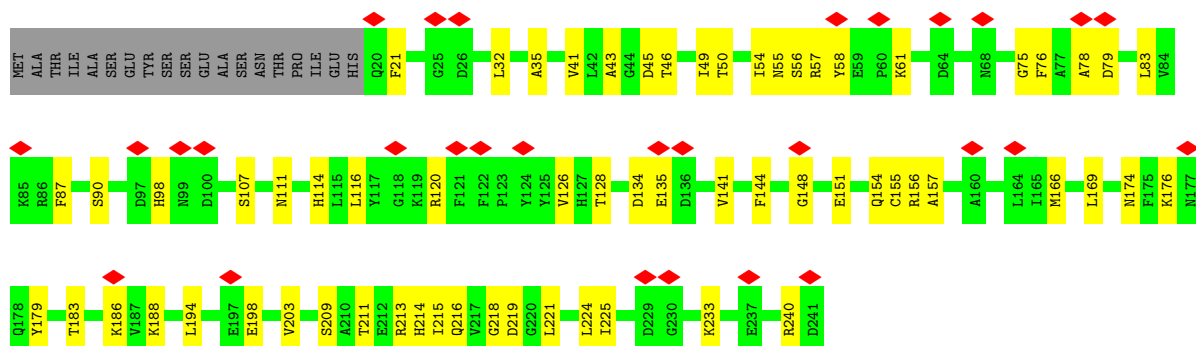




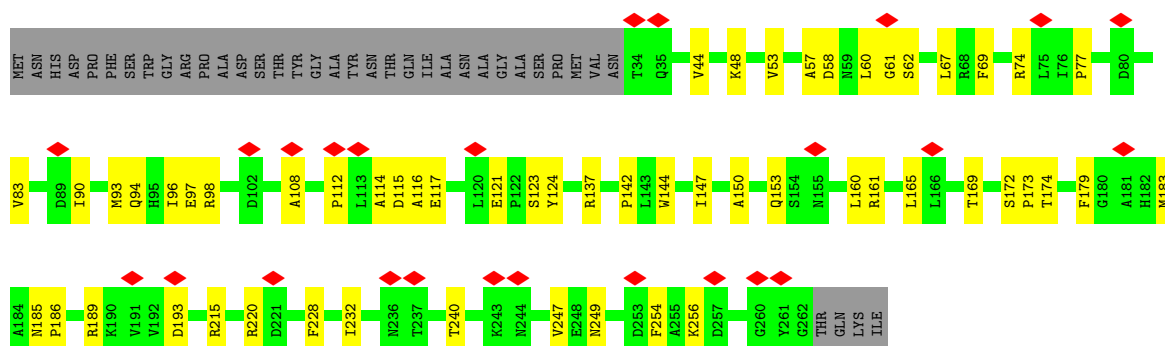
• Molecule 6: Proteasome subunit beta type-6



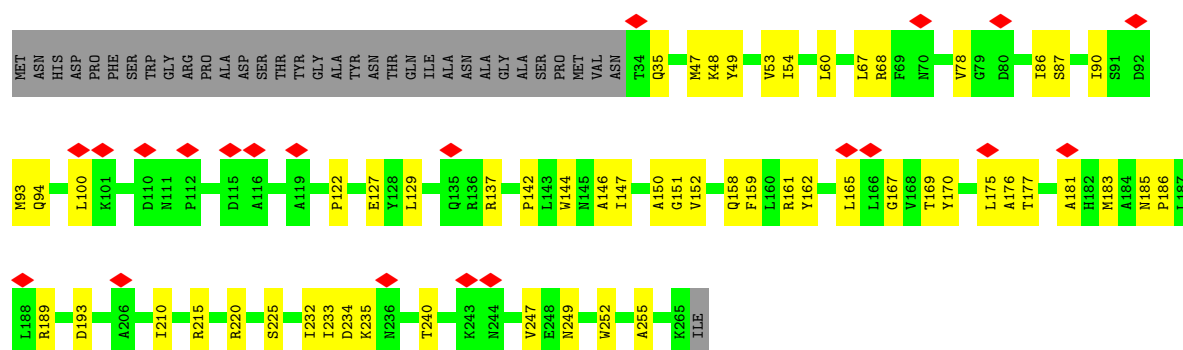
• Molecule 6: Proteasome subunit beta type-6



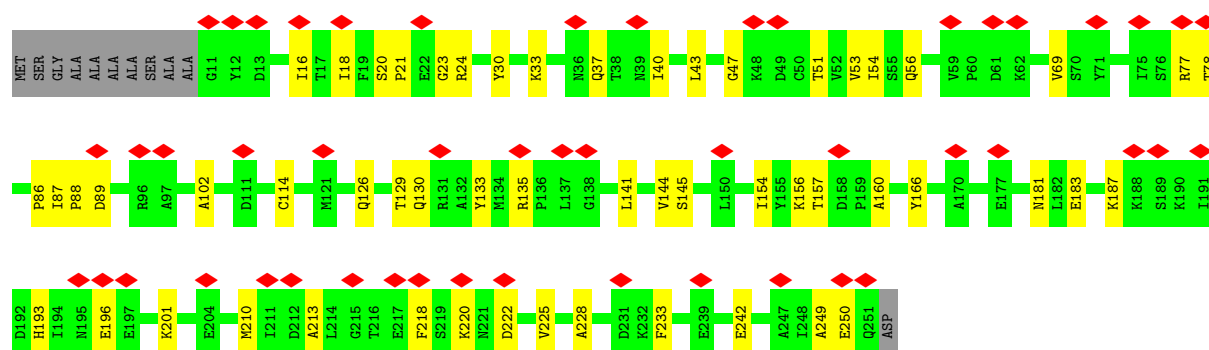
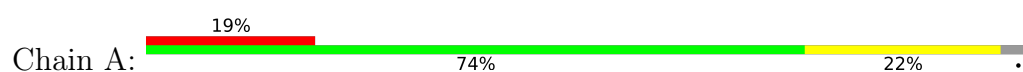
• Molecule 7: Proteasome subunit beta type-7



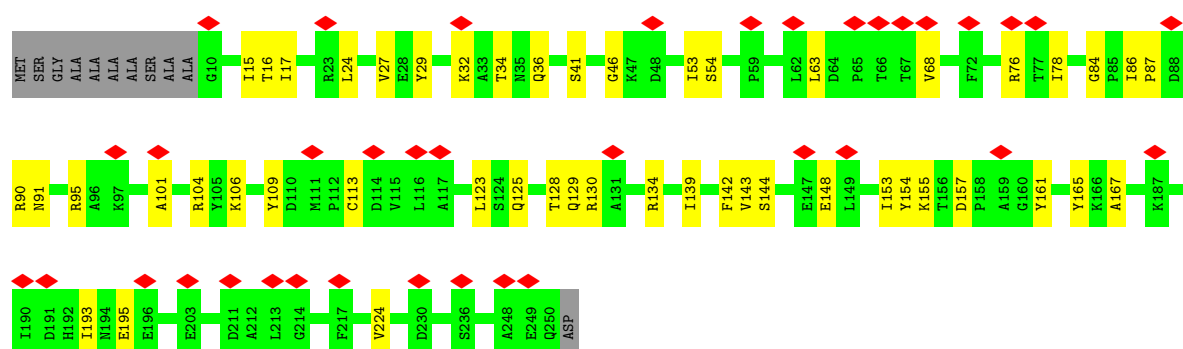
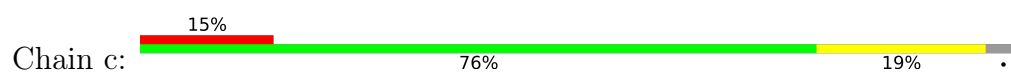
• Molecule 7: Proteasome subunit beta type-7



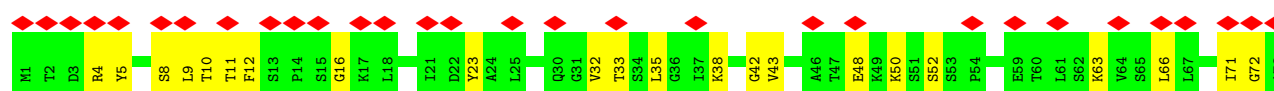
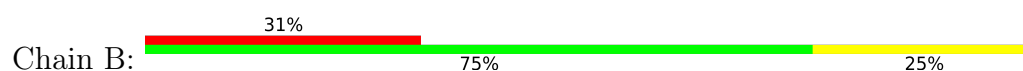
• Molecule 8: Proteasome subunit alpha type-1

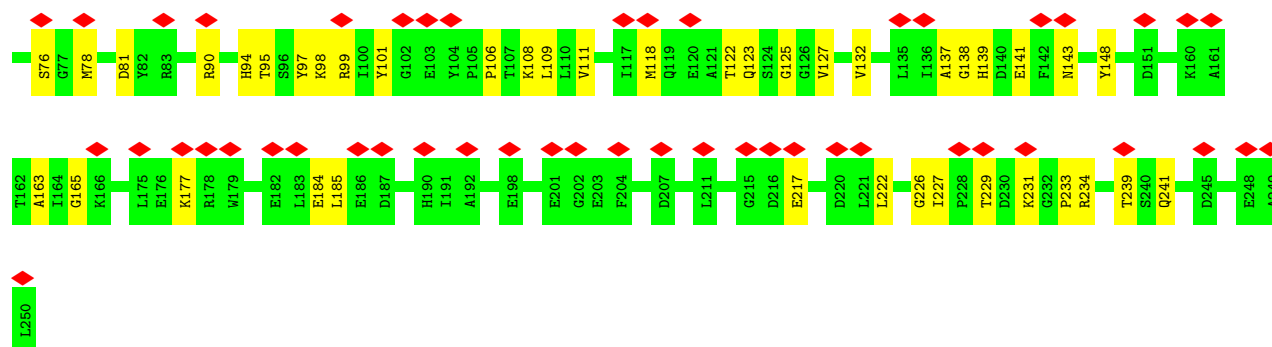


• Molecule 8: Proteasome subunit alpha type-1

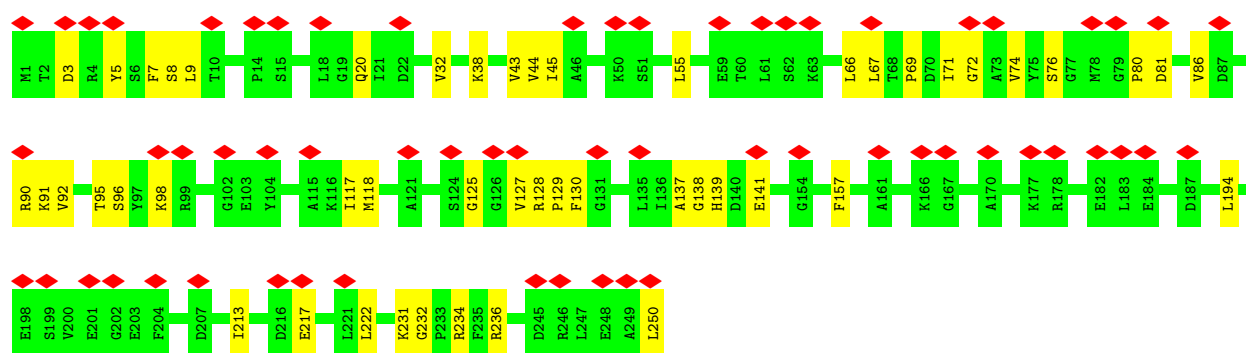
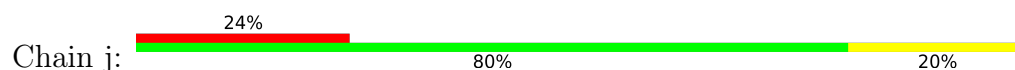


• Molecule 9: Proteasome subunit alpha type-2

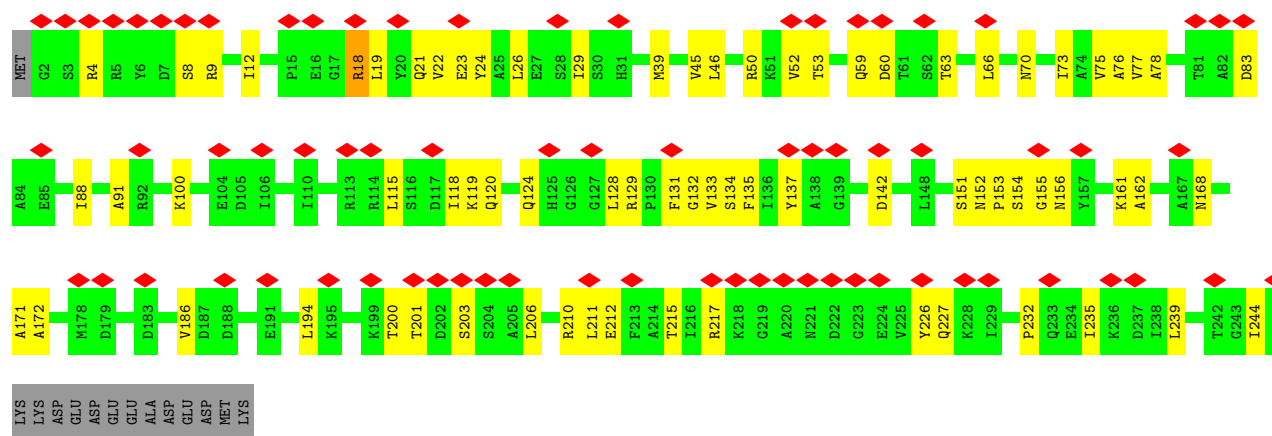




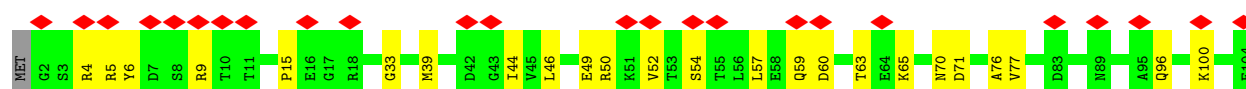
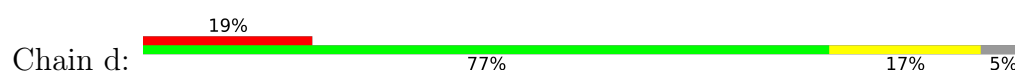
• Molecule 9: Proteasome subunit alpha type-2

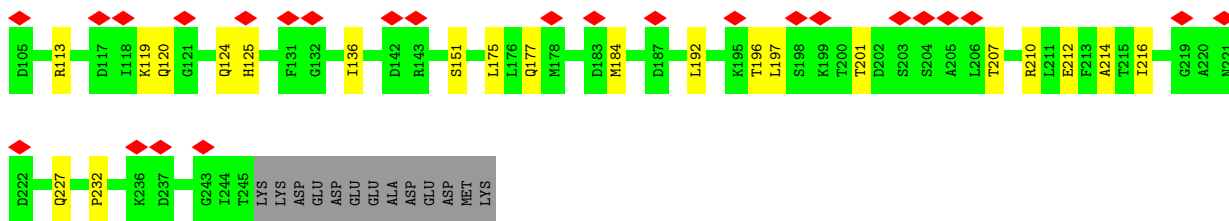


• Molecule 10: Proteasome subunit alpha type-3

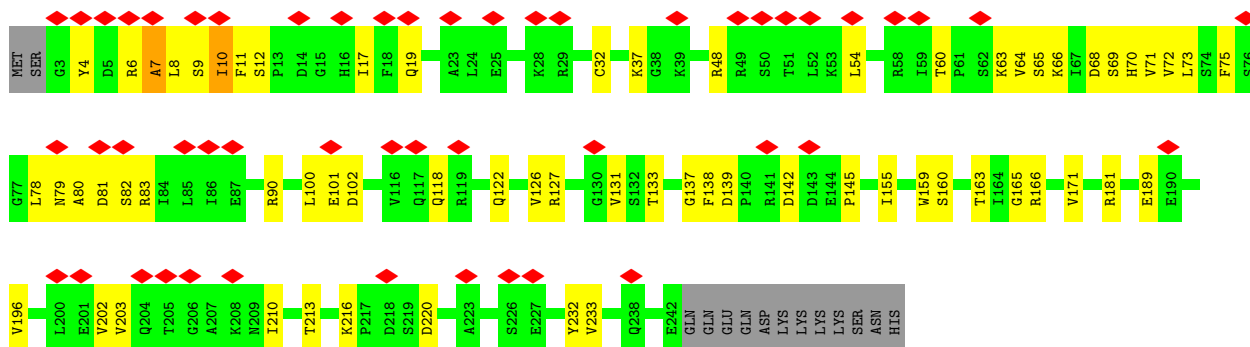


• Molecule 10: Proteasome subunit alpha type-3

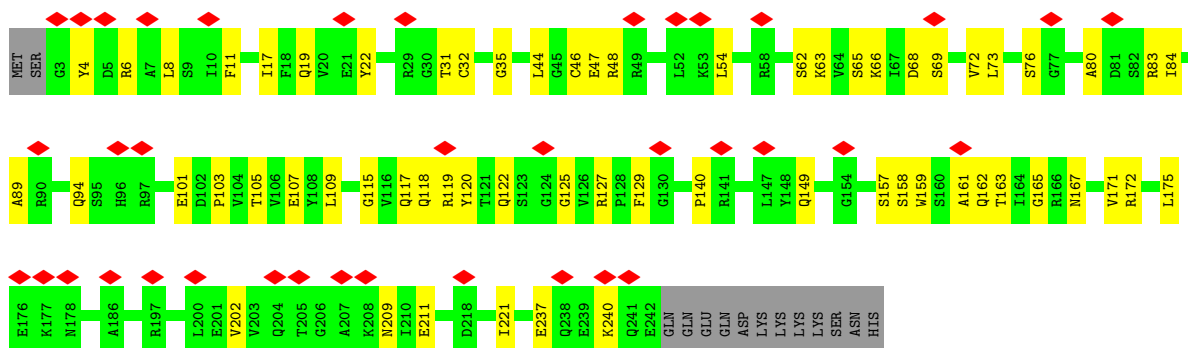




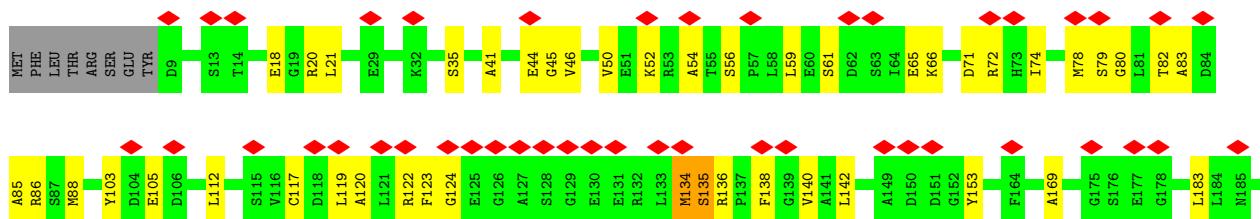
• Molecule 11: Proteasome subunit alpha type-4

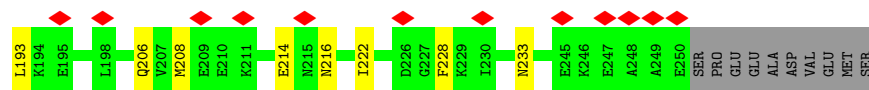


• Molecule 11: Proteasome subunit alpha type-4

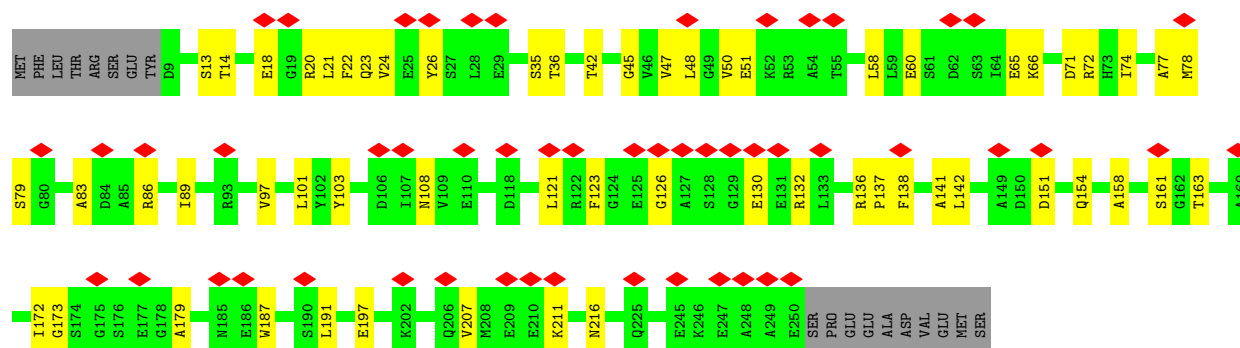


• Molecule 12: Proteasome subunit alpha type-5

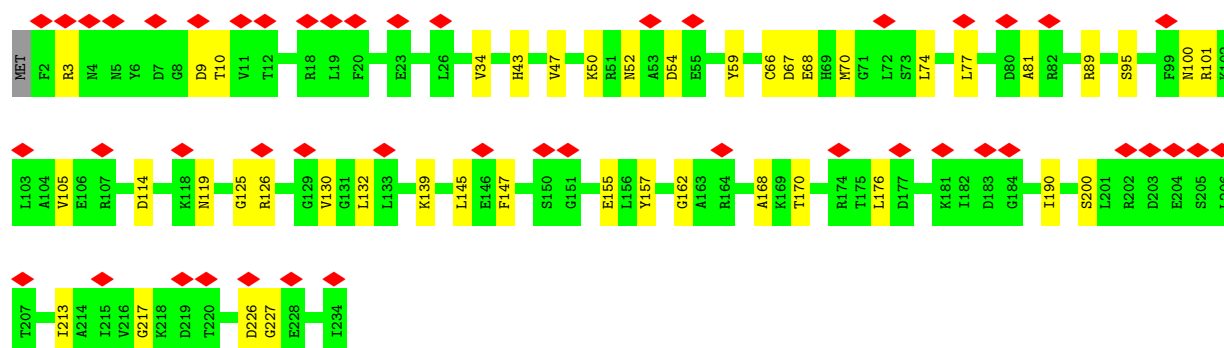
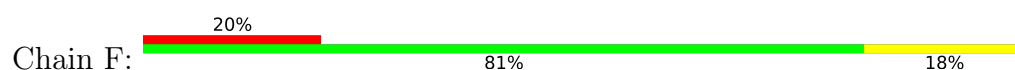




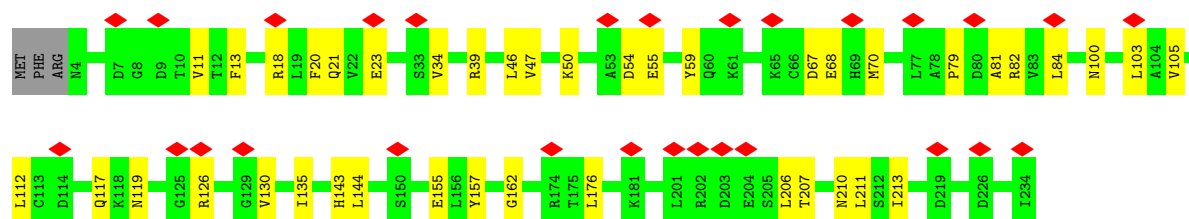
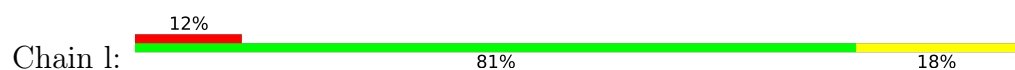
• Molecule 12: Proteasome subunit alpha type-5



• Molecule 13: Proteasome subunit alpha type-6

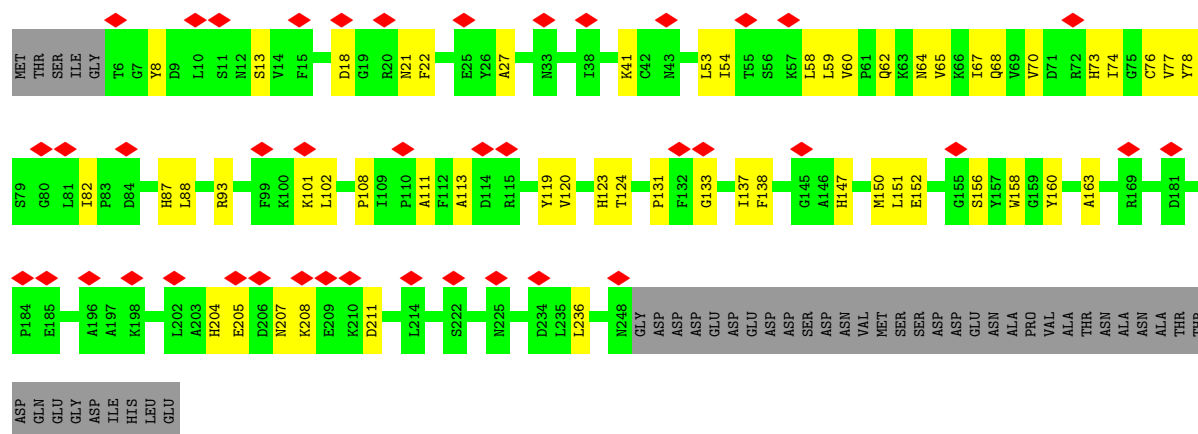


• Molecule 13: Proteasome subunit alpha type-6

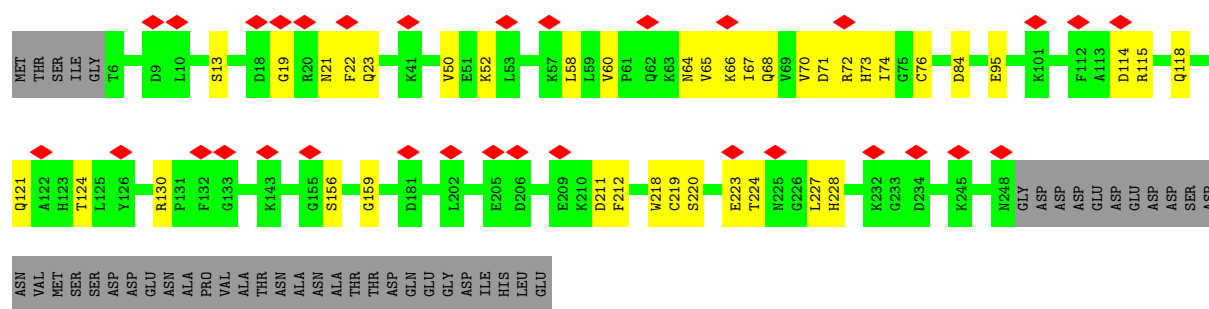


• Molecule 14: Probable proteasome subunit alpha type-7

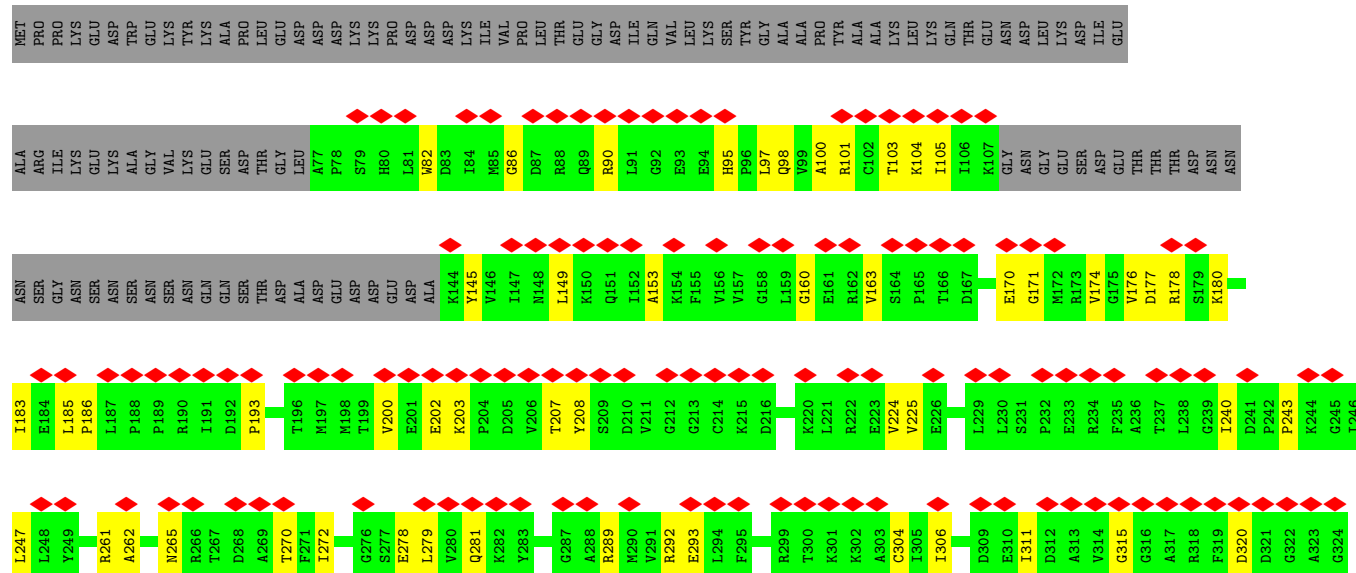
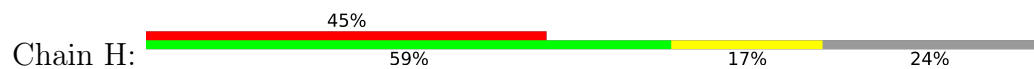


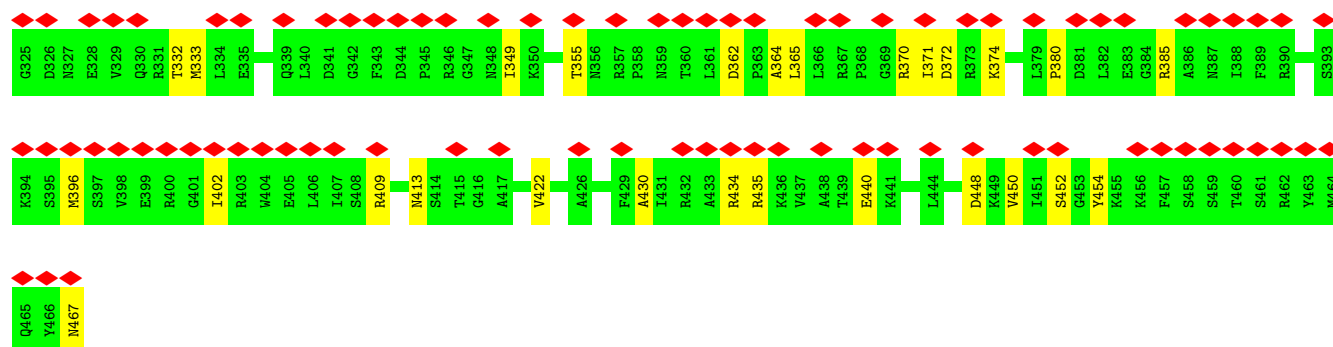


• Molecule 14: Probable proteasome subunit alpha type-7



• Molecule 15: 26S proteasome regulatory subunit 7 homolog





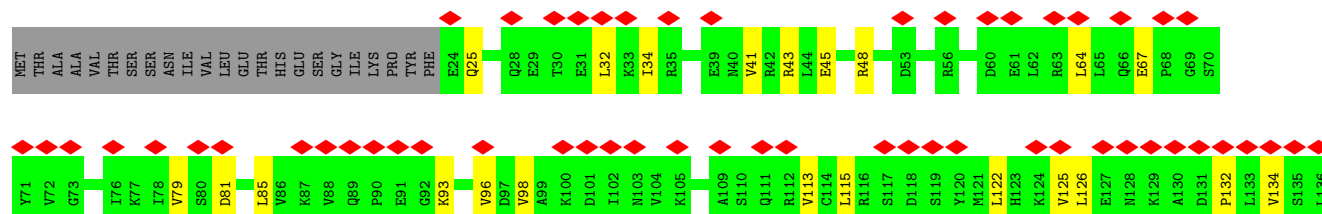
- Molecule 16: 26S proteasome regulatory subunit 4 homolog

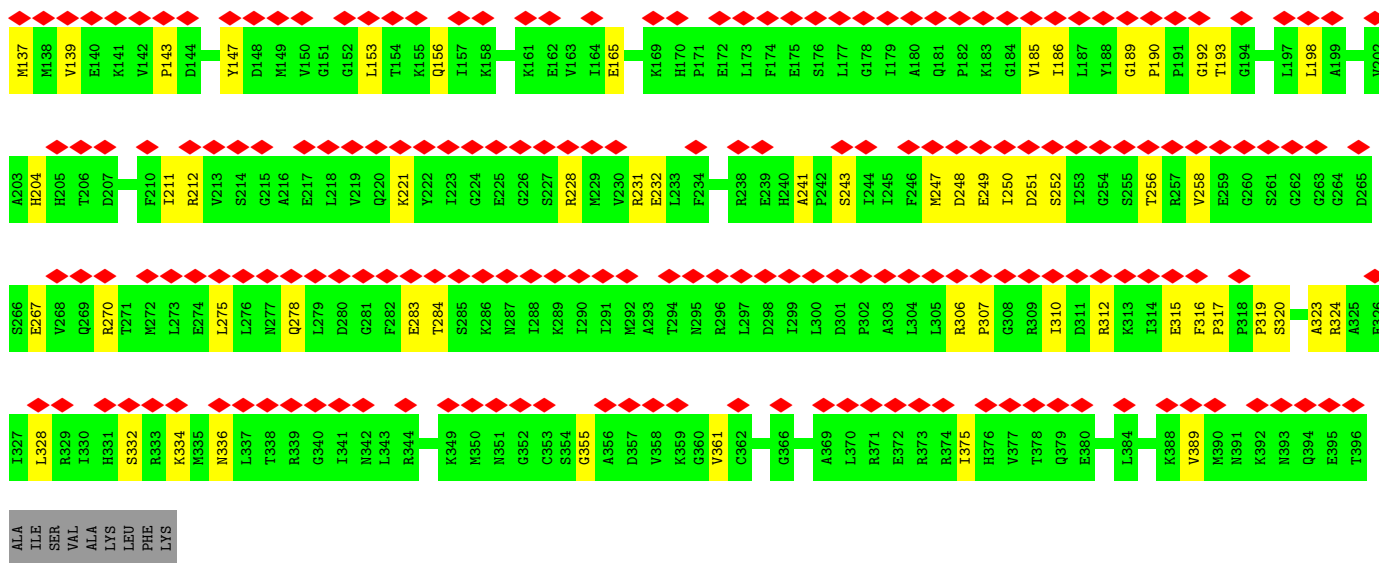
Chain I:



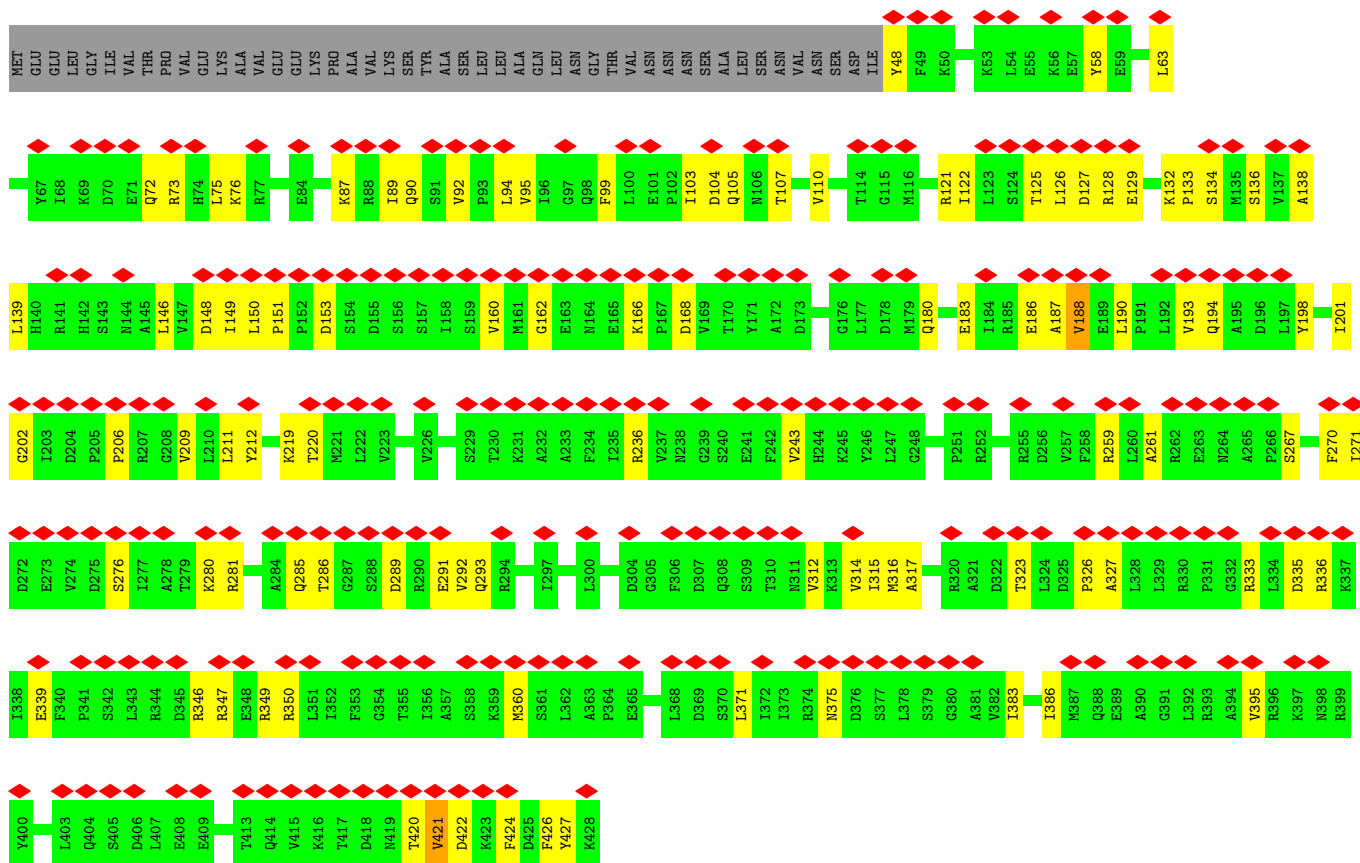
- Molecule 17: 26S proteasome regulatory subunit 8 homolog

Chain J:



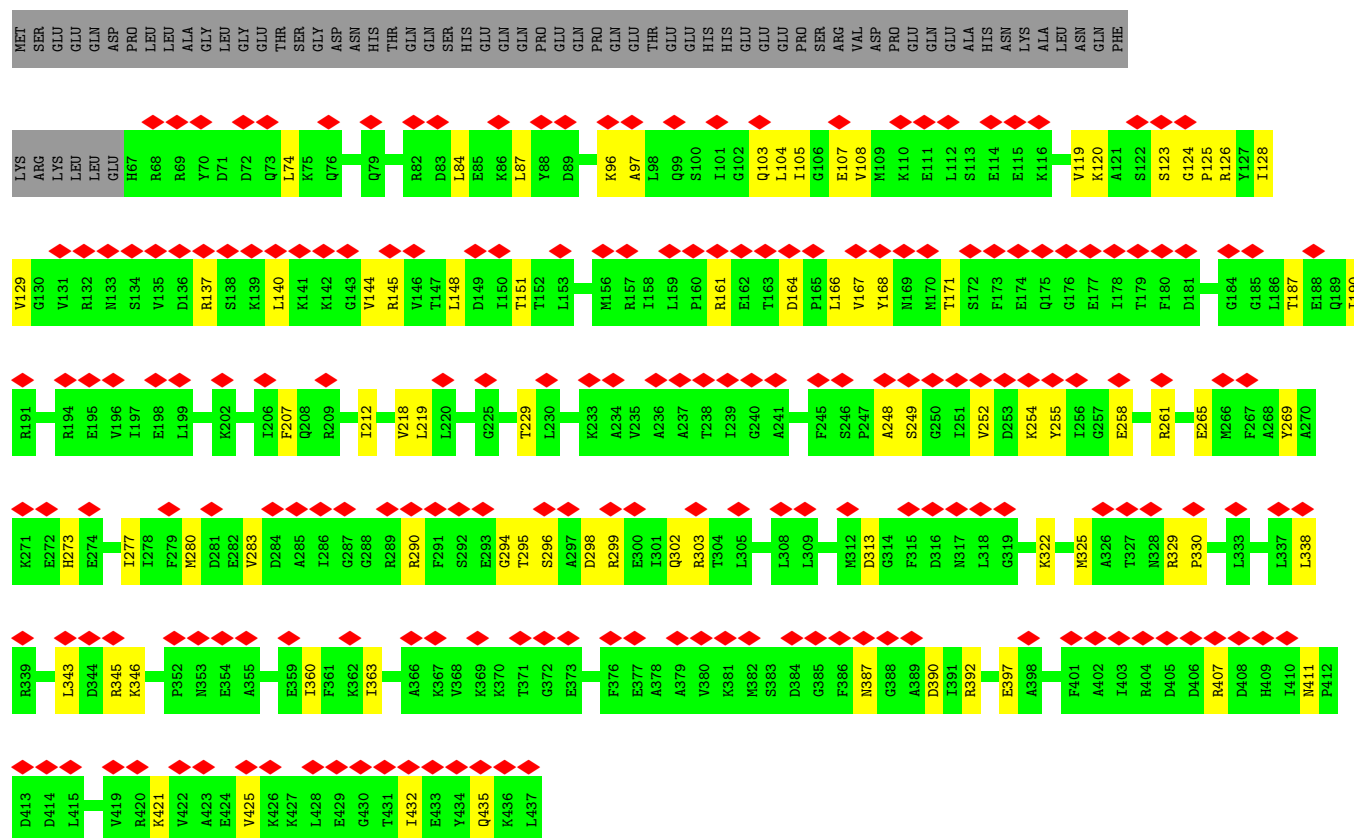


- Molecule 18: 26S proteasome regulatory subunit 6B homolog

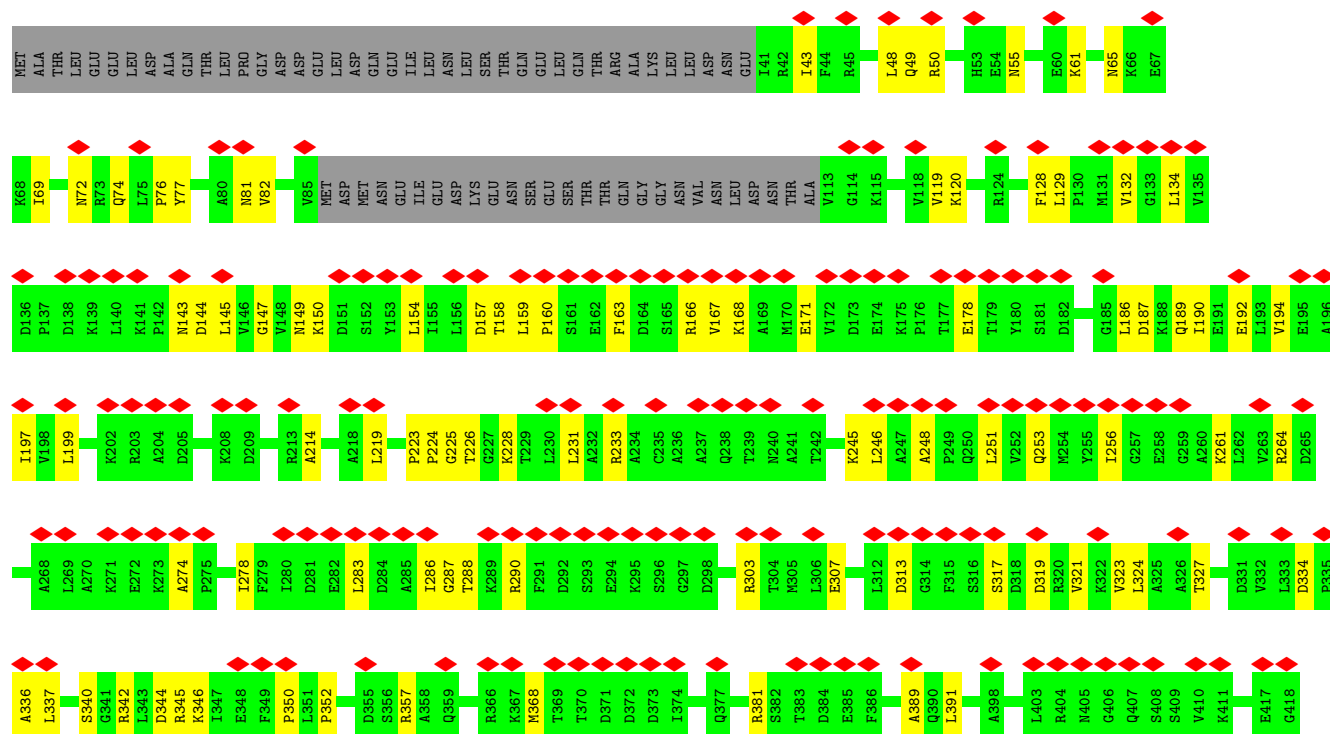


- Molecule 19: 26S proteasome subunit RPT4



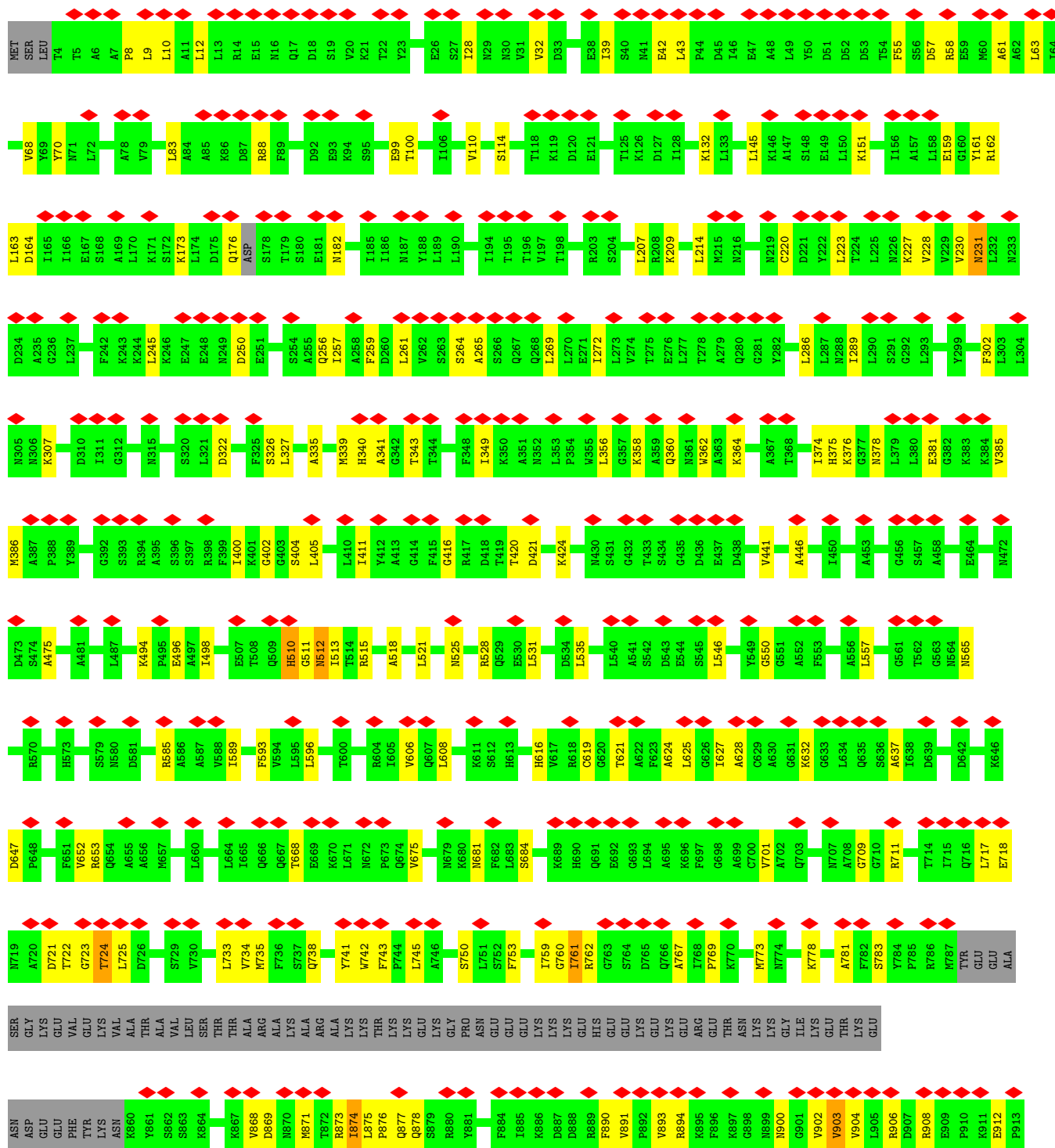


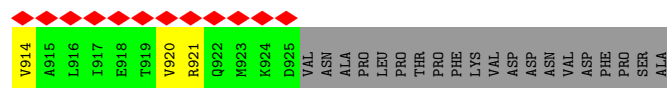
• Molecule 20: 26S proteasome regulatory subunit 6A



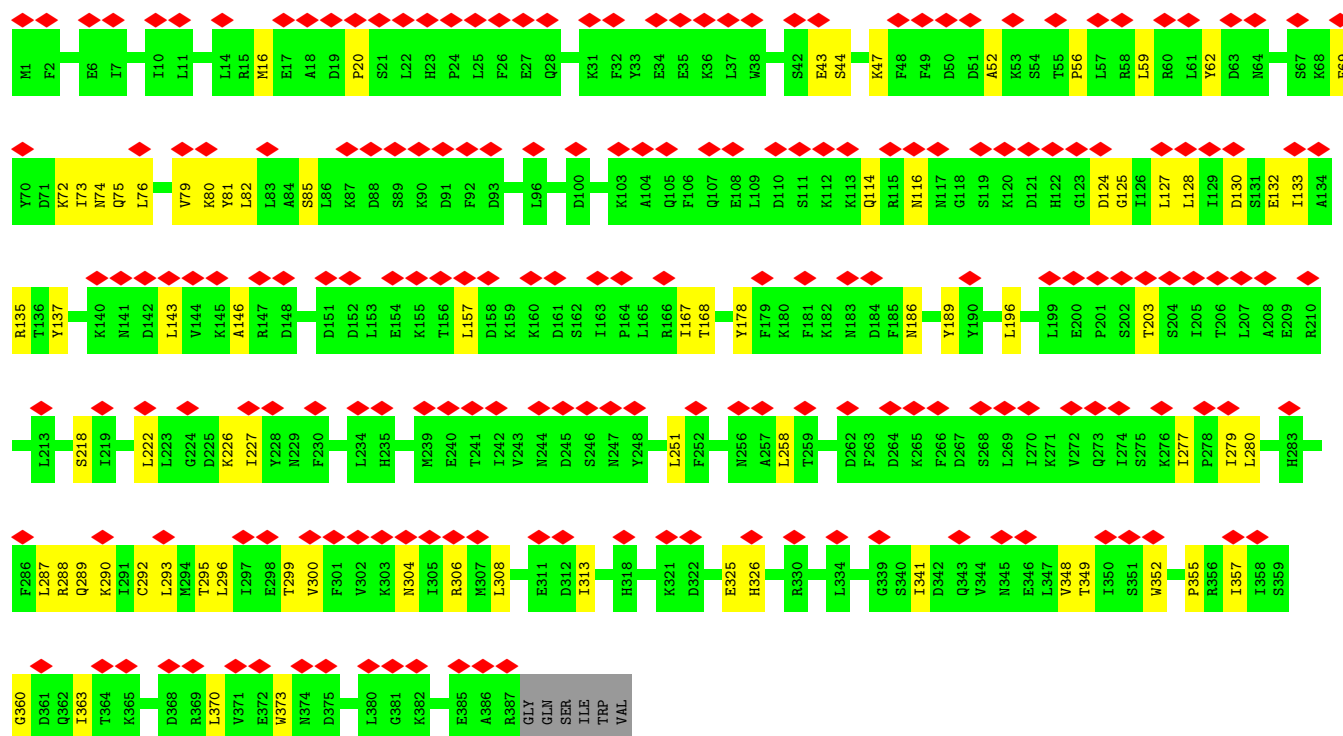
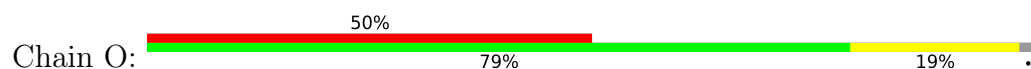


• Molecule 21: 26S proteasome regulatory subunit RPN2

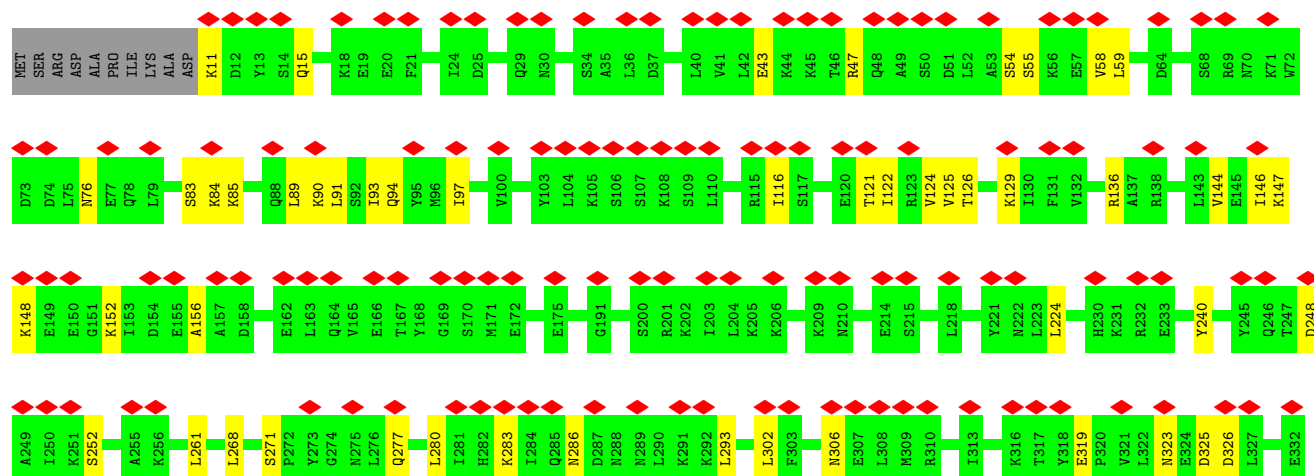
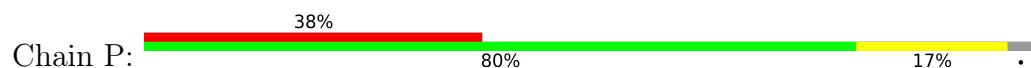


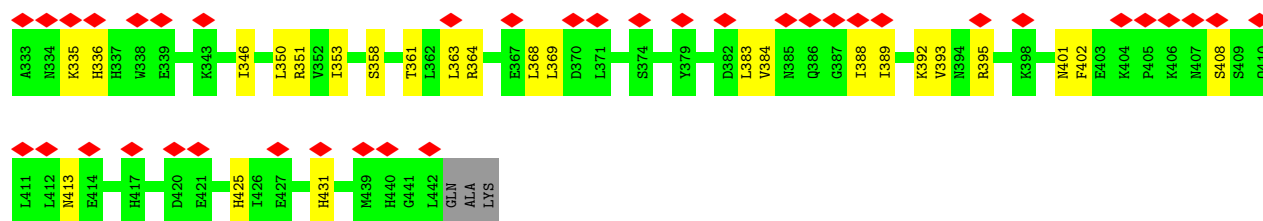


• Molecule 22: 26S proteasome regulatory subunit RPN9



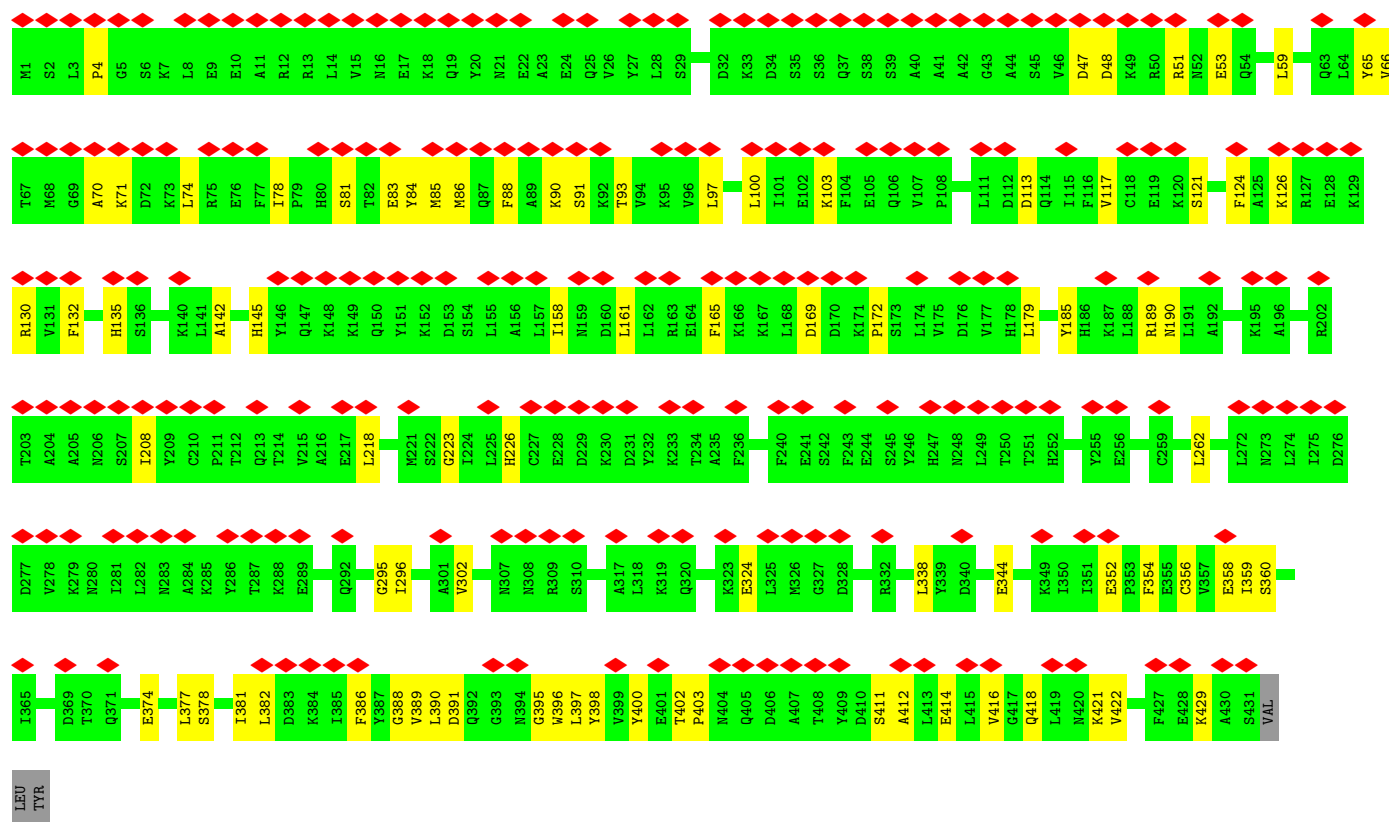
• Molecule 23: 26S proteasome regulatory subunit RPN5





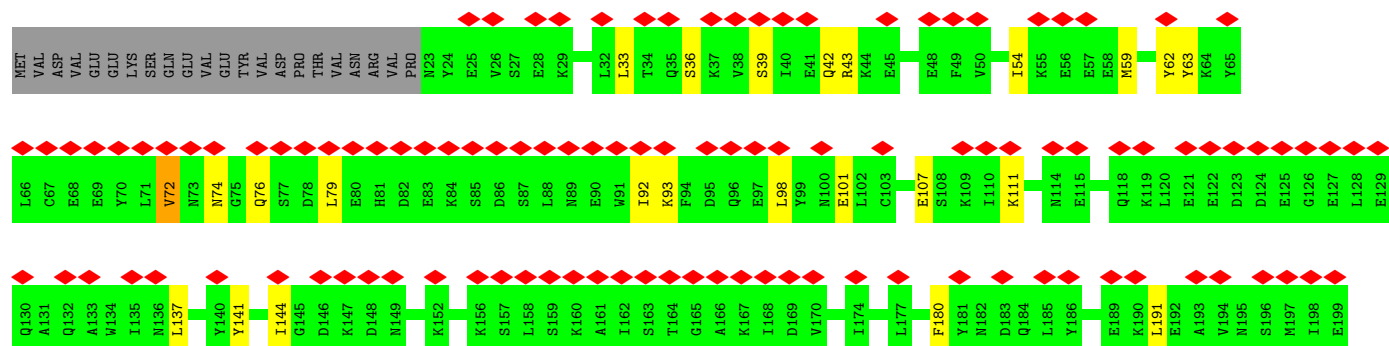
• Molecule 24: 26S proteasome regulatory subunit RPN6

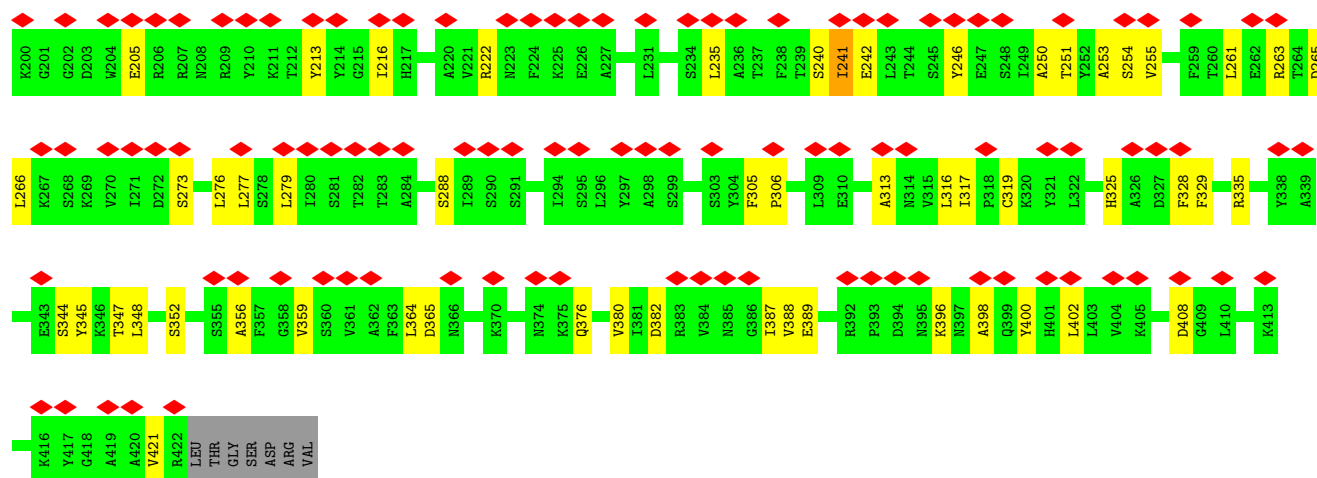
Chain Q: 53% 80% 20%



• Molecule 25: 26S proteasome regulatory subunit RPN7

Chain R: 50% 75% 18% 7%

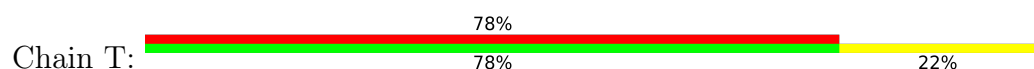


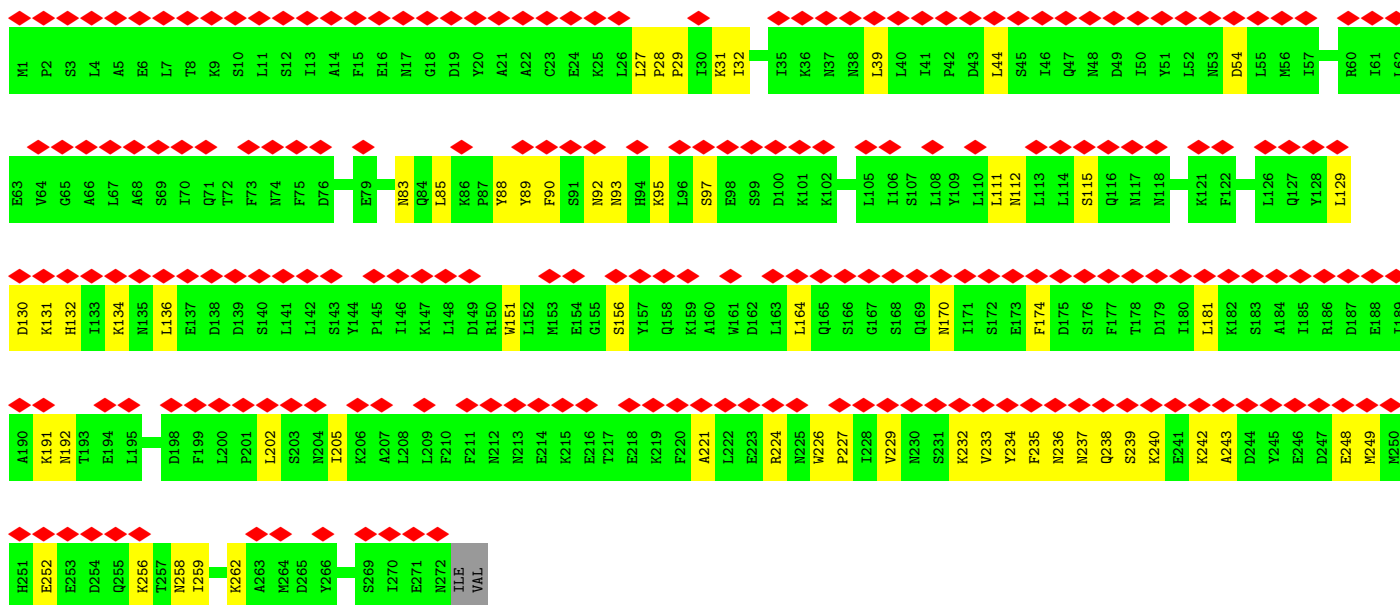


• Molecule 26: 26S proteasome regulatory subunit RPN3

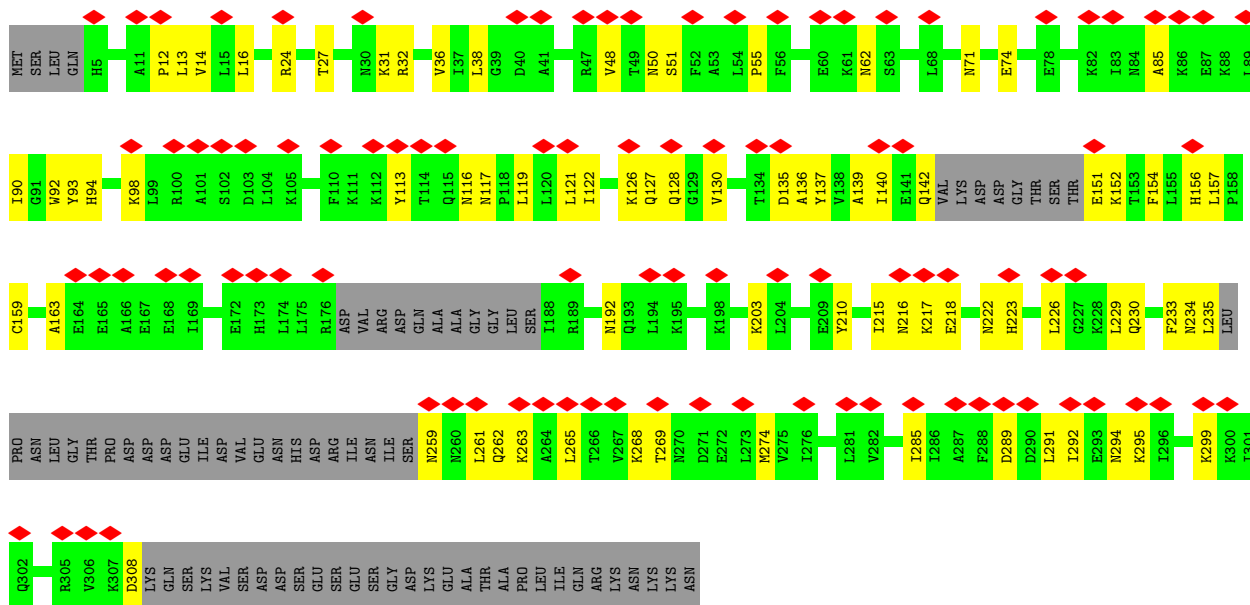


• Molecule 27: 26S proteasome regulatory subunit RPN12

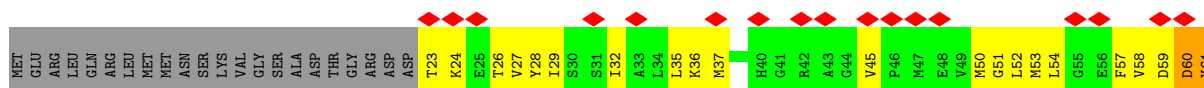


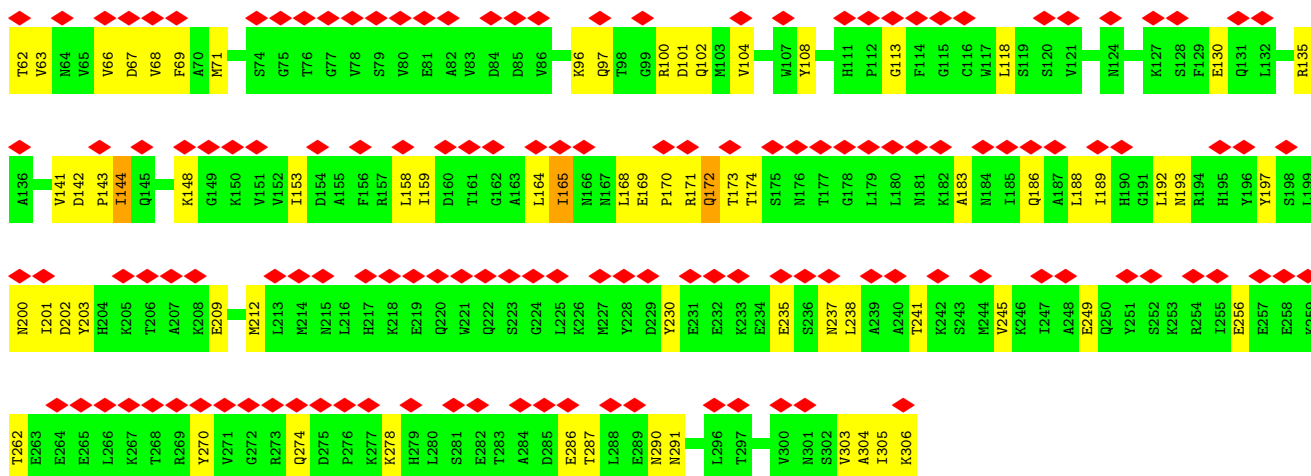


- Molecule 28: 26S proteasome regulatory subunit RPN8

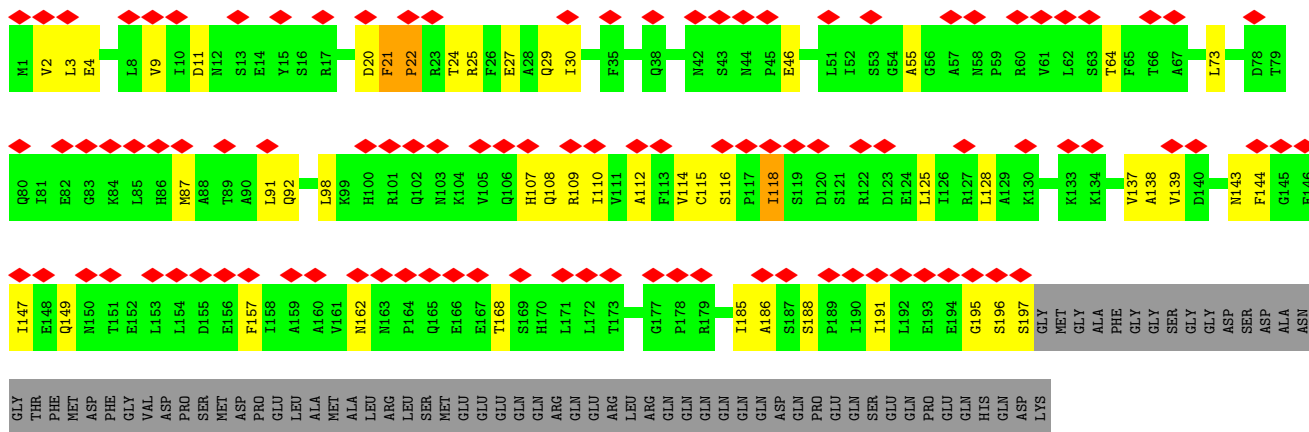
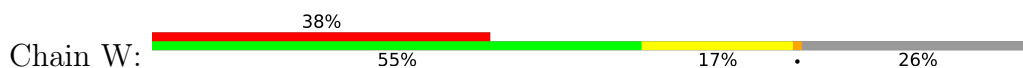


- Molecule 29: Ubiquitin carboxyl-terminal hydrolase RPN11

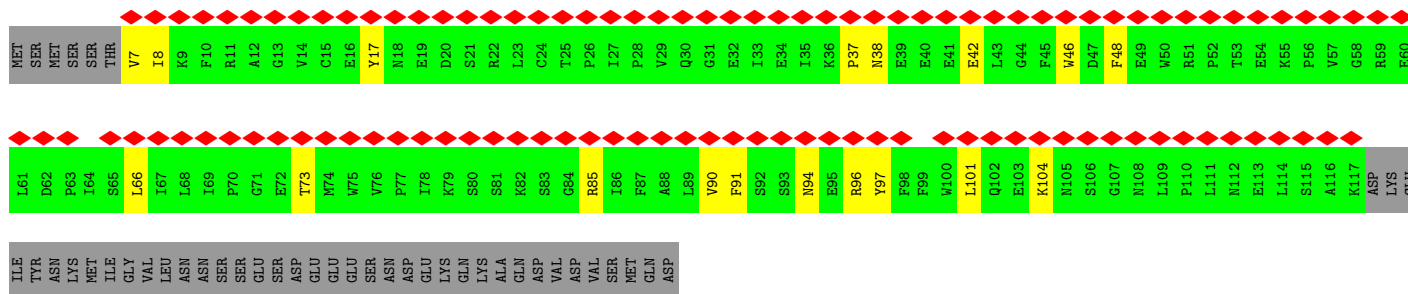




• Molecule 30: 26S proteasome regulatory subunit RPN10



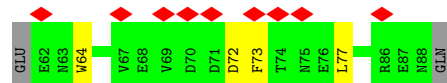
• Molecule 31: 26S proteasome regulatory subunit RPN13



• Molecule 32: 26S proteasome complex subunit SEM1



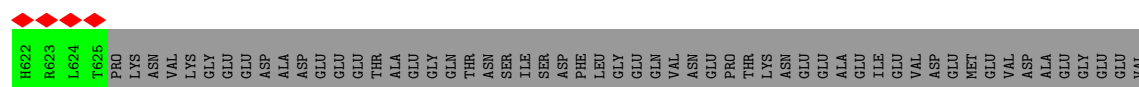
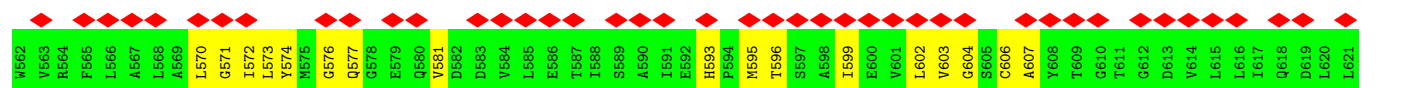
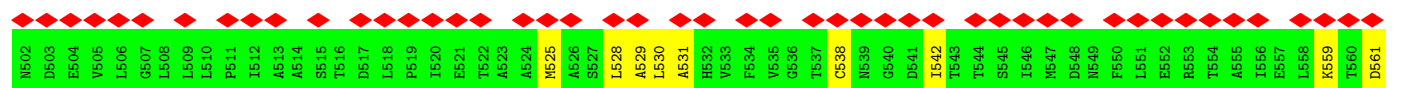
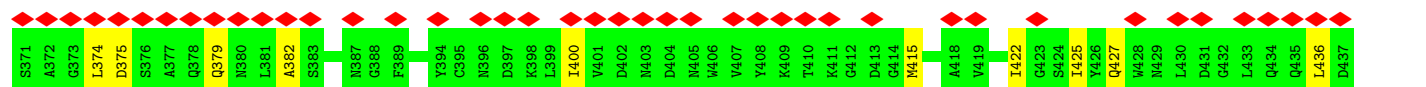
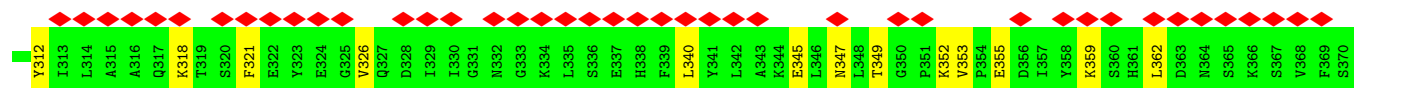
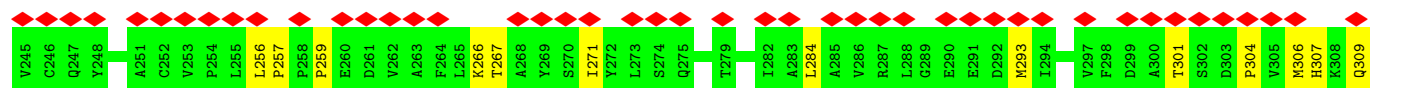
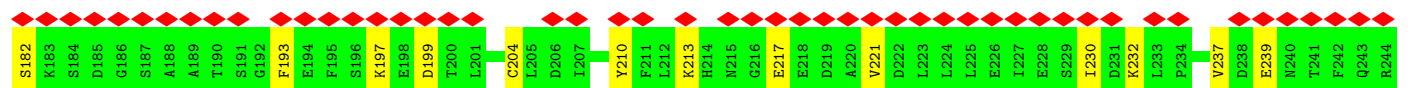
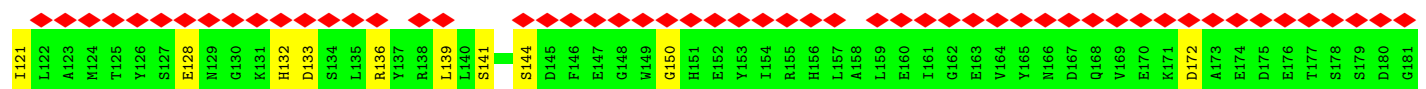
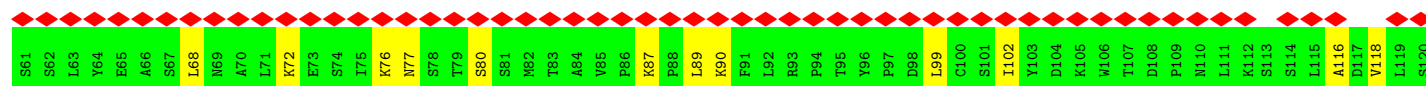
MET SER THR ASP VAL ALA ALA GLN ALA GLN SER LYS ILE ASP LEU THR LYS LYS ASN GLU ILE ASN LYS LYS SER LEU GLU GLU ASP PHE GLU ASP PHE PRO ILE ASP THR TRP ALA ASN GLY THR ILE LYS SER ASN VAL THR GLN THR ILE TRP



● Molecule 33: 26S proteasome regulatory subunit RPN1



MET VAL ASP GLU ASP ASP LYS LYS GLN THR ILE ASP GLU GLN SER LEU THR LYS SER ASN LYS LYS SER LEU THR LYS LYS ASP THR ASP ALA LYS LEU LYS THR ASP L49 E50 L51 L52 V53 E54 R55 L56 K57 E58 D59 D60





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 40585                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 38                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 2.122                                   | Depositor |
| Minimum map value                    | -1.006                                  | Depositor |
| Average map value                    | 0.011                                   | Depositor |
| Map value standard deviation         | 0.088                                   | Depositor |
| Recommended contour level            | 0.686                                   | Depositor |
| Map size (Å)                         | 474.47998, 474.47998, 474.47998         | wwPDB     |
| Map dimensions                       | 360, 360, 360                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.318, 1.318, 1.318                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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     | 0.06         | 0/1541        | 0.21        | 0/2087      |
| 1   | b     | 0.06         | 0/1541        | 0.21        | 0/2087      |
| 2   | 2     | 0.06         | 0/1750        | 0.21        | 0/2373      |
| 2   | i     | 0.06         | 0/1750        | 0.20        | 0/2373      |
| 3   | 3     | 0.07         | 0/1611        | 0.24        | 0/2174      |
| 3   | h     | 0.07         | 0/1611        | 0.24        | 0/2174      |
| 4   | 4     | 0.07         | 0/1589        | 0.24        | 0/2142      |
| 4   | g     | 0.07         | 0/1589        | 0.23        | 0/2142      |
| 5   | 5     | 0.07         | 0/1681        | 0.22        | 0/2274      |
| 5   | f     | 0.07         | 0/1681        | 0.21        | 0/2274      |
| 6   | 6     | 0.07         | 0/1795        | 0.23        | 0/2420      |
| 6   | e     | 0.07         | 0/1795        | 0.23        | 0/2420      |
| 7   | 7     | 0.08         | 0/1821        | 0.24        | 0/2470      |
| 7   | a     | 0.08         | 0/1846        | 0.25        | 0/2503      |
| 8   | A     | 0.07         | 0/1945        | 0.22        | 0/2634      |
| 8   | c     | 0.08         | 0/1945        | 0.23        | 0/2634      |
| 9   | B     | 0.08         | 0/1952        | 0.28        | 0/2642      |
| 9   | j     | 0.07         | 0/1952        | 0.23        | 0/2642      |
| 10  | C     | 0.07         | 0/1934        | 0.24        | 0/2618      |
| 10  | d     | 0.08         | 0/1934        | 0.27        | 0/2618      |
| 11  | D     | 0.09         | 0/1910        | 0.28        | 0/2586      |
| 11  | n     | 0.08         | 0/1910        | 0.24        | 0/2586      |
| 12  | E     | 0.06         | 0/1886        | 0.21        | 0/2541      |
| 12  | m     | 0.07         | 0/1886        | 0.23        | 0/2541      |
| 13  | F     | 0.07         | 0/1823        | 0.24        | 0/2463      |
| 13  | l     | 0.07         | 0/1800        | 0.22        | 0/2433      |
| 14  | G     | 0.07         | 0/1932        | 0.22        | 0/2609      |
| 14  | k     | 0.08         | 0/1932        | 0.22        | 0/2609      |
| 15  | H     | 0.09         | 0/2834        | 0.28        | 0/3816      |
| 16  | I     | 0.08         | 0/2860        | 0.27        | 0/3856      |
| 17  | J     | 0.09         | 0/2964        | 0.28        | 0/3981      |
| 18  | K     | 0.10         | 0/3062        | 0.34        | 0/4132      |
| 19  | L     | 0.09         | 0/2981        | 0.29        | 0/4008      |
| 20  | M     | 0.21         | 1/2903 (0.0%) | 0.29        | 0/3909      |

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5         |
| 21  | N     | 0.10         | 0/6670          | 0.29        | 0/9023          |
| 22  | O     | 0.07         | 0/3243          | 0.25        | 0/4374          |
| 23  | P     | 0.07         | 0/3599          | 0.23        | 0/4854          |
| 24  | Q     | 0.08         | 0/3527          | 0.25        | 0/4748          |
| 25  | R     | 0.08         | 0/3272          | 0.28        | 0/4412          |
| 26  | S     | 0.09         | 0/3966          | 0.35        | 3/5355 (0.1%)   |
| 27  | T     | 0.11         | 0/2279          | 0.36        | 0/3077          |
| 28  | U     | 0.08         | 0/2146          | 0.28        | 0/2893          |
| 29  | V     | 0.10         | 0/2271          | 0.33        | 0/3064          |
| 30  | W     | 0.16         | 0/1557          | 0.32        | 0/2111          |
| 31  | X     | 0.07         | 0/931           | 0.23        | 0/1262          |
| 32  | Y     | 0.10         | 0/239           | 0.33        | 0/322           |
| 33  | Z     | 0.11         | 1/6404 (0.0%)   | 0.26        | 0/8686          |
| All | All   | 0.09         | 2/108050 (0.0%) | 0.26        | 3/145952 (0.0%) |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 20  | M     | 274 | ALA  | C-N   | 10.45 | 1.58        | 1.33     |
| 33  | Z     | 468 | GLU  | C-N   | 6.49  | 1.49        | 1.33     |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 26  | S     | 477 | VAL  | N-CA-C | 12.68 | 123.19      | 111.91   |
| 26  | S     | 477 | VAL  | CA-C-N | -7.12 | 113.00      | 123.11   |
| 26  | S     | 477 | VAL  | C-N-CA | -7.12 | 113.00      | 123.11   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 1     | 1512  | 0        | 1478     | 26      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | b     | 1512  | 0        | 1478     | 32      | 0            |
| 2   | 2     | 1719  | 0        | 1716     | 31      | 0            |
| 2   | i     | 1719  | 0        | 1716     | 36      | 0            |
| 3   | 3     | 1581  | 0        | 1571     | 49      | 0            |
| 3   | h     | 1581  | 0        | 1571     | 33      | 0            |
| 4   | 4     | 1561  | 0        | 1569     | 22      | 0            |
| 4   | g     | 1561  | 0        | 1569     | 30      | 0            |
| 5   | 5     | 1644  | 0        | 1592     | 34      | 0            |
| 5   | f     | 1644  | 0        | 1592     | 28      | 0            |
| 6   | 6     | 1757  | 0        | 1708     | 31      | 0            |
| 6   | e     | 1757  | 0        | 1708     | 46      | 0            |
| 7   | 7     | 1790  | 0        | 1790     | 42      | 0            |
| 7   | a     | 1815  | 0        | 1818     | 40      | 0            |
| 8   | A     | 1907  | 0        | 1901     | 38      | 0            |
| 8   | c     | 1907  | 0        | 1901     | 41      | 0            |
| 9   | B     | 1915  | 0        | 1929     | 45      | 0            |
| 9   | j     | 1915  | 0        | 1929     | 34      | 0            |
| 10  | C     | 1904  | 0        | 1901     | 66      | 0            |
| 10  | d     | 1904  | 0        | 1901     | 36      | 0            |
| 11  | D     | 1881  | 0        | 1892     | 56      | 0            |
| 11  | n     | 1881  | 0        | 1892     | 50      | 0            |
| 12  | E     | 1861  | 0        | 1836     | 38      | 0            |
| 12  | m     | 1861  | 0        | 1836     | 45      | 0            |
| 13  | F     | 1795  | 0        | 1797     | 28      | 0            |
| 13  | l     | 1773  | 0        | 1775     | 28      | 0            |
| 14  | G     | 1892  | 0        | 1883     | 36      | 0            |
| 14  | k     | 1892  | 0        | 1883     | 32      | 0            |
| 15  | H     | 2787  | 0        | 2851     | 57      | 0            |
| 16  | I     | 2822  | 0        | 2870     | 46      | 0            |
| 17  | J     | 2928  | 0        | 3057     | 59      | 0            |
| 18  | K     | 3019  | 0        | 3084     | 74      | 0            |
| 19  | L     | 2937  | 0        | 3011     | 58      | 0            |
| 20  | M     | 2866  | 0        | 2938     | 71      | 0            |
| 21  | N     | 6562  | 0        | 6625     | 124     | 0            |
| 22  | O     | 3182  | 0        | 3207     | 50      | 0            |
| 23  | P     | 3545  | 0        | 3629     | 52      | 0            |
| 24  | Q     | 3471  | 0        | 3495     | 57      | 0            |
| 25  | R     | 3218  | 0        | 3216     | 50      | 0            |
| 26  | S     | 3894  | 0        | 3938     | 58      | 0            |
| 27  | T     | 2235  | 0        | 2207     | 56      | 0            |
| 28  | U     | 2118  | 0        | 2177     | 66      | 0            |
| 29  | V     | 2236  | 0        | 2242     | 85      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 30  | W     | 1534   | 0        | 1542     | 30      | 0            |
| 31  | X     | 906    | 0        | 888      | 14      | 0            |
| 32  | Y     | 236    | 0        | 203      | 4       | 0            |
| 33  | Z     | 6290   | 0        | 6236     | 102     | 0            |
| All | All   | 106227 | 0        | 106548   | 1836    | 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 9.

All (1836) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:C:18:ARG:NE    | 10:C:23:GLU:HG2   | 1.67                     | 1.09              |
| 29:V:59:ASP:O     | 29:V:60:ASP:HB2   | 1.56                     | 1.05              |
| 10:C:18:ARG:CZ    | 10:C:23:GLU:HG2   | 1.91                     | 0.98              |
| 28:U:152:LYS:HE3  | 28:U:154:PHE:CE1  | 1.99                     | 0.96              |
| 10:C:18:ARG:NE    | 10:C:23:GLU:CG    | 2.31                     | 0.93              |
| 3:3:107:PRO:HD2   | 3:3:124:PHE:HB2   | 1.53                     | 0.91              |
| 28:U:152:LYS:HE3  | 28:U:154:PHE:HE1  | 1.38                     | 0.89              |
| 21:N:475:ALA:HB1  | 29:V:61:TYR:CE2   | 2.09                     | 0.87              |
| 21:N:230:VAL:HB   | 21:N:723:GLY:HA3  | 1.56                     | 0.85              |
| 11:D:8:LEU:HD23   | 11:D:17:ILE:HG21  | 1.56                     | 0.85              |
| 28:U:222:ASN:O    | 28:U:223:HIS:ND1  | 2.09                     | 0.84              |
| 5:5:165:TYR:HB3   | 6:6:120:ARG:HH12  | 1.41                     | 0.83              |
| 1:1:20:THR:N      | 1:1:188:SER:HG    | 1.78                     | 0.81              |
| 29:V:61:TYR:HD1   | 29:V:62:THR:H     | 1.29                     | 0.80              |
| 9:B:10:THR:O      | 9:B:12:PHE:CD2    | 2.36                     | 0.79              |
| 12:E:120:ALA:HA   | 12:E:134:MET:HE1  | 1.65                     | 0.78              |
| 10:C:18:ARG:HH11  | 10:C:18:ARG:HG3   | 1.49                     | 0.78              |
| 29:V:118:LEU:HD22 | 29:V:193:ASN:HD21 | 1.49                     | 0.78              |
| 10:C:53:THR:HA    | 10:C:210:ARG:HH12 | 1.49                     | 0.77              |
| 29:V:23:THR:HG22  | 29:V:171:ARG:CZ   | 2.14                     | 0.77              |
| 27:T:242:LYS:HG3  | 27:T:243:ALA:H    | 1.48                     | 0.77              |
| 27:T:233:VAL:HG12 | 27:T:234:TYR:H    | 1.48                     | 0.76              |
| 20:M:74:GLN:HG3   | 20:M:76:PRO:HD2   | 1.66                     | 0.76              |
| 9:B:33:THR:HA     | 9:B:165:GLY:HA3   | 1.65                     | 0.76              |
| 9:B:9:LEU:HD21    | 9:B:125:GLY:HA2   | 1.69                     | 0.75              |
| 11:D:78:LEU:HD13  | 16:I:436:TYR:HE1  | 1.51                     | 0.75              |
| 29:V:50:MET:HG3   | 29:V:71:MET:HB2   | 1.68                     | 0.75              |
| 17:J:306:ARG:HD3  | 17:J:307:PRO:HD2  | 1.69                     | 0.75              |
| 5:5:106:VAL:HA    | 6:6:151:GLU:HG2   | 1.69                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:c:90:ARG:HB2    | 14:k:121:GLN:HE22 | 1.52                     | 0.74              |
| 21:N:223:LEU:HD11 | 21:N:721:ASP:O    | 1.88                     | 0.74              |
| 22:O:304:ASN:HD22 | 29:V:306:LYS:HE3  | 1.52                     | 0.74              |
| 1:b:20:THR:N      | 1:b:148:SER:HG    | 1.84                     | 0.73              |
| 11:n:6:ARG:HB3    | 11:n:125:GLY:HA3  | 1.70                     | 0.73              |
| 10:d:52:VAL:HG23  | 10:d:59:GLN:HE21  | 1.54                     | 0.73              |
| 10:C:18:ARG:NH1   | 16:I:432:LEU:HD23 | 2.04                     | 0.72              |
| 30:W:25:ARG:NH2   | 30:W:115:CYS:SG   | 2.61                     | 0.72              |
| 13:F:155:GLU:H    | 14:G:64:ASN:HD21  | 1.35                     | 0.72              |
| 18:K:285:GLN:HG2  | 19:L:299:ARG:HH11 | 1.55                     | 0.72              |
| 25:R:72:VAL:HA    | 25:R:76:GLN:HE22  | 1.54                     | 0.72              |
| 21:N:475:ALA:CB   | 29:V:61:TYR:OH    | 2.37                     | 0.72              |
| 25:R:33:LEU:O     | 25:R:74:ASN:ND2   | 2.23                     | 0.72              |
| 27:T:224:ARG:HE   | 27:T:235:PHE:HD1  | 1.37                     | 0.72              |
| 4:4:1:MET:HG2     | 4:4:2:ASP:H       | 1.54                     | 0.72              |
| 2:i:79:ALA:HA     | 3:h:129:CYS:HB3   | 1.71                     | 0.71              |
| 15:H:278:GLU:HB2  | 16:I:265:ARG:HH22 | 1.55                     | 0.71              |
| 18:K:132:LYS:HD2  | 18:K:259:ARG:HH22 | 1.55                     | 0.71              |
| 5:f:136:SER:HB3   | 12:m:97:VAL:HG13  | 1.73                     | 0.71              |
| 26:S:428:ARG:HH12 | 27:T:191:LYS:HB2  | 1.54                     | 0.71              |
| 10:C:18:ARG:HH12  | 16:I:432:LEU:HD23 | 1.55                     | 0.71              |
| 21:N:307:LYS:HD3  | 21:N:343:THR:HG21 | 1.72                     | 0.71              |
| 5:f:93:SER:HB2    | 5:f:249:SER:H     | 1.56                     | 0.71              |
| 30:W:162:ASN:HA   | 30:W:168:THR:HG21 | 1.73                     | 0.71              |
| 29:V:23:THR:OG1   | 29:V:172:GLN:HB2  | 1.90                     | 0.70              |
| 18:K:160:VAL:HG12 | 18:K:162:GLY:H    | 1.56                     | 0.70              |
| 24:Q:418:GLN:HE22 | 28:U:292:ILE:HD11 | 1.57                     | 0.70              |
| 20:M:336:ALA:O    | 20:M:342:ARG:NH2  | 2.25                     | 0.70              |
| 9:B:10:THR:HG23   | 10:C:21:GLN:HE21  | 1.57                     | 0.69              |
| 11:D:37:LYS:HE2   | 11:D:160:SER:HA   | 1.73                     | 0.69              |
| 21:N:735:MET:HB3  | 21:N:745:LEU:HB3  | 1.74                     | 0.69              |
| 9:B:108:LYS:HE3   | 9:B:143:ASN:HD22  | 1.58                     | 0.69              |
| 9:j:67:LEU:O      | 9:j:90:ARG:NH1    | 2.24                     | 0.69              |
| 17:J:43:ARG:HE    | 26:S:480:ARG:HB3  | 1.56                     | 0.69              |
| 18:K:280:LYS:HE3  | 18:K:281:ARG:HE   | 1.58                     | 0.69              |
| 28:U:263:LYS:HG3  | 29:V:306:LYS:HD3  | 1.75                     | 0.68              |
| 29:V:59:ASP:O     | 29:V:60:ASP:CB    | 2.38                     | 0.68              |
| 26:S:235:ASN:HD22 | 26:S:268:LEU:HD22 | 1.58                     | 0.68              |
| 8:c:17:ILE:HD13   | 9:j:9:LEU:HD21    | 1.75                     | 0.68              |
| 10:d:49:GLU:O     | 10:d:65:LYS:NZ    | 2.26                     | 0.68              |
| 12:E:123:PHE:CE1  | 12:E:134:MET:SD   | 2.87                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:b:63:CYS:HB2    | 1:b:117:ILE:HB    | 1.76                     | 0.68              |
| 26:S:173:LEU:O    | 26:S:177:ASN:ND2  | 2.27                     | 0.68              |
| 7:7:161:ARG:HD3   | 7:7:169:THR:HB    | 1.75                     | 0.67              |
| 11:D:118:GLN:NE2  | 12:E:83:ALA:O     | 2.26                     | 0.67              |
| 1:1:40:THR:HG22   | 1:1:45:ILE:HG12   | 1.77                     | 0.67              |
| 15:H:185:LEU:HD12 | 15:H:186:PRO:HD2  | 1.76                     | 0.67              |
| 33:Z:530:LEU:HB3  | 33:Z:542:ILE:HD11 | 1.76                     | 0.67              |
| 3:h:124:PHE:HB3   | 3:h:128:GLY:HA2   | 1.75                     | 0.67              |
| 18:K:286:THR:HB   | 19:L:294:GLY:HA2  | 1.75                     | 0.67              |
| 21:N:475:ALA:HB1  | 29:V:61:TYR:HE2   | 1.54                     | 0.67              |
| 11:D:32:CYS:HA    | 11:D:165:GLY:HA3  | 1.75                     | 0.67              |
| 10:C:22:VAL:HG11  | 16:I:433:GLU:HG2  | 1.76                     | 0.66              |
| 20:M:82:VAL:HG22  | 20:M:119:VAL:HG12 | 1.77                     | 0.66              |
| 21:N:920:VAL:HG23 | 21:N:921:ARG:H    | 1.58                     | 0.66              |
| 8:A:37:GLN:NE2    | 14:G:18:ASP:O     | 2.29                     | 0.66              |
| 29:V:45:VAL:HG13  | 29:V:144:ILE:HG13 | 1.76                     | 0.66              |
| 1:1:57:HIS:HB3    | 1:1:60:ILE:HB     | 1.77                     | 0.66              |
| 10:d:50:ARG:NH2   | 10:d:63:THR:OG1   | 2.28                     | 0.66              |
| 33:Z:150:GLY:H    | 33:Z:210:TYR:HE1  | 1.42                     | 0.66              |
| 10:C:18:ARG:CD    | 10:C:23:GLU:HG3   | 2.26                     | 0.66              |
| 2:2:196:LEU:HB3   | 6:e:215:ILE:HB    | 1.78                     | 0.66              |
| 10:d:50:ARG:NH1   | 10:d:59:GLN:O     | 2.29                     | 0.66              |
| 12:E:120:ALA:HA   | 12:E:134:MET:CE   | 2.25                     | 0.66              |
| 9:j:7:PHE:HB3     | 9:j:125:GLY:H     | 1.60                     | 0.66              |
| 24:Q:93:THR:OG1   | 24:Q:130:ARG:NH2  | 2.29                     | 0.65              |
| 10:C:78:ALA:HB3   | 10:C:134:SER:HB3  | 1.76                     | 0.65              |
| 19:L:254:LYS:HB2  | 20:M:256:ILE:HB   | 1.77                     | 0.65              |
| 11:n:66:LYS:HG2   | 11:n:72:VAL:HG12  | 1.79                     | 0.65              |
| 17:J:32:LEU:HD21  | 26:S:174:ARG:HH12 | 1.60                     | 0.65              |
| 21:N:762:ARG:HG3  | 21:N:767:ALA:HB2  | 1.78                     | 0.65              |
| 30:W:143:ASN:ND2  | 30:W:149:GLN:O    | 2.30                     | 0.65              |
| 31:X:38:ASN:HD22  | 31:X:42:GLU:H     | 1.42                     | 0.65              |
| 5:5:146:LYS:NZ    | 12:E:65:GLU:OE1   | 2.28                     | 0.65              |
| 21:N:223:LEU:CD1  | 21:N:721:ASP:O    | 2.45                     | 0.65              |
| 29:V:23:THR:HG22  | 29:V:171:ARG:NE   | 2.11                     | 0.65              |
| 3:3:8:ASN:ND2     | 3:3:30:GLY:O      | 2.25                     | 0.65              |
| 8:A:126:GLN:NE2   | 9:B:81:ASP:OD1    | 2.30                     | 0.65              |
| 22:O:143:LEU:HD13 | 22:O:178:TYR:HA   | 1.79                     | 0.65              |
| 24:Q:51:ARG:HD2   | 24:Q:88:PHE:HA    | 1.76                     | 0.65              |
| 11:D:78:LEU:HD22  | 16:I:436:TYR:OH   | 1.96                     | 0.65              |
| 29:V:188:LEU:HB3  | 29:V:192:LEU:HA   | 1.79                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:X:91:PHE:H     | 31:X:96:ARG:HD3   | 1.62                     | 0.65              |
| 33:Z:925:VAL:HG13 | 33:Z:992:GLU:HB3  | 1.79                     | 0.65              |
| 7:7:58:ASP:OD1    | 7:7:74:ARG:NH2    | 2.29                     | 0.65              |
| 1:1:80:TYR:HB2    | 8:A:102:ALA:HB1   | 1.79                     | 0.65              |
| 1:b:138:VAL:O     | 7:a:94:GLN:NE2    | 2.30                     | 0.65              |
| 16:I:223:GLY:HA3  | 16:I:350:PHE:HB2  | 1.78                     | 0.65              |
| 2:2:63:LEU:HD11   | 2:2:71:TRP:HB3    | 1.79                     | 0.65              |
| 13:F:3:ARG:NH1    | 15:H:467:ASN:OD1  | 2.30                     | 0.65              |
| 27:T:129:LEU:HD12 | 27:T:136:LEU:HD12 | 1.79                     | 0.65              |
| 17:J:336:ASN:ND2  | 25:R:205:GLU:OE1  | 2.31                     | 0.64              |
| 23:P:125:VAL:HA   | 23:P:136:ARG:HG2  | 1.78                     | 0.64              |
| 10:C:60:ASP:HA    | 10:C:232:PRO:HG2  | 1.80                     | 0.64              |
| 8:c:63:LEU:HD23   | 14:k:159:GLY:H    | 1.60                     | 0.64              |
| 10:C:18:ARG:HG3   | 10:C:18:ARG:NH1   | 2.08                     | 0.64              |
| 14:G:108:PRO:HG2  | 14:G:111:ALA:HB3  | 1.80                     | 0.64              |
| 8:A:53:VAL:HG21   | 8:A:144:VAL:HG21  | 1.78                     | 0.64              |
| 28:U:55:PRO:HB3   | 29:V:97:GLN:HB3   | 1.79                     | 0.64              |
| 28:U:217:LYS:HG2  | 28:U:218:GLU:HG3  | 1.80                     | 0.64              |
| 9:j:118:MET:HE1   | 9:j:130:PHE:HB2   | 1.80                     | 0.64              |
| 10:C:119:LYS:HD3  | 10:C:153:PRO:HA   | 1.79                     | 0.63              |
| 28:U:265:LEU:O    | 28:U:269:THR:N    | 2.31                     | 0.63              |
| 7:a:137:ARG:HA    | 7:a:142:PRO:HG3   | 1.80                     | 0.63              |
| 10:d:4:ARG:HG3    | 10:d:5:ARG:H      | 1.63                     | 0.63              |
| 12:m:24:VAL:HG13  | 12:m:161:SER:HB2  | 1.79                     | 0.63              |
| 18:K:271:ILE:HB   | 18:K:316:MET:HG2  | 1.81                     | 0.63              |
| 11:D:66:LYS:HG2   | 11:D:72:VAL:HG12  | 1.79                     | 0.63              |
| 24:Q:85:MET:HB3   | 24:Q:91:SER:HA    | 1.81                     | 0.63              |
| 3:h:11:ILE:HD12   | 3:h:146:LEU:HD11  | 1.80                     | 0.63              |
| 29:V:52:LEU:HD11  | 29:V:104:VAL:HG13 | 1.79                     | 0.63              |
| 1:b:47:ASN:ND2    | 2:i:150:VAL:O     | 2.32                     | 0.63              |
| 21:N:525:ASN:HD21 | 21:N:535:LEU:HD23 | 1.64                     | 0.63              |
| 33:Z:819:GLY:HA3  | 33:Z:827:LEU:HD21 | 1.80                     | 0.63              |
| 4:g:183:ILE:HB    | 4:g:190:ARG:HB2   | 1.79                     | 0.62              |
| 7:a:161:ARG:HD3   | 7:a:169:THR:HB    | 1.79                     | 0.62              |
| 9:B:16:GLY:HA2    | 10:C:24:TYR:HB3   | 1.80                     | 0.62              |
| 28:U:152:LYS:CE   | 28:U:154:PHE:CE1  | 2.78                     | 0.62              |
| 33:Z:72:LYS:NZ    | 33:Z:144:SER:O    | 2.31                     | 0.62              |
| 1:1:47:ASN:ND2    | 2:2:150:VAL:O     | 2.32                     | 0.62              |
| 3:3:28:ARG:HB2    | 3:3:183:TRP:HB2   | 1.81                     | 0.62              |
| 4:g:17:SER:HB2    | 4:g:34:LYS:HB2    | 1.81                     | 0.62              |
| 21:N:619:CYS:HB2  | 21:N:652:VAL:HG22 | 1.82                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:Z:257:PRO:HB2  | 33:Z:259:PRO:HD2  | 1.80                     | 0.62              |
| 4:4:29:LYS:HD2    | 5:5:199:GLY:HA2   | 1.80                     | 0.62              |
| 5:f:170:LEU:HG    | 5:f:192:SER:HB2   | 1.80                     | 0.62              |
| 1:b:198:THR:HG23  | 1:b:200:ALA:H     | 1.64                     | 0.62              |
| 8:A:144:VAL:HG12  | 8:A:154:ILE:HG12  | 1.81                     | 0.62              |
| 10:d:124:GLN:NE2  | 11:n:127:ARG:O    | 2.32                     | 0.62              |
| 18:K:220:THR:HG21 | 19:L:313:ASP:HB3  | 1.80                     | 0.62              |
| 25:R:359:VAL:HG21 | 25:R:364:LEU:HD13 | 1.81                     | 0.62              |
| 28:U:259:ASN:HA   | 29:V:306:LYS:H    | 1.65                     | 0.62              |
| 29:V:286:GLU:O    | 29:V:290:ASN:ND2  | 2.33                     | 0.62              |
| 4:4:96:ARG:NH1    | 4:4:97:PRO:O      | 2.33                     | 0.62              |
| 5:f:138:CYS:HB3   | 5:f:149:ILE:HG13  | 1.81                     | 0.62              |
| 18:K:134:SER:OG   | 18:K:259:ARG:NH1  | 2.33                     | 0.62              |
| 20:M:334:ASP:HB3  | 20:M:337:LEU:HG   | 1.81                     | 0.62              |
| 33:Z:352:LYS:HE2  | 33:Z:462:VAL:HG23 | 1.82                     | 0.62              |
| 11:D:78:LEU:HB2   | 16:I:436:TYR:CE1  | 2.35                     | 0.62              |
| 22:O:306:ARG:HH12 | 22:O:349:THR:HB   | 1.64                     | 0.62              |
| 33:Z:375:ASP:H    | 33:Z:379:GLN:HE21 | 1.45                     | 0.62              |
| 16:I:426:ASN:HB2  | 17:J:306:ARG:HH12 | 1.65                     | 0.62              |
| 2:2:81:THR:HG23   | 2:2:127:LEU:HD21  | 1.81                     | 0.62              |
| 10:C:120:GLN:NE2  | 11:D:81:ASP:OD1   | 2.32                     | 0.62              |
| 28:U:116:ASN:OD1  | 28:U:117:ASN:N    | 2.31                     | 0.62              |
| 1:1:198:THR:HG23  | 1:1:200:ALA:H     | 1.65                     | 0.61              |
| 5:f:106:VAL:HA    | 6:e:151:GLU:HG2   | 1.81                     | 0.61              |
| 14:G:113:ALA:HB2  | 14:G:138:PHE:HZ   | 1.64                     | 0.61              |
| 19:L:219:LEU:HB2  | 19:L:343:LEU:HD21 | 1.81                     | 0.61              |
| 21:N:421:ASP:HA   | 21:N:424:LYS:HE2  | 1.81                     | 0.61              |
| 21:N:515:ARG:HB2  | 21:N:546:LEU:HD22 | 1.82                     | 0.61              |
| 33:Z:436:LEU:HD22 | 33:Z:455:ILE:HG13 | 1.81                     | 0.61              |
| 5:5:283:ASN:ND2   | 4:g:148:TYR:O     | 2.33                     | 0.61              |
| 20:M:422:VAL:HG13 | 20:M:426:LYS:HB2  | 1.80                     | 0.61              |
| 22:O:44:SER:O     | 22:O:47:LYS:N     | 2.34                     | 0.61              |
| 26:S:264:VAL:HB   | 26:S:268:LEU:HB2  | 1.81                     | 0.61              |
| 26:S:389:LYS:HZ3  | 26:S:425:ARG:HG3  | 1.64                     | 0.61              |
| 33:Z:570:LEU:HD23 | 33:Z:573:LEU:HD12 | 1.82                     | 0.61              |
| 5:f:273:TRP:HA    | 5:f:276:LYS:HE2   | 1.83                     | 0.61              |
| 14:G:27:ALA:HB1   | 14:G:133:GLY:HA2  | 1.81                     | 0.61              |
| 2:i:66:ILE:HG23   | 2:i:89:GLY:HA2    | 1.82                     | 0.61              |
| 6:e:49:ILE:HG22   | 6:e:54:ILE:HA     | 1.81                     | 0.61              |
| 14:G:68:GLN:O     | 14:G:76:CYS:N     | 2.30                     | 0.61              |
| 12:m:151:ASP:O    | 12:m:154:GLN:NE2  | 2.33                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 15:H:364:ALA:O   | 15:H:370:ARG:NH1  | 2.33                     | 0.61              |
| 33:Z:347:ASN:HA  | 33:Z:352:LYS:HD2  | 1.82                     | 0.61              |
| 9:B:184:GLU:OE1  | 24:Q:90:LYS:NZ    | 2.27                     | 0.61              |
| 21:N:528:ARG:HB3 | 21:N:531:LEU:HB2  | 1.83                     | 0.61              |
| 10:C:4:ARG:HG3   | 16:I:289:THR:HG21 | 1.82                     | 0.61              |
| 12:E:85:ALA:HB2  | 12:E:140:VAL:HG21 | 1.83                     | 0.61              |
| 4:g:66:LEU:HB2   | 11:n:94:GLN:HG3   | 1.83                     | 0.61              |
| 21:N:227:LYS:HA  | 21:N:723:GLY:HA2  | 1.83                     | 0.61              |
| 21:N:511:GLY:O   | 21:N:515:ARG:NH1  | 2.34                     | 0.61              |
| 3:3:7:ILE:HG23   | 3:3:32:GLN:HG3    | 1.83                     | 0.61              |
| 7:7:48:LYS:HG2   | 7:7:53:VAL:HG12   | 1.83                     | 0.61              |
| 2:i:47:THR:HB    | 2:i:60:CYS:H      | 1.65                     | 0.61              |
| 10:C:63:THR:HB   | 10:C:66:LEU:HB3   | 1.82                     | 0.61              |
| 8:c:167:ALA:HB3  | 9:j:55:LEU:HD13   | 1.83                     | 0.61              |
| 18:K:187:ALA:HB2 | 18:K:336:ARG:HE   | 1.66                     | 0.61              |
| 9:j:3:ASP:HB3    | 11:n:4:TYR:HB2    | 1.83                     | 0.61              |
| 12:m:130:GLU:HB2 | 12:m:132:ARG:HH12 | 1.66                     | 0.61              |
| 20:M:278:ILE:HB  | 20:M:323:VAL:HG22 | 1.82                     | 0.61              |
| 21:N:512:ASN:N   | 21:N:512:ASN:OD1  | 2.34                     | 0.61              |
| 23:P:147:LYS:HB3 | 23:P:152:LYS:HB2  | 1.82                     | 0.61              |
| 1:b:182:ILE:HG12 | 1:b:189:GLY:HA2   | 1.83                     | 0.60              |
| 6:e:78:ALA:HB2   | 7:a:167:GLY:HA3   | 1.82                     | 0.60              |
| 19:L:103:GLN:HB2 | 20:M:128:PHE:HB3  | 1.82                     | 0.60              |
| 33:Z:774:ARG:HD3 | 33:Z:810:ASN:HD21 | 1.65                     | 0.60              |
| 3:3:190:ILE:HA   | 3:3:195:VAL:HG22  | 1.83                     | 0.60              |
| 33:Z:784:SER:O   | 33:Z:826:ARG:NH1  | 2.34                     | 0.60              |
| 27:T:89:TYR:H    | 27:T:97:SER:HB3   | 1.66                     | 0.60              |
| 3:3:27:LEU:HB3   | 3:3:39:LYS:HA     | 1.83                     | 0.60              |
| 4:g:59:TYR:O     | 4:g:63:ASN:ND2    | 2.35                     | 0.60              |
| 20:M:171:GLU:HG3 | 20:M:245:LYS:HE3  | 1.82                     | 0.60              |
| 26:S:477:VAL:O   | 26:S:477:VAL:HG12 | 2.02                     | 0.60              |
| 2:2:70:ILE:HG12  | 2:2:131:GLY:HA3   | 1.83                     | 0.60              |
| 1:b:110:ASP:OD2  | 7:a:35:GLN:NE2    | 2.34                     | 0.60              |
| 4:g:19:LYS:HB3   | 4:g:31:SER:HA     | 1.83                     | 0.60              |
| 1:1:145:ILE:HD11 | 1:1:154:TYR:HD1   | 1.66                     | 0.60              |
| 3:h:172:LEU:HD22 | 3:h:202:MET:HB3   | 1.84                     | 0.60              |
| 15:H:243:PRO:HB3 | 15:H:372:ASP:HB2  | 1.81                     | 0.60              |
| 21:N:230:VAL:CB  | 21:N:723:GLY:HA3  | 2.29                     | 0.60              |
| 3:h:30:GLY:HA2   | 3:h:36:VAL:HG23   | 1.84                     | 0.60              |
| 24:Q:185:TYR:HB3 | 24:Q:190:ASN:HB3  | 1.84                     | 0.60              |
| 27:T:39:LEU:HD13 | 27:T:54:ASP:HB2   | 1.83                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:3:173:ASN:ND2   | 6:e:176:LYS:O     | 2.33                     | 0.60              |
| 1:b:40:THR:HG22   | 1:b:45:ILE:HG12   | 1.83                     | 0.60              |
| 11:n:163:THR:O    | 11:n:172:ARG:NH2  | 2.35                     | 0.60              |
| 18:K:89:ILE:HG23  | 29:V:148:LYS:HB3  | 1.84                     | 0.60              |
| 22:O:341:ILE:HG22 | 22:O:348:VAL:HG13 | 1.83                     | 0.60              |
| 4:g:4:ILE:HG22    | 4:g:103:LEU:HD12  | 1.84                     | 0.60              |
| 7:a:232:ILE:HB    | 7:a:240:THR:HB    | 1.84                     | 0.60              |
| 11:n:118:GLN:HE22 | 12:m:86:ARG:HB3   | 1.66                     | 0.60              |
| 15:H:247:LEU:HB3  | 15:H:374:LYS:HA   | 1.83                     | 0.60              |
| 19:L:74:LEU:HD23  | 20:M:48:LEU:HB2   | 1.82                     | 0.60              |
| 29:V:96:LYS:HA    | 29:V:101:ASP:HB2  | 1.83                     | 0.60              |
| 33:Z:796:LEU:HD13 | 33:Z:815:MET:HG2  | 1.82                     | 0.60              |
| 1:1:113:THR:HG23  | 1:1:134:LEU:HD13  | 1.84                     | 0.60              |
| 3:3:103:TYR:OH    | 4:4:93:ARG:NH1    | 2.35                     | 0.60              |
| 7:7:58:ASP:HA     | 7:7:228:PHE:HA    | 1.84                     | 0.60              |
| 2:i:192:ILE:HG23  | 2:i:199:GLY:HA2   | 1.84                     | 0.60              |
| 2:i:201:ASN:ND2   | 2:i:218:ASN:OD1   | 2.35                     | 0.60              |
| 6:e:75:GLY:HA3    | 6:e:126:VAL:HA    | 1.82                     | 0.60              |
| 9:j:92:VAL:HG21   | 9:j:117:ILE:HD11  | 1.84                     | 0.60              |
| 11:n:162:GLN:OE1  | 11:n:172:ARG:NH2  | 2.33                     | 0.60              |
| 2:i:104:ARG:NH2   | 8:c:148:GLU:OE2   | 2.35                     | 0.59              |
| 9:B:217:GLU:HG2   | 9:B:231:LYS:HB3   | 1.84                     | 0.59              |
| 14:G:70:VAL:N     | 14:G:74:ILE:O     | 2.35                     | 0.59              |
| 21:N:261:LEU:HA   | 21:N:264:SER:HB2  | 1.84                     | 0.59              |
| 25:R:382:ASP:HB3  | 25:R:387:ILE:H    | 1.67                     | 0.59              |
| 6:6:29:GLY:O      | 6:6:216:GLN:NE2   | 2.35                     | 0.59              |
| 2:i:93:GLU:O      | 9:j:90:ARG:NH2    | 2.30                     | 0.59              |
| 10:C:155:GLY:O    | 11:D:83:ARG:NH1   | 2.34                     | 0.59              |
| 28:U:48:VAL:HG22  | 28:U:90:ILE:HD11  | 1.84                     | 0.59              |
| 33:Z:446:GLU:HG2  | 33:Z:484:LYS:HG3  | 1.84                     | 0.59              |
| 5:5:244:ALA:HB1   | 3:h:179:ALA:HB1   | 1.83                     | 0.59              |
| 6:6:43:ALA:HB1    | 6:6:221:LEU:HD11  | 1.84                     | 0.59              |
| 6:6:57:ARG:NH1    | 7:7:193:ASP:O     | 2.34                     | 0.59              |
| 10:C:18:ARG:HD3   | 10:C:23:GLU:HG3   | 1.85                     | 0.59              |
| 10:C:201:THR:HG22 | 10:C:203:SER:H    | 1.67                     | 0.59              |
| 8:c:41:SER:HA     | 8:c:54:SER:HA     | 1.84                     | 0.59              |
| 10:d:54:SER:H     | 10:d:210:ARG:HH21 | 1.49                     | 0.59              |
| 15:H:101:ARG:HE   | 15:H:171:GLY:HA2  | 1.67                     | 0.59              |
| 21:N:494:LYS:HE2  | 21:N:496:GLU:HB3  | 1.84                     | 0.59              |
| 29:V:53:MET:HA    | 29:V:68:VAL:HG12  | 1.83                     | 0.59              |
| 33:Z:914:LEU:HB2  | 33:Z:980:VAL:HG13 | 1.84                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:b:76:ASP:OD2   | 2:i:113:LYS:NZ    | 2.35                     | 0.59              |
| 7:a:129:LEU:HD13 | 7:a:147:ILE:HD13  | 1.83                     | 0.59              |
| 10:d:70:ASN:OD1  | 10:d:71:ASP:N     | 2.34                     | 0.59              |
| 33:Z:230:ILE:HB  | 33:Z:267:THR:HG21 | 1.82                     | 0.59              |
| 8:c:129:GLN:HB3  | 9:j:127:VAL:HA    | 1.85                     | 0.59              |
| 13:l:207:THR:OG1 | 13:l:210:ASN:ND2  | 2.35                     | 0.59              |
| 15:H:98:GLN:N    | 15:H:176:VAL:O    | 2.32                     | 0.59              |
| 8:c:87:PRO:O     | 14:k:121:GLN:NE2  | 2.35                     | 0.59              |
| 26:S:400:LYS:HG3 | 26:S:445:THR:HB   | 1.84                     | 0.59              |
| 20:M:192:GLU:OE1 | 20:M:345:ARG:NH1  | 2.32                     | 0.59              |
| 27:T:248:GLU:HG3 | 27:T:249:MET:HG2  | 1.85                     | 0.59              |
| 6:6:170:ASP:HB3  | 6:6:176:LYS:HD2   | 1.84                     | 0.59              |
| 10:C:26:LEU:HD23 | 10:C:29:ILE:HD12  | 1.85                     | 0.59              |
| 25:R:380:VAL:HB  | 25:R:389:GLU:HB3  | 1.85                     | 0.59              |
| 12:m:48:LEU:HD21 | 12:m:77:ALA:HB2   | 1.83                     | 0.59              |
| 15:H:380:PRO:O   | 15:H:385:ARG:NH1  | 2.36                     | 0.59              |
| 28:U:71:ASN:ND2  | 30:W:64:THR:OG1   | 2.35                     | 0.59              |
| 28:U:126:LYS:HB3 | 28:U:128:GLN:HE21 | 1.67                     | 0.59              |
| 7:a:215:ARG:HG2  | 7:a:247:VAL:HG13  | 1.83                     | 0.59              |
| 11:D:48:ARG:NH1  | 11:D:60:THR:O     | 2.35                     | 0.59              |
| 8:c:15:ILE:HD12  | 8:c:17:ILE:HD12   | 1.84                     | 0.59              |
| 12:m:18:GLU:OE1  | 12:m:20:ARG:NH2   | 2.36                     | 0.59              |
| 15:H:103:THR:O   | 20:M:166:ARG:NH2  | 2.35                     | 0.59              |
| 7:7:215:ARG:HG2  | 7:7:247:VAL:HG13  | 1.85                     | 0.58              |
| 8:c:157:ASP:OD1  | 8:c:161:TYR:N     | 2.36                     | 0.58              |
| 10:d:39:MET:HA   | 10:d:44:ILE:HG12  | 1.84                     | 0.58              |
| 13:l:47:VAL:HG22 | 13:l:213:ILE:HG12 | 1.85                     | 0.58              |
| 21:N:10:LEU:HB3  | 21:N:42:GLU:HG3   | 1.84                     | 0.58              |
| 6:e:35:ALA:HB2   | 6:e:141:VAL:HG23  | 1.85                     | 0.58              |
| 12:E:117:CYS:HA  | 12:E:120:ALA:HB3  | 1.85                     | 0.58              |
| 8:c:63:LEU:HD12  | 8:c:68:VAL:HG13   | 1.84                     | 0.58              |
| 18:K:276:SER:O   | 19:L:299:ARG:NH2  | 2.37                     | 0.58              |
| 19:L:269:TYR:HB3 | 19:L:273:HIS:HD2  | 1.68                     | 0.58              |
| 22:O:16:MET:HB3  | 22:O:20:PRO:HB3   | 1.84                     | 0.58              |
| 33:Z:837:TYR:HB3 | 33:Z:848:THR:HG22 | 1.84                     | 0.58              |
| 10:d:46:LEU:HB2  | 10:d:214:ALA:HB3  | 1.86                     | 0.58              |
| 17:J:212:ARG:HB3 | 17:J:248:ASP:HB2  | 1.85                     | 0.58              |
| 18:K:94:LEU:HB2  | 19:L:128:ILE:HD12 | 1.86                     | 0.58              |
| 21:N:475:ALA:HB1 | 29:V:61:TYR:CZ    | 2.38                     | 0.58              |
| 1:1:38:ARG:NH1   | 1:1:186:GLY:O     | 2.36                     | 0.58              |
| 3:3:185:ALA:HB3  | 3:3:200:LEU:HB2   | 1.86                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:7:232:ILE:HB    | 7:7:240:THR:HB    | 1.84                     | 0.58              |
| 13:F:119:ASN:ND2  | 13:F:126:ARG:O    | 2.36                     | 0.58              |
| 10:d:216:ILE:HG12 | 10:d:227:GLN:HG2  | 1.86                     | 0.58              |
| 3:3:11:ILE:HD12   | 3:3:146:LEU:HD11  | 1.84                     | 0.58              |
| 17:J:189:GLY:HA3  | 17:J:316:PHE:HB3  | 1.85                     | 0.58              |
| 20:M:283:LEU:HB3  | 20:M:327:THR:HB   | 1.85                     | 0.58              |
| 21:N:873:ARG:HG3  | 21:N:874:ILE:H    | 1.69                     | 0.58              |
| 22:O:74:ASN:OD1   | 22:O:75:GLN:N     | 2.36                     | 0.58              |
| 28:U:140:ILE:HG12 | 28:U:142:GLN:H    | 1.69                     | 0.58              |
| 28:U:152:LYS:CE   | 28:U:154:PHE:HE1  | 2.12                     | 0.58              |
| 28:U:216:ASN:OD1  | 28:U:217:LYS:N    | 2.37                     | 0.58              |
| 6:6:162:ALA:HB1   | 6:6:166:MET:HE2   | 1.85                     | 0.58              |
| 7:a:152:VAL:HG22  | 7:a:158:GLN:HG3   | 1.86                     | 0.58              |
| 10:C:77:VAL:HG21  | 10:C:88:ILE:HD11  | 1.85                     | 0.58              |
| 26:S:418:THR:HG22 | 26:S:422:MET:HE2  | 1.86                     | 0.58              |
| 7:7:137:ARG:HA    | 7:7:142:PRO:HG3   | 1.85                     | 0.58              |
| 5:f:260:TRP:HZ3   | 5:f:262:TYR:HB2   | 1.69                     | 0.58              |
| 20:M:261:LYS:HG2  | 20:M:264:ARG:HH21 | 1.68                     | 0.58              |
| 33:Z:77:ASN:HB2   | 33:Z:80:SER:HB2   | 1.86                     | 0.58              |
| 33:Z:813:PHE:HB2  | 33:Z:850:LEU:HD13 | 1.86                     | 0.58              |
| 7:a:86:ILE:HG12   | 7:a:147:ILE:HG12  | 1.86                     | 0.58              |
| 14:k:65:VAL:HG12  | 14:k:67:ILE:H     | 1.68                     | 0.58              |
| 15:H:104:LYS:NZ   | 20:M:160:PRO:O    | 2.35                     | 0.58              |
| 15:H:247:LEU:HB2  | 15:H:371:ILE:HG21 | 1.86                     | 0.58              |
| 28:U:122:ILE:HD12 | 28:U:137:TYR:HE2  | 1.68                     | 0.58              |
| 33:Z:87:LYS:HD3   | 33:Z:90:LYS:HG3   | 1.86                     | 0.58              |
| 12:m:142:LEU:HB2  | 12:m:158:ALA:HB3  | 1.85                     | 0.57              |
| 15:H:149:LEU:HD12 | 15:H:153:ALA:HB3  | 1.85                     | 0.57              |
| 21:N:207:LEU:HB3  | 21:N:228:VAL:HG13 | 1.86                     | 0.57              |
| 21:N:738:GLN:HB3  | 21:N:745:LEU:HD12 | 1.85                     | 0.57              |
| 23:P:11:LYS:HG2   | 23:P:15:GLN:HG3   | 1.86                     | 0.57              |
| 25:R:408:ASP:OD1  | 26:S:464:ARG:NH2  | 2.36                     | 0.57              |
| 27:T:170:ASN:HA   | 27:T:174:PHE:HB2  | 1.86                     | 0.57              |
| 33:Z:574:TYR:HB2  | 33:Z:581:VAL:HG12 | 1.86                     | 0.57              |
| 33:Z:964:GLU:HG3  | 33:Z:965:LEU:HG   | 1.85                     | 0.57              |
| 1:1:23:MET:HE2    | 1:1:174:ILE:HG12  | 1.86                     | 0.57              |
| 2:i:63:LEU:HD23   | 2:i:73:ALA:HB2    | 1.86                     | 0.57              |
| 3:h:155:GLU:HB3   | 3:h:158:LEU:HD21  | 1.86                     | 0.57              |
| 8:A:126:GLN:O     | 8:A:129:THR:OG1   | 2.21                     | 0.57              |
| 14:k:72:ARG:HH21  | 14:k:227:LEU:HD13 | 1.69                     | 0.57              |
| 17:J:247:MET:HB2  | 17:J:250:ILE:HD13 | 1.86                     | 0.57              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 20:M:147:GLY:HA3  | 20:M:157:ASP:HB3 | 1.86                     | 0.57              |
| 20:M:228:LYS:NZ   | 20:M:327:THR:O   | 2.37                     | 0.57              |
| 8:A:54:ILE:HG12   | 8:A:225:VAL:HG22 | 1.85                     | 0.57              |
| 9:B:71:ILE:HG12   | 9:B:138:GLY:HA3  | 1.87                     | 0.57              |
| 12:E:35:SER:HG    | 12:E:66:LYS:HZ3  | 1.51                     | 0.57              |
| 16:I:417:LYS:HA   | 16:I:420:LYS:HE2 | 1.85                     | 0.57              |
| 24:Q:389:VAL:HG23 | 24:Q:398:TYR:HB2 | 1.87                     | 0.57              |
| 10:C:162:ALA:HB3  | 11:D:54:LEU:HD23 | 1.85                     | 0.57              |
| 18:K:73:ARG:HA    | 18:K:76:LYS:HE2  | 1.85                     | 0.57              |
| 21:N:778:LYS:HG3  | 21:N:875:LEU:HB3 | 1.86                     | 0.57              |
| 26:S:93:LEU:O     | 26:S:98:SER:OG   | 2.20                     | 0.57              |
| 26:S:428:ARG:HH11 | 27:T:192:ASN:HB2 | 1.68                     | 0.57              |
| 2:2:126:TYR:HB3   | 2:2:156:LEU:HD21 | 1.86                     | 0.57              |
| 7:a:60:LEU:HD22   | 7:a:225:SER:HB3  | 1.85                     | 0.57              |
| 7:a:215:ARG:NH2   | 7:a:249:ASN:O    | 2.37                     | 0.57              |
| 7:7:121:GLU:OE2   | 13:F:139:LYS:NZ  | 2.36                     | 0.57              |
| 2:i:39:ASN:HB3    | 2:i:208:GLU:HG3  | 1.86                     | 0.57              |
| 11:D:166:ARG:NH2  | 11:D:202:VAL:O   | 2.37                     | 0.57              |
| 14:k:68:GLN:O     | 14:k:76:CYS:N    | 2.36                     | 0.57              |
| 20:M:43:ILE:HG21  | 30:W:27:GLU:HB3  | 1.87                     | 0.57              |
| 26:S:311:GLN:NE2  | 26:S:341:SER:OG  | 2.38                     | 0.57              |
| 31:X:48:PHE:HB2   | 31:X:66:LEU:HB3  | 1.87                     | 0.57              |
| 6:6:128:THR:HB    | 6:6:144:PHE:HB2  | 1.84                     | 0.57              |
| 6:e:49:ILE:HD11   | 6:e:216:GLN:HE21 | 1.69                     | 0.57              |
| 6:e:57:ARG:NH1    | 7:a:193:ASP:O    | 2.37                     | 0.57              |
| 10:d:60:ASP:HA    | 10:d:232:PRO:HG2 | 1.86                     | 0.57              |
| 11:n:163:THR:HG21 | 11:n:171:VAL:HB  | 1.86                     | 0.57              |
| 12:m:121:LEU:HB3  | 13:l:79:PRO:HB3  | 1.87                     | 0.57              |
| 22:O:352:TRP:O    | 28:U:234:ASN:ND2 | 2.37                     | 0.57              |
| 28:U:50:ASN:OD1   | 28:U:51:SER:N    | 2.37                     | 0.57              |
| 31:X:91:PHE:HB3   | 31:X:94:ASN:HD22 | 1.69                     | 0.57              |
| 9:B:222:LEU:HB2   | 9:B:233:PRO:HD3  | 1.85                     | 0.57              |
| 11:n:17:ILE:HG12  | 11:n:19:GLN:H    | 1.70                     | 0.57              |
| 21:N:378:ASN:HD21 | 21:N:381:GLU:HB2 | 1.68                     | 0.57              |
| 21:N:893:VAL:HG22 | 21:N:908:ARG:HD2 | 1.87                     | 0.57              |
| 25:R:396:LYS:HG3  | 25:R:400:TYR:HB2 | 1.87                     | 0.57              |
| 12:E:18:GLU:OE1   | 12:E:20:ARG:NH2  | 2.36                     | 0.57              |
| 12:m:13:SER:O     | 13:l:21:GLN:NE2  | 2.37                     | 0.57              |
| 17:J:320:SER:H    | 17:J:323:ALA:HB3 | 1.70                     | 0.57              |
| 18:K:104:ASP:HB3  | 18:K:107:THR:HB  | 1.86                     | 0.57              |
| 24:Q:124:PHE:HB2  | 24:Q:130:ARG:HG3 | 1.86                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:Z:531:ALA:HB1  | 33:Z:572:ILE:HB   | 1.87                     | 0.57              |
| 5:5:76:THR:N      | 5:5:245:TYR:O     | 2.37                     | 0.57              |
| 8:c:143:VAL:HG12  | 8:c:153:ILE:HG12  | 1.86                     | 0.57              |
| 33:Z:491:LEU:HD13 | 33:Z:525:MET:HG3  | 1.87                     | 0.57              |
| 11:n:47:GLU:O     | 11:n:63:LYS:NZ    | 2.36                     | 0.56              |
| 21:N:742:TRP:HE3  | 21:N:743:PHE:HD1  | 1.51                     | 0.56              |
| 24:Q:78:ILE:HG12  | 24:Q:100:LEU:HD13 | 1.87                     | 0.56              |
| 5:f:82:ARG:NH1    | 5:f:185:PRO:O     | 2.36                     | 0.56              |
| 6:e:174:ASN:HB3   | 6:e:176:LYS:HE2   | 1.88                     | 0.56              |
| 15:H:160:GLY:H    | 15:H:163:VAL:HB   | 1.69                     | 0.56              |
| 22:O:357:ILE:HG13 | 28:U:223:HIS:CD2  | 2.40                     | 0.56              |
| 33:Z:306:MET:HG2  | 33:Z:973:TYR:HB3  | 1.86                     | 0.56              |
| 33:Z:873:LEU:HD23 | 33:Z:878:LEU:HD21 | 1.86                     | 0.56              |
| 3:3:152:SER:HG    | 6:e:209:SER:HG    | 1.50                     | 0.56              |
| 10:C:18:ARG:HD2   | 10:C:18:ARG:C     | 2.30                     | 0.56              |
| 10:C:70:ASN:OD1   | 10:C:73:ILE:N     | 2.37                     | 0.56              |
| 9:j:20:GLN:HE21   | 9:j:129:PRO:HG3   | 1.70                     | 0.56              |
| 12:m:163:THR:OG1  | 13:l:82:ARG:NH1   | 2.39                     | 0.56              |
| 14:k:95:GLU:OE1   | 14:k:115:ARG:NH2  | 2.39                     | 0.56              |
| 16:I:423:VAL:O    | 17:J:306:ARG:NH2  | 2.37                     | 0.56              |
| 21:N:162:ARG:HE   | 21:N:164:ASP:HB3  | 1.70                     | 0.56              |
| 29:V:23:THR:HG22  | 29:V:171:ARG:NH2  | 2.19                     | 0.56              |
| 23:P:83:SER:HB2   | 23:P:90:LYS:HE3   | 1.87                     | 0.56              |
| 3:h:7:ILE:HG23    | 3:h:32:GLN:HG3    | 1.88                     | 0.56              |
| 8:A:135:ARG:NE    | 14:G:13:SER:O     | 2.38                     | 0.56              |
| 12:E:41:ALA:HA    | 12:E:46:VAL:HG22  | 1.86                     | 0.56              |
| 19:L:187:THR:HA   | 19:L:190:ILE:HB   | 1.87                     | 0.56              |
| 12:E:78:MET:HA    | 12:E:142:LEU:HG   | 1.88                     | 0.56              |
| 24:Q:142:ALA:HA   | 24:Q:145:HIS:HD2  | 1.69                     | 0.56              |
| 3:3:51:LEU:HD11   | 3:3:107:PRO:HB3   | 1.87                     | 0.56              |
| 7:7:144:TRP:HA    | 7:7:165:LEU:HD23  | 1.87                     | 0.56              |
| 27:T:226:TRP:CH2  | 27:T:233:VAL:HA   | 2.41                     | 0.56              |
| 25:R:398:ALA:HA   | 25:R:402:LEU:HB2  | 1.88                     | 0.56              |
| 33:Z:867:PHE:O    | 33:Z:909:ARG:NH1  | 2.39                     | 0.56              |
| 3:3:16:THR:HG22   | 3:3:21:VAL:HG12   | 1.88                     | 0.56              |
| 29:V:235:GLU:HA   | 29:V:238:LEU:HG   | 1.88                     | 0.56              |
| 4:4:41:HIS:HE2    | 4:4:74:GLU:HB3    | 1.71                     | 0.56              |
| 7:a:144:TRP:HA    | 7:a:165:LEU:HD23  | 1.88                     | 0.56              |
| 12:E:35:SER:O     | 12:E:79:SER:OG    | 2.21                     | 0.56              |
| 15:H:224:VAL:HG23 | 15:H:225:VAL:HG23 | 1.88                     | 0.56              |
| 17:J:85:LEU:HD11  | 17:J:93:LYS:HB3   | 1.88                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:N:632:LYS:NZ   | 21:N:717:LEU:O    | 2.40                     | 0.56              |
| 24:Q:66:VAL:HA    | 24:Q:71:LYS:HB3   | 1.88                     | 0.56              |
| 12:m:50:VAL:HG21  | 12:m:66:LYS:HB2   | 1.87                     | 0.55              |
| 15:H:320:ASP:O    | 20:M:290:ARG:NH2  | 2.27                     | 0.55              |
| 20:M:352:PRO:O    | 20:M:357:ARG:NH1  | 2.40                     | 0.55              |
| 21:N:405:LEU:HD13 | 21:N:446:ALA:HB2  | 1.88                     | 0.55              |
| 28:U:32:ARG:NH1   | 28:U:98:LYS:O     | 2.38                     | 0.55              |
| 33:Z:604:GLY:HA2  | 33:Z:607:ALA:HB3  | 1.87                     | 0.55              |
| 2:i:200:SER:HA    | 2:i:223:ASN:HD21  | 1.71                     | 0.55              |
| 15:H:278:GLU:O    | 15:H:281:GLN:NE2  | 2.38                     | 0.55              |
| 30:W:30:ILE:HG23  | 30:W:73:LEU:HD22  | 1.88                     | 0.55              |
| 18:K:110:VAL:HG21 | 18:K:139:LEU:HD21 | 1.88                     | 0.55              |
| 9:j:157:PHE:HB3   | 10:d:57:LEU:HD11  | 1.88                     | 0.55              |
| 20:M:132:VAL:HG12 | 20:M:134:LEU:H    | 1.70                     | 0.55              |
| 21:N:557:LEU:HD21 | 21:N:734:VAL:HG21 | 1.89                     | 0.55              |
| 30:W:110:ILE:N    | 30:W:138:ALA:O    | 2.37                     | 0.55              |
| 22:O:79:VAL:HB    | 22:O:127:LEU:HD23 | 1.88                     | 0.55              |
| 30:W:92:GLN:HE21  | 30:W:128:LEU:HD21 | 1.70                     | 0.55              |
| 3:h:189:ILE:HB    | 3:h:196:VAL:HB    | 1.88                     | 0.55              |
| 17:J:221:LYS:NZ   | 18:K:289:ASP:O    | 2.36                     | 0.55              |
| 25:R:54:ILE:HG13  | 25:R:59:MET:H     | 1.72                     | 0.55              |
| 26:S:204:ASP:H    | 27:T:93:ASN:HD21  | 1.53                     | 0.55              |
| 17:J:185:VAL:HG22 | 17:J:312:ARG:HB2  | 1.89                     | 0.55              |
| 22:O:62:TYR:HB2   | 22:O:69:PHE:HZ    | 1.71                     | 0.55              |
| 27:T:258:ASN:O    | 27:T:262:LYS:N    | 2.40                     | 0.55              |
| 33:Z:957:LEU:HD12 | 33:Z:961:GLU:HB3  | 1.88                     | 0.55              |
| 1:l:193:ARG:NH2   | 7:a:255:ALA:O     | 2.40                     | 0.55              |
| 2:2:225:ARG:NH1   | 3:3:151:GLU:OE2   | 2.39                     | 0.55              |
| 5:5:82:ARG:HH21   | 5:5:200:ASP:HA    | 1.70                     | 0.55              |
| 25:R:107:GLU:HG2  | 25:R:111:LYS:HD2  | 1.89                     | 0.55              |
| 3:3:27:LEU:HD13   | 3:3:39:LYS:HG3    | 1.87                     | 0.55              |
| 12:E:88:MET:HE3   | 12:E:138:PHE:HD2  | 1.71                     | 0.55              |
| 17:J:186:ILE:HG22 | 17:J:310:ILE:HG21 | 1.89                     | 0.55              |
| 21:N:259:PHE:CG   | 21:N:904:VAL:HG11 | 2.42                     | 0.55              |
| 27:T:236:ASN:OD1  | 27:T:237:ASN:N    | 2.40                     | 0.55              |
| 11:D:6:ARG:O      | 12:E:135:SER:OG   | 2.24                     | 0.55              |
| 10:d:197:LEU:O    | 10:d:201:THR:OG1  | 2.24                     | 0.55              |
| 16:I:133:LEU:HD12 | 16:I:157:VAL:HA   | 1.89                     | 0.55              |
| 28:U:127:GLN:HE22 | 29:V:212:MET:HA   | 1.72                     | 0.55              |
| 1:b:23:MET:HE2    | 1:b:174:ILE:HG12  | 1.88                     | 0.54              |
| 8:c:129:GLN:HG2   | 9:j:128:ARG:HG2   | 1.88                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:J:156:GLN:HE21 | 17:J:317:PRO:HD3  | 1.72                     | 0.54              |
| 24:Q:172:PRO:HB3  | 24:Q:208:ILE:HG21 | 1.87                     | 0.54              |
| 32:Y:73:PHE:HA    | 32:Y:77:LEU:HD13  | 1.89                     | 0.54              |
| 2:i:93:GLU:OE1    | 9:j:98:LYS:NZ     | 2.35                     | 0.54              |
| 10:C:18:ARG:CD    | 10:C:23:GLU:CG    | 2.85                     | 0.54              |
| 11:D:71:VAL:HG22  | 11:D:137:GLY:HA3  | 1.88                     | 0.54              |
| 11:D:78:LEU:HD13  | 16:I:436:TYR:CE1  | 2.38                     | 0.54              |
| 12:E:80:GLY:HA3   | 12:E:140:VAL:HG23 | 1.89                     | 0.54              |
| 12:m:179:ALA:HB2  | 12:m:207:VAL:HG11 | 1.89                     | 0.54              |
| 13:l:84:LEU:HD22  | 13:l:112:LEU:HD22 | 1.88                     | 0.54              |
| 18:K:212:TYR:HB2  | 18:K:339:GLU:HA   | 1.89                     | 0.54              |
| 30:W:21:PHE:N     | 30:W:24:THR:O     | 2.36                     | 0.54              |
| 14:G:124:THR:HG22 | 14:G:131:PRO:HB3  | 1.90                     | 0.54              |
| 7:7:60:LEU:HD11   | 7:7:67:LEU:HD22   | 1.88                     | 0.54              |
| 9:B:66:LEU:O      | 9:B:90:ARG:NH2    | 2.40                     | 0.54              |
| 12:m:79:SER:HB3   | 12:m:141:ALA:HB3  | 1.90                     | 0.54              |
| 27:T:252:GLU:HB2  | 27:T:256:LYS:HE3  | 1.89                     | 0.54              |
| 33:Z:68:LEU:HD22  | 33:Z:118:VAL:HG21 | 1.89                     | 0.54              |
| 2:i:114:GLN:HE22  | 8:c:106:LYS:HA    | 1.72                     | 0.54              |
| 9:B:10:THR:O      | 9:B:11:THR:C      | 2.50                     | 0.54              |
| 16:I:284:ILE:HB   | 16:I:328:THR:HB   | 1.89                     | 0.54              |
| 19:L:145:ARG:H    | 19:L:161:ARG:HG2  | 1.72                     | 0.54              |
| 26:S:314:ASN:HD22 | 26:S:338:MET:HE1  | 1.72                     | 0.54              |
| 2:i:48:ARG:HE     | 2:i:199:GLY:HA3   | 1.73                     | 0.54              |
| 9:B:43:VAL:HG11   | 9:B:137:ALA:HB1   | 1.90                     | 0.54              |
| 13:F:47:VAL:HG22  | 13:F:213:ILE:HG12 | 1.89                     | 0.54              |
| 15:H:207:THR:HA   | 15:H:265:ASN:HD22 | 1.71                     | 0.54              |
| 21:N:340:HIS:HB2  | 21:N:374:ILE:HG12 | 1.89                     | 0.54              |
| 33:Z:87:LYS:HE2   | 33:Z:89:LEU:HB2   | 1.88                     | 0.54              |
| 2:2:129:VAL:HB    | 2:2:140:PHE:HB2   | 1.89                     | 0.54              |
| 8:A:220:LYS:HD3   | 8:A:242:GLU:HB2   | 1.89                     | 0.54              |
| 10:d:120:GLN:NE2  | 11:n:80:ALA:O     | 2.40                     | 0.54              |
| 24:Q:421:LYS:NZ   | 29:V:256:GLU:O    | 2.40                     | 0.54              |
| 26:S:423:VAL:HG11 | 26:S:443:ILE:HD13 | 1.89                     | 0.54              |
| 5:f:168:ALA:HB3   | 6:e:120:ARG:HH22  | 1.72                     | 0.54              |
| 9:B:32:VAL:O      | 9:B:76:SER:OG     | 2.21                     | 0.54              |
| 11:D:6:ARG:O      | 11:D:7:ALA:HB2    | 2.06                     | 0.54              |
| 11:D:6:ARG:HH21   | 13:F:125:GLY:H    | 1.56                     | 0.54              |
| 14:k:70:VAL:N     | 14:k:74:ILE:O     | 2.41                     | 0.54              |
| 22:O:43:GLU:HA    | 22:O:82:LEU:HD21  | 1.89                     | 0.54              |
| 5:f:172:MET:HB3   | 5:f:192:SER:HB3   | 1.89                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:B:9:LEU:HD12    | 10:C:128:LEU:HA   | 1.90                     | 0.54              |
| 12:m:36:THR:HA    | 12:m:173:GLY:HA3  | 1.89                     | 0.54              |
| 12:m:126:GLY:HA2  | 12:m:132:ARG:HG3  | 1.90                     | 0.54              |
| 21:N:63:LEU:HD22  | 21:N:88:ARG:HB3   | 1.90                     | 0.54              |
| 21:N:718:GLU:HA   | 21:N:725:LEU:HG   | 1.90                     | 0.54              |
| 6:6:41:VAL:HG12   | 6:6:225:ILE:HA    | 1.89                     | 0.54              |
| 2:i:172:LYS:HB3   | 2:i:175:LEU:HD21  | 1.90                     | 0.54              |
| 7:a:122:PRO:HB2   | 7:a:159:PHE:HB3   | 1.90                     | 0.54              |
| 8:A:249:ALA:HB1   | 23:P:85:LYS:HA    | 1.90                     | 0.54              |
| 13:F:170:THR:HG21 | 20:M:381:ARG:HD3  | 1.90                     | 0.54              |
| 7:a:181:ALA:O     | 7:a:185:ASN:ND2   | 2.40                     | 0.53              |
| 9:B:95:THR:HA     | 9:B:99:ARG:HD2    | 1.90                     | 0.53              |
| 8:c:125:GLN:O     | 8:c:128:THR:OG1   | 2.22                     | 0.53              |
| 11:n:122:GLN:HE22 | 12:m:136:ARG:HG2  | 1.73                     | 0.53              |
| 18:K:187:ALA:O    | 18:K:188:VAL:HG23 | 2.08                     | 0.53              |
| 21:N:256:GLN:OE1  | 21:N:894:ARG:NH1  | 2.41                     | 0.53              |
| 33:Z:737:ALA:HA   | 33:Z:772:ILE:HD13 | 1.88                     | 0.53              |
| 20:M:149:ASN:OD1  | 20:M:150:LYS:N    | 2.42                     | 0.53              |
| 28:U:93:TYR:HB3   | 28:U:121:LEU:HD12 | 1.90                     | 0.53              |
| 28:U:121:LEU:HD23 | 28:U:136:ALA:HA   | 1.91                     | 0.53              |
| 4:g:3:ILE:HG12    | 4:g:136:SER:HB2   | 1.89                     | 0.53              |
| 6:e:32:LEU:HD11   | 6:e:169:LEU:HD11  | 1.89                     | 0.53              |
| 13:l:119:ASN:ND2  | 13:l:126:ARG:O    | 2.41                     | 0.53              |
| 26:S:445:THR:HG22 | 26:S:447:GLU:H    | 1.73                     | 0.53              |
| 1:1:196:VAL:HB    | 1:1:203:GLU:HB3   | 1.91                     | 0.53              |
| 8:A:40:ILE:HG23   | 8:A:56:GLN:HB2    | 1.89                     | 0.53              |
| 10:C:39:MET:HE2   | 10:C:161:LYS:HA   | 1.90                     | 0.53              |
| 15:H:82:TRP:CD1   | 16:I:134:SER:HG   | 2.25                     | 0.53              |
| 16:I:255:LYS:HD3  | 16:I:297:GLY:HA2  | 1.90                     | 0.53              |
| 19:L:338:LEU:O    | 19:L:346:LYS:NZ   | 2.35                     | 0.53              |
| 9:B:35:LEU:HA     | 9:B:163:ALA:HA    | 1.90                     | 0.53              |
| 13:F:114:ASP:OD1  | 14:G:87:HIS:ND1   | 2.42                     | 0.53              |
| 20:M:317:SER:H    | 20:M:321:VAL:HG21 | 1.74                     | 0.53              |
| 21:N:525:ASN:HA   | 21:N:528:ARG:HD3  | 1.89                     | 0.53              |
| 22:O:168:THR:HG21 | 28:U:142:GLN:NE2  | 2.22                     | 0.53              |
| 29:V:61:TYR:HD1   | 29:V:62:THR:N     | 2.02                     | 0.53              |
| 13:l:176:LEU:HD22 | 14:k:58:LEU:HD23  | 1.91                     | 0.53              |
| 15:H:193:PRO:HG3  | 15:H:293:GLU:HG2  | 1.90                     | 0.53              |
| 15:H:261:ARG:NH2  | 16:I:315:GLY:O    | 2.42                     | 0.53              |
| 21:N:759:ILE:HG23 | 21:N:761:ILE:HG12 | 1.91                     | 0.53              |
| 25:R:335:ARG:HD2  | 25:R:376:GLN:HB3  | 1.91                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:Z:362:LEU:O    | 33:Z:859:LYS:NZ   | 2.42                     | 0.53              |
| 3:h:37:SER:HB2    | 4:g:128:LEU:HD21  | 1.89                     | 0.53              |
| 5:f:96:THR:HA     | 5:f:102:ALA:H     | 1.73                     | 0.53              |
| 11:D:155:ILE:HG22 | 12:E:82:THR:HB    | 1.91                     | 0.53              |
| 14:k:220:SER:O    | 14:k:224:THR:OG1  | 2.26                     | 0.53              |
| 15:H:448:ASP:HA   | 15:H:452:SER:HB2  | 1.91                     | 0.53              |
| 18:K:90:GLN:HB3   | 18:K:94:LEU:HD21  | 1.91                     | 0.53              |
| 21:N:475:ALA:HB2  | 29:V:61:TYR:OH    | 2.08                     | 0.53              |
| 29:V:61:TYR:CD1   | 29:V:62:THR:N     | 2.69                     | 0.53              |
| 30:W:2:VAL:HG22   | 30:W:196:SER:HB2  | 1.90                     | 0.53              |
| 33:Z:301:THR:O    | 33:Z:307:HIS:NE2  | 2.37                     | 0.53              |
| 33:Z:304:PRO:HB3  | 33:Z:340:LEU:HD13 | 1.91                     | 0.53              |
| 8:c:46:GLY:HA2    | 8:c:193:ILE:HB    | 1.91                     | 0.53              |
| 9:j:139:HIS:O     | 9:j:234:ARG:NH2   | 2.42                     | 0.53              |
| 18:K:243:VAL:HG11 | 19:L:303:ARG:HH22 | 1.73                     | 0.53              |
| 18:K:280:LYS:HB3  | 18:K:323:THR:HB   | 1.91                     | 0.53              |
| 33:Z:868:ASN:HA   | 33:Z:909:ARG:HH12 | 1.74                     | 0.53              |
| 5:5:196:ARG:NH2   | 11:D:101:GLU:OE1  | 2.42                     | 0.53              |
| 2:i:104:ARG:HB2   | 8:c:109:TYR:HE2   | 1.74                     | 0.53              |
| 13:l:67:ASP:HB3   | 13:l:70:MET:HB3   | 1.91                     | 0.53              |
| 21:N:518:ALA:HB1  | 21:N:550:GLY:HA3  | 1.91                     | 0.53              |
| 29:V:36:LYS:NZ    | 29:V:67:ASP:OD1   | 2.42                     | 0.53              |
| 3:3:203:ARG:HH22  | 6:e:176:LYS:HB3   | 1.73                     | 0.53              |
| 9:B:5:TYR:O       | 9:B:8:SER:N       | 2.40                     | 0.53              |
| 25:R:255:VAL:HG11 | 25:R:316:LEU:HD21 | 1.91                     | 0.53              |
| 30:W:114:VAL:HG11 | 30:W:118:ILE:HD11 | 1.91                     | 0.53              |
| 33:Z:914:LEU:H    | 33:Z:980:VAL:HG22 | 1.74                     | 0.53              |
| 8:c:161:TYR:HB2   | 9:j:80:PRO:HD3    | 1.91                     | 0.52              |
| 21:N:647:ASP:O    | 21:N:653:ARG:NE   | 2.41                     | 0.52              |
| 23:P:431:HIS:CG   | 28:U:156:HIS:HB3  | 2.45                     | 0.52              |
| 25:R:39:SER:HB3   | 25:R:42:GLN:HG3   | 1.90                     | 0.52              |
| 26:S:480:ARG:HD2  | 26:S:483:GLU:HB2  | 1.90                     | 0.52              |
| 27:T:256:LYS:HZ3  | 27:T:259:ILE:HD12 | 1.75                     | 0.52              |
| 2:2:192:ILE:HG12  | 2:2:199:GLY:HA2   | 1.91                     | 0.52              |
| 4:g:53:THR:HG22   | 4:g:100:VAL:HG22  | 1.91                     | 0.52              |
| 11:n:46:CYS:HB2   | 11:n:211:GLU:HB3  | 1.91                     | 0.52              |
| 15:H:105:ILE:HG23 | 15:H:145:TYR:HE1  | 1.74                     | 0.52              |
| 17:J:67:GLU:HG3   | 29:V:186:GLN:HE22 | 1.74                     | 0.52              |
| 20:M:219:LEU:HD23 | 20:M:346:LYS:HG3  | 1.90                     | 0.52              |
| 21:N:761:ILE:HG21 | 21:N:904:VAL:HG13 | 1.90                     | 0.52              |
| 26:S:201:ILE:O    | 27:T:92:ASN:ND2   | 2.42                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:V:57:PHE:O     | 29:V:135:ARG:NH1  | 2.43                     | 0.52              |
| 2:i:126:TYR:HB3   | 2:i:156:LEU:HD21  | 1.91                     | 0.52              |
| 11:n:237:GLU:HA   | 11:n:240:LYS:HD3  | 1.90                     | 0.52              |
| 13:l:143:HIS:ND1  | 13:l:155:GLU:OE2  | 2.42                     | 0.52              |
| 22:O:341:ILE:O    | 23:P:358:SER:OG   | 2.25                     | 0.52              |
| 26:S:234:ILE:HG23 | 26:S:253:PHE:HE2  | 1.74                     | 0.52              |
| 4:4:36:ARG:HG3    | 4:4:57:ALA:HB1    | 1.90                     | 0.52              |
| 7:7:98:ARG:HD2    | 14:G:101:LYS:HA   | 1.90                     | 0.52              |
| 15:H:315:GLY:HA2  | 15:H:333:MET:HG3  | 1.92                     | 0.52              |
| 28:U:117:ASN:ND2  | 28:U:139:ALA:O    | 2.40                     | 0.52              |
| 33:Z:913:ILE:HD12 | 33:Z:963:ALA:HB3  | 1.90                     | 0.52              |
| 1:1:103:GLU:HG3   | 14:G:102:LEU:HD12 | 1.92                     | 0.52              |
| 4:4:107:TYR:HA    | 4:4:114:PRO:HA    | 1.91                     | 0.52              |
| 5:5:272:PHE:HZ    | 5:5:285:VAL:HG21  | 1.74                     | 0.52              |
| 1:b:27:PHE:HE2    | 1:b:32:ILE:HG13   | 1.74                     | 0.52              |
| 10:d:52:VAL:HG21  | 10:d:57:LEU:HD22  | 1.92                     | 0.52              |
| 17:J:48:ARG:HH22  | 21:N:608:LEU:HB3  | 1.74                     | 0.52              |
| 18:K:211:LEU:HD12 | 18:K:317:ALA:HB2  | 1.91                     | 0.52              |
| 19:L:252:VAL:HG21 | 20:M:303:ARG:HD2  | 1.90                     | 0.52              |
| 20:M:171:GLU:HG3  | 20:M:245:LYS:HB3  | 1.91                     | 0.52              |
| 21:N:265:ALA:HB1  | 21:N:269:LEU:HB3  | 1.90                     | 0.52              |
| 11:D:181:ARG:NH1  | 12:E:59:LEU:O     | 2.43                     | 0.52              |
| 12:E:71:ASP:HB3   | 12:E:74:ILE:HB    | 1.92                     | 0.52              |
| 8:c:142:PHE:N     | 8:c:154:TYR:O     | 2.41                     | 0.52              |
| 12:m:211:LYS:O    | 12:m:216:ASN:ND2  | 2.43                     | 0.52              |
| 20:M:194:VAL:HG12 | 20:M:199:LEU:HG   | 1.92                     | 0.52              |
| 20:M:428:LYS:HB3  | 20:M:430:VAL:HG12 | 1.91                     | 0.52              |
| 21:N:110:VAL:HG11 | 21:N:159:GLU:HG2  | 1.91                     | 0.52              |
| 33:Z:99:LEU:HD23  | 33:Z:102:ILE:HD12 | 1.91                     | 0.52              |
| 8:A:250:GLU:HA    | 23:P:84:LYS:HE2   | 1.91                     | 0.52              |
| 10:C:75:VAL:HG12  | 10:C:137:TYR:HA   | 1.90                     | 0.52              |
| 17:J:319:PRO:HB2  | 17:J:324:ARG:HH11 | 1.74                     | 0.52              |
| 18:K:187:ALA:O    | 18:K:188:VAL:CG2  | 2.58                     | 0.52              |
| 19:L:397:GLU:OE1  | 20:M:345:ARG:NH2  | 2.34                     | 0.52              |
| 20:M:72:ASN:O     | 20:M:77:TYR:OH    | 2.25                     | 0.52              |
| 26:S:109:GLU:OE2  | 26:S:111:ARG:NE   | 2.40                     | 0.52              |
| 33:Z:139:LEU:HD22 | 33:Z:199:ASP:HB3  | 1.91                     | 0.52              |
| 5:5:102:ALA:HB1   | 6:6:156:ARG:HH22  | 1.74                     | 0.52              |
| 4:g:92:ILE:HD12   | 4:g:97:PRO:HB3    | 1.91                     | 0.52              |
| 11:n:62:SER:OG    | 11:n:211:GLU:OE2  | 2.28                     | 0.52              |
| 19:L:104:LEU:O    | 19:L:148:LEU:N    | 2.36                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:N:890:PHE:O    | 21:N:891:VAL:HG12 | 2.09                     | 0.52              |
| 22:O:137:TYR:HB2  | 22:O:146:ALA:HB2  | 1.91                     | 0.52              |
| 25:R:240:SER:O    | 25:R:241:ILE:HG22 | 2.10                     | 0.52              |
| 26:S:472:HIS:O    | 26:S:476:LEU:N    | 2.42                     | 0.52              |
| 5:5:199:GLY:H     | 5:5:202:PHE:HZ    | 1.57                     | 0.52              |
| 15:H:95:HIS:O     | 15:H:97:LEU:N     | 2.42                     | 0.52              |
| 21:N:39:ILE:HG21  | 21:N:68:VAL:HG21  | 1.92                     | 0.52              |
| 22:O:258:LEU:HA   | 22:O:288:ARG:HG2  | 1.92                     | 0.52              |
| 6:6:167:PRO:HG3   | 3:h:177:ARG:HE    | 1.74                     | 0.52              |
| 10:C:22:VAL:HG11  | 16:I:433:GLU:CG   | 2.39                     | 0.52              |
| 13:F:67:ASP:OD1   | 13:F:68:GLU:N     | 2.43                     | 0.52              |
| 14:G:68:GLN:OE1   | 14:G:93:ARG:NH2   | 2.43                     | 0.52              |
| 13:l:206:LEU:HD22 | 13:l:211:LEU:HD11 | 1.92                     | 0.52              |
| 20:M:225:GLY:O    | 20:M:389:ALA:N    | 2.40                     | 0.52              |
| 5:5:96:THR:HG22   | 5:5:101:VAL:HG22  | 1.91                     | 0.51              |
| 1:b:146:ALA:HB2   | 7:a:68:ARG:HH22   | 1.74                     | 0.51              |
| 5:f:102:ALA:O     | 6:e:156:ARG:NH1   | 2.32                     | 0.51              |
| 6:e:134:ASP:OD1   | 6:e:135:GLU:N     | 2.43                     | 0.51              |
| 10:d:120:GLN:HB3  | 11:n:84:ILE:HD11  | 1.91                     | 0.51              |
| 11:n:8:LEU:HB2    | 11:n:19:GLN:HE22  | 1.75                     | 0.51              |
| 11:n:149:GLN:OE1  | 11:n:162:GLN:NE2  | 2.43                     | 0.51              |
| 24:Q:429:LYS:HG3  | 28:U:299:LYS:HE3  | 1.90                     | 0.51              |
| 27:T:95:LYS:NZ    | 27:T:130:ASP:OD2  | 2.28                     | 0.51              |
| 28:U:36:VAL:HA    | 28:U:92:TRP:HA    | 1.92                     | 0.51              |
| 33:Z:382:ALA:HB1  | 33:Z:849:ARG:HD2  | 1.90                     | 0.51              |
| 33:Z:595:MET:HG2  | 33:Z:737:ALA:HB3  | 1.91                     | 0.51              |
| 12:E:206:GLN:OE1  | 15:H:409:ARG:NH2  | 2.42                     | 0.51              |
| 12:m:141:ALA:HB1  | 12:m:172:ILE:HD12 | 1.92                     | 0.51              |
| 17:J:43:ARG:NH1   | 26:S:478:SER:HA   | 2.25                     | 0.51              |
| 27:T:248:GLU:O    | 27:T:249:MET:HE2  | 2.10                     | 0.51              |
| 28:U:16:LEU:HB2   | 29:V:212:MET:HG2  | 1.90                     | 0.51              |
| 5:5:127:CYS:HA    | 5:5:172:MET:HE3   | 1.92                     | 0.51              |
| 31:X:73:THR:HG23  | 31:X:90:VAL:H     | 1.75                     | 0.51              |
| 1:b:145:ILE:HG22  | 1:b:150:SER:HB2   | 1.92                     | 0.51              |
| 17:J:143:PRO:O    | 17:J:204:HIS:ND1  | 2.44                     | 0.51              |
| 28:U:230:GLN:HA   | 28:U:233:PHE:HD2  | 1.76                     | 0.51              |
| 29:V:27:VAL:HA    | 29:V:63:VAL:HB    | 1.91                     | 0.51              |
| 5:5:94:ARG:NH2    | 3:h:205:ASP:OD2   | 2.44                     | 0.51              |
| 3:h:56:LEU:HD11   | 4:g:122:LEU:HD13  | 1.92                     | 0.51              |
| 3:h:58:THR:OG1    | 4:g:124:THR:OG1   | 2.24                     | 0.51              |
| 23:P:54:SER:HA    | 23:P:58:VAL:HB    | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:6:46:THR:HB     | 6:6:59:GLU:H      | 1.75                     | 0.51              |
| 24:Q:93:THR:O     | 24:Q:97:LEU:N     | 2.44                     | 0.51              |
| 33:Z:415:MET:HE2  | 33:Z:447:VAL:HG22 | 1.92                     | 0.51              |
| 5:5:82:ARG:HH11   | 5:5:186:THR:HA    | 1.76                     | 0.51              |
| 6:e:194:LEU:HB3   | 6:e:198:GLU:HB2   | 1.92                     | 0.51              |
| 6:e:179:TYR:HA    | 6:e:188:LYS:HA    | 1.92                     | 0.51              |
| 7:a:90:ILE:HG23   | 7:a:93:MET:HE2    | 1.92                     | 0.51              |
| 17:J:139:VAL:HG22 | 17:J:211:ILE:HG12 | 1.93                     | 0.51              |
| 19:L:108:VAL:HG22 | 19:L:119:VAL:HG22 | 1.92                     | 0.51              |
| 29:V:141:VAL:HG22 | 29:V:153:ILE:HG22 | 1.92                     | 0.51              |
| 3:3:30:GLY:HA2    | 3:3:36:VAL:HG23   | 1.92                     | 0.51              |
| 1:b:80:TYR:HB2    | 8:c:101:ALA:HB1   | 1.92                     | 0.51              |
| 9:j:71:ILE:HG12   | 9:j:138:GLY:HA3   | 1.92                     | 0.51              |
| 18:K:122:ILE:HG23 | 18:K:146:LEU:HD22 | 1.93                     | 0.51              |
| 25:R:250:ALA:HB1  | 25:R:279:LEU:HD21 | 1.93                     | 0.51              |
| 25:R:348:LEU:HB2  | 25:R:388:VAL:HB   | 1.92                     | 0.51              |
| 8:A:181:ASN:HD22  | 8:A:213:ALA:HB2   | 1.76                     | 0.51              |
| 14:k:219:CYS:HB2  | 14:k:228:HIS:HD2  | 1.75                     | 0.51              |
| 27:T:227:PRO:HB2  | 27:T:232:LYS:HE2  | 1.92                     | 0.51              |
| 2:2:253:GLN:HG2   | 10:C:226:TYR:HA   | 1.93                     | 0.50              |
| 3:3:51:LEU:HD22   | 3:3:87:PHE:HZ     | 1.76                     | 0.50              |
| 12:m:187:TRP:HA   | 12:m:191:LEU:HD11 | 1.93                     | 0.50              |
| 14:k:211:ASP:OD1  | 14:k:212:PHE:N    | 2.44                     | 0.50              |
| 22:O:296:LEU:HD11 | 22:O:308:LEU:HD22 | 1.93                     | 0.50              |
| 22:O:326:HIS:HE1  | 23:P:368:LEU:HD11 | 1.74                     | 0.50              |
| 24:Q:391:ASP:OD1  | 25:R:347:THR:OG1  | 2.28                     | 0.50              |
| 33:Z:957:LEU:HA   | 33:Z:961:GLU:HG2  | 1.93                     | 0.50              |
| 11:D:63:LYS:NZ    | 11:D:79:ASN:OD1   | 2.43                     | 0.50              |
| 13:l:67:ASP:OD1   | 13:l:68:GLU:N     | 2.44                     | 0.50              |
| 17:J:43:ARG:HD3   | 26:S:479:MET:H    | 1.77                     | 0.50              |
| 29:V:164:LEU:HB2  | 29:V:165:ILE:HD12 | 1.93                     | 0.50              |
| 30:W:11:ASP:HA    | 30:W:55:ALA:HB3   | 1.93                     | 0.50              |
| 33:Z:128:GLU:HB3  | 33:Z:132:HIS:CD2  | 2.46                     | 0.50              |
| 33:Z:400:ILE:HG12 | 33:Z:422:ILE:HG12 | 1.92                     | 0.50              |
| 1:1:33:LEU:HD21   | 1:1:119:ALA:HB3   | 1.93                     | 0.50              |
| 1:1:54:THR:HG21   | 1:1:75:ALA:HB1    | 1.94                     | 0.50              |
| 10:C:206:LEU:HD11 | 10:C:211:LEU:HD21 | 1.93                     | 0.50              |
| 13:F:105:VAL:HG12 | 13:F:145:LEU:HD13 | 1.93                     | 0.50              |
| 13:F:176:LEU:HD13 | 14:G:58:LEU:HD23  | 1.94                     | 0.50              |
| 28:U:16:LEU:HD21  | 29:V:209:GLU:HG2  | 1.92                     | 0.50              |
| 30:W:108:GLN:HB2  | 30:W:137:VAL:HA   | 1.94                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:3:38:ASN:HD22   | 5:f:285:VAL:HG22  | 1.76                     | 0.50              |
| 3:3:175:ALA:HB1   | 3:3:182:GLY:HA2   | 1.94                     | 0.50              |
| 3:h:169:GLN:O     | 3:h:173:ASN:ND2   | 2.34                     | 0.50              |
| 4:g:8:ARG:HG3     | 4:g:13:VAL:HG22   | 1.92                     | 0.50              |
| 10:C:18:ARG:HD3   | 10:C:19:LEU:O     | 2.12                     | 0.50              |
| 17:J:43:ARG:NH1   | 26:S:477:VAL:O    | 2.30                     | 0.50              |
| 17:J:267:GLU:OE1  | 17:J:270:ARG:NH2  | 2.45                     | 0.50              |
| 24:Q:179:LEU:HD13 | 24:Q:218:LEU:HD23 | 1.93                     | 0.50              |
| 31:X:85:ARG:HD2   | 31:X:101:LEU:HD12 | 1.93                     | 0.50              |
| 4:g:35:THR:HA     | 4:g:45:SER:HA     | 1.93                     | 0.50              |
| 4:g:149:ARG:NH2   | 4:g:156:GLU:OE1   | 2.44                     | 0.50              |
| 19:L:129:VAL:HG11 | 19:L:148:LEU:HD22 | 1.93                     | 0.50              |
| 23:P:350:LEU:HA   | 23:P:353:ILE:HD12 | 1.93                     | 0.50              |
| 6:6:134:ASP:OD1   | 6:6:135:GLU:N     | 2.43                     | 0.50              |
| 10:d:207:THR:OG1  | 10:d:210:ARG:NH1  | 2.41                     | 0.50              |
| 16:I:190:GLN:HB3  | 16:I:348:ILE:HG23 | 1.93                     | 0.50              |
| 21:N:302:PHE:HA   | 21:N:871:MET:HE3  | 1.92                     | 0.50              |
| 21:N:326:SER:HB3  | 21:N:360:GLN:HE22 | 1.77                     | 0.50              |
| 23:P:248:ASP:HA   | 23:P:252:SER:HB3  | 1.93                     | 0.50              |
| 23:P:268:LEU:HD11 | 23:P:277:GLN:HA   | 1.94                     | 0.50              |
| 33:Z:318:LYS:HD2  | 33:Z:874:ASN:HD21 | 1.77                     | 0.50              |
| 3:3:20:CYS:HA     | 3:3:112:ILE:HD11  | 1.93                     | 0.50              |
| 3:3:138:VAL:HG11  | 3:3:146:LEU:HB2   | 1.93                     | 0.50              |
| 13:F:34:VAL:HA    | 13:F:162:GLY:HA3  | 1.92                     | 0.50              |
| 13:F:66:CYS:O     | 13:F:89:ARG:NH1   | 2.43                     | 0.50              |
| 20:M:357:ARG:HD2  | 20:M:391:LEU:HD21 | 1.94                     | 0.50              |
| 26:S:208:ILE:HD13 | 27:T:44:LEU:HD22  | 1.93                     | 0.50              |
| 29:V:142:ASP:HB3  | 29:V:143:PRO:HD3  | 1.93                     | 0.50              |
| 1:1:102:LYS:NZ    | 7:7:94:GLN:OE1    | 2.31                     | 0.50              |
| 2:2:194:ASN:OD1   | 7:a:189:ARG:NH1   | 2.45                     | 0.50              |
| 2:2:254:GLU:HB2   | 10:C:227:GLN:HG2  | 1.93                     | 0.50              |
| 3:3:177:ARG:HH12  | 6:e:166:MET:HB3   | 1.77                     | 0.50              |
| 7:7:44:VAL:HG13   | 7:7:57:ALA:HB2    | 1.94                     | 0.50              |
| 6:e:224:LEU:HG    | 6:e:233:LYS:HG2   | 1.93                     | 0.50              |
| 9:j:72:GLY:N      | 9:j:137:ALA:O     | 2.43                     | 0.50              |
| 10:d:33:GLY:HA3   | 10:d:65:LYS:HZ3   | 1.77                     | 0.50              |
| 21:N:43:LEU:HD21  | 21:N:68:VAL:HG11  | 1.93                     | 0.50              |
| 29:V:29:ILE:HD13  | 29:V:37:MET:HE1   | 1.93                     | 0.50              |
| 6:e:56:SER:HB2    | 7:a:170:TYR:HB2   | 1.94                     | 0.50              |
| 15:H:200:VAL:HG13 | 15:H:270:THR:HG23 | 1.93                     | 0.50              |
| 16:I:136:VAL:HG11 | 16:I:158:GLY:HA2  | 1.94                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:W:29:GLN:HE21  | 30:W:144:PHE:HE2  | 1.60                     | 0.50              |
| 2:2:189:GLN:HA    | 2:2:192:ILE:HD12  | 1.94                     | 0.49              |
| 3:3:115:LYS:NZ    | 9:B:141:GLU:OE1   | 2.33                     | 0.49              |
| 5:5:271:LEU:HD23  | 5:5:274:LYS:HD2   | 1.94                     | 0.49              |
| 2:i:189:GLN:HA    | 2:i:192:ILE:HD12  | 1.93                     | 0.49              |
| 4:g:29:LYS:HD3    | 4:g:32:ASP:HB2    | 1.94                     | 0.49              |
| 4:g:139:TYR:HE2   | 4:g:172:MET:HG3   | 1.76                     | 0.49              |
| 12:E:44:GLU:OE1   | 12:E:193:LEU:N    | 2.45                     | 0.49              |
| 21:N:227:LYS:HG2  | 21:N:722:THR:O    | 2.11                     | 0.49              |
| 27:T:221:ALA:HB1  | 27:T:226:TRP:HB2  | 1.94                     | 0.49              |
| 28:U:234:ASN:OD1  | 28:U:235:LEU:N    | 2.45                     | 0.49              |
| 1:b:55:ARG:HH21   | 1:b:58:ASP:HA     | 1.76                     | 0.49              |
| 8:A:130:GLN:HB3   | 9:B:127:VAL:HG13  | 1.93                     | 0.49              |
| 13:F:52:ASN:ND2   | 13:F:54:ASP:O     | 2.45                     | 0.49              |
| 15:H:208:TYR:HA   | 15:H:262:ALA:HB1  | 1.94                     | 0.49              |
| 19:L:248:ALA:HB2  | 19:L:283:VAL:HG22 | 1.94                     | 0.49              |
| 21:N:627:ILE:HG23 | 21:N:733:LEU:HD13 | 1.93                     | 0.49              |
| 22:O:81:TYR:HA    | 22:O:85:SER:HB3   | 1.94                     | 0.49              |
| 24:Q:135:HIS:ND1  | 24:Q:169:ASP:OD2  | 2.44                     | 0.49              |
| 5:5:82:ARG:NH2    | 5:5:199:GLY:O     | 2.45                     | 0.49              |
| 11:D:189:GLU:HG3  | 11:D:232:TYR:HE1  | 1.77                     | 0.49              |
| 13:l:18:ARG:NE    | 13:l:23:GLU:OE2   | 2.42                     | 0.49              |
| 15:H:385:ARG:NH1  | 15:H:413:ASN:OD1  | 2.40                     | 0.49              |
| 17:J:190:PRO:HD2  | 17:J:316:PHE:HD2  | 1.77                     | 0.49              |
| 20:M:159:LEU:HD12 | 20:M:160:PRO:HD2  | 1.94                     | 0.49              |
| 21:N:876:PRO:HB3  | 21:N:900:ASN:HB3  | 1.93                     | 0.49              |
| 24:Q:295:GLY:N    | 24:Q:324:GLU:OE1  | 2.40                     | 0.49              |
| 27:T:226:TRP:HE1  | 27:T:235:PHE:HB3  | 1.77                     | 0.49              |
| 27:T:233:VAL:HG12 | 27:T:234:TYR:N    | 2.23                     | 0.49              |
| 28:U:285:ILE:O    | 28:U:289:ASP:N    | 2.45                     | 0.49              |
| 33:Z:116:ALA:HB3  | 33:Z:141:SER:HB2  | 1.95                     | 0.49              |
| 33:Z:559:LYS:HG3  | 33:Z:561:ASP:H    | 1.77                     | 0.49              |
| 18:K:126:LEU:HD13 | 18:K:149:ILE:HG13 | 1.94                     | 0.49              |
| 19:L:218:VAL:HA   | 19:L:345:ARG:HB2  | 1.95                     | 0.49              |
| 21:N:114:SER:HA   | 21:N:161:TYR:HD2  | 1.76                     | 0.49              |
| 9:B:122:THR:HB    | 10:C:129:ARG:HH22 | 1.77                     | 0.49              |
| 11:D:6:ARG:HD2    | 12:E:124:GLY:HA2  | 1.95                     | 0.49              |
| 11:D:75:PHE:HB3   | 11:D:133:THR:HG22 | 1.95                     | 0.49              |
| 13:F:226:ASP:OD1  | 13:F:227:GLY:N    | 2.46                     | 0.49              |
| 10:d:119:LYS:NZ   | 10:d:151:SER:OG   | 2.38                     | 0.49              |
| 15:H:289:ARG:NE   | 20:M:253:GLN:OE1  | 2.43                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:J:248:ASP:OD1  | 17:J:249:GLU:N    | 2.46                     | 0.49              |
| 18:K:420:THR:O    | 18:K:421:VAL:HG22 | 2.11                     | 0.49              |
| 24:Q:4:PRO:HB2    | 24:Q:53:GLU:HB2   | 1.94                     | 0.49              |
| 2:2:149:ASP:OD1   | 2:2:150:VAL:N     | 2.45                     | 0.49              |
| 5:5:80:ALA:HB3    | 5:5:202:PHE:HB2   | 1.95                     | 0.49              |
| 7:7:96:ILE:HD13   | 7:7:147:ILE:HD11  | 1.94                     | 0.49              |
| 7:7:179:PHE:HZ    | 1:b:44:TYR:HD1    | 1.59                     | 0.49              |
| 2:i:236:ARG:HA    | 3:h:165:GLU:HG3   | 1.95                     | 0.49              |
| 12:E:71:ASP:OD1   | 12:E:72:ARG:N     | 2.43                     | 0.49              |
| 9:j:213:ILE:HD11  | 9:j:236:ARG:HD2   | 1.93                     | 0.49              |
| 12:m:71:ASP:OD1   | 12:m:72:ARG:N     | 2.45                     | 0.49              |
| 12:m:121:LEU:HD23 | 13:l:79:PRO:HB3   | 1.94                     | 0.49              |
| 22:O:168:THR:HG21 | 28:U:142:GLN:HE22 | 1.78                     | 0.49              |
| 28:U:38:LEU:HB2   | 28:U:50:ASN:HB3   | 1.94                     | 0.49              |
| 3:h:115:LYS:NZ    | 9:j:141:GLU:OE1   | 2.43                     | 0.49              |
| 4:g:70:ARG:O      | 10:d:113:ARG:NH1  | 2.42                     | 0.49              |
| 11:D:65:SER:O     | 11:D:73:LEU:N     | 2.45                     | 0.49              |
| 11:D:159:TRP:HZ3  | 12:E:56:SER:HB3   | 1.78                     | 0.49              |
| 14:k:218:TRP:HH2  | 14:k:223:GLU:HB2  | 1.77                     | 0.49              |
| 14:k:219:CYS:HB2  | 14:k:228:HIS:CD2  | 2.48                     | 0.49              |
| 18:K:187:ALA:C    | 18:K:188:VAL:HG23 | 2.36                     | 0.49              |
| 18:K:371:LEU:O    | 18:K:375:ASN:ND2  | 2.45                     | 0.49              |
| 22:O:130:ASP:HA   | 22:O:133:ILE:HD12 | 1.94                     | 0.49              |
| 25:R:325:HIS:HB2  | 25:R:329:PHE:CE2  | 2.47                     | 0.49              |
| 26:S:330:LEU:HB2  | 32:Y:64:TRP:CD1   | 2.48                     | 0.49              |
| 11:D:82:SER:HB3   | 11:D:131:VAL:HG21 | 1.94                     | 0.49              |
| 11:n:161:ALA:HB1  | 11:n:175:LEU:HD13 | 1.94                     | 0.49              |
| 20:M:61:LYS:O     | 20:M:65:ASN:ND2   | 2.45                     | 0.49              |
| 25:R:261:LEU:HD23 | 25:R:266:LEU:HD23 | 1.94                     | 0.49              |
| 26:S:399:TYR:HD2  | 26:S:402:ILE:HD12 | 1.78                     | 0.49              |
| 32:Y:72:ASP:CG    | 32:Y:73:PHE:H     | 2.20                     | 0.49              |
| 5:5:125:ALA:HA    | 6:6:149:SER:HB2   | 1.94                     | 0.49              |
| 6:e:211:THR:HG23  | 6:e:218:GLY:HA2   | 1.94                     | 0.49              |
| 9:B:4:ARG:HG3     | 9:B:5:TYR:H       | 1.78                     | 0.49              |
| 8:c:34:THR:HA     | 8:c:84:GLY:HA2    | 1.93                     | 0.49              |
| 18:K:63:LEU:HD13  | 21:N:565:ASN:HD22 | 1.77                     | 0.49              |
| 23:P:388:ILE:HG22 | 23:P:389:ILE:HG23 | 1.95                     | 0.49              |
| 26:S:222:SER:HA   | 26:S:230:LYS:HD3  | 1.95                     | 0.49              |
| 28:U:262:GLN:N    | 29:V:306:LYS:HD2  | 2.28                     | 0.49              |
| 29:V:153:ILE:HD11 | 29:V:201:ILE:HG21 | 1.95                     | 0.49              |
| 1:1:64:ARG:HA     | 1:1:116:ILE:HG12  | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:3:11:ILE:HG21   | 3:3:142:ALA:HB3   | 1.95                     | 0.49              |
| 3:3:123:GLY:HA3   | 3:3:137:ILE:HG21  | 1.94                     | 0.49              |
| 10:C:132:GLY:HA2  | 10:C:153:PRO:HB3  | 1.95                     | 0.49              |
| 12:m:123:PHE:CD1  | 12:m:137:PRO:HB3  | 2.48                     | 0.49              |
| 17:J:228:ARG:O    | 17:J:232:GLU:N    | 2.46                     | 0.49              |
| 19:L:84:LEU:HD12  | 20:M:55:ASN:HD21  | 1.78                     | 0.49              |
| 21:N:521:LEU:HB3  | 21:N:535:LEU:HD21 | 1.95                     | 0.49              |
| 24:Q:388:GLY:HA2  | 24:Q:400:TYR:HB3  | 1.94                     | 0.49              |
| 25:R:273:SER:HB3  | 25:R:276:LEU:HB2  | 1.94                     | 0.49              |
| 27:T:224:ARG:HB2  | 27:T:235:PHE:HB2  | 1.93                     | 0.49              |
| 30:W:114:VAL:HG12 | 30:W:116:SER:H    | 1.77                     | 0.49              |
| 31:X:48:PHE:HD2   | 31:X:66:LEU:HD23  | 1.78                     | 0.49              |
| 5:5:266:HIS:HB3   | 5:5:271:LEU:HD11  | 1.94                     | 0.48              |
| 24:Q:402:THR:HB   | 24:Q:403:PRO:HD3  | 1.95                     | 0.48              |
| 27:T:224:ARG:CZ   | 27:T:235:PHE:HA   | 2.42                     | 0.48              |
| 28:U:119:LEU:HD11 | 28:U:136:ALA:HB1  | 1.94                     | 0.48              |
| 30:W:87:MET:HE3   | 30:W:91:LEU:HD11  | 1.95                     | 0.48              |
| 33:Z:796:LEU:HA   | 33:Z:799:PHE:HB3  | 1.95                     | 0.48              |
| 8:A:51:THR:HB     | 8:A:228:ALA:HB3   | 1.96                     | 0.48              |
| 10:C:152:ASN:O    | 10:C:154:SER:N    | 2.46                     | 0.48              |
| 13:l:105:VAL:HG21 | 13:l:143:HIS:HB2  | 1.94                     | 0.48              |
| 17:J:256:THR:HG22 | 18:K:326:PRO:HB2  | 1.95                     | 0.48              |
| 18:K:347:ARG:O    | 18:K:350:ARG:HG2  | 2.13                     | 0.48              |
| 22:O:79:VAL:HG23  | 22:O:80:LYS:HG2   | 1.94                     | 0.48              |
| 25:R:254:SER:HB3  | 25:R:288:SER:HB2  | 1.93                     | 0.48              |
| 5:f:146:LYS:NZ    | 12:m:65:GLU:OE1   | 2.38                     | 0.48              |
| 7:a:127:GLU:HG2   | 13:l:100:ASN:HB2  | 1.94                     | 0.48              |
| 16:I:172:LYS:HB3  | 16:I:246:ARG:HB2  | 1.95                     | 0.48              |
| 20:M:357:ARG:HG2  | 20:M:391:LEU:HD11 | 1.95                     | 0.48              |
| 23:P:124:VAL:HG22 | 23:P:129:LYS:HG3  | 1.95                     | 0.48              |
| 23:P:392:LYS:HB3  | 23:P:401:ASN:H    | 1.78                     | 0.48              |
| 6:6:29:GLY:N      | 6:6:216:GLN:HE21  | 2.12                     | 0.48              |
| 18:K:104:ASP:OD1  | 18:K:105:GLN:N    | 2.43                     | 0.48              |
| 19:L:249:SER:OG   | 20:M:307:GLU:OE2  | 2.26                     | 0.48              |
| 33:Z:266:LYS:HA   | 33:Z:293:MET:HE1  | 1.95                     | 0.48              |
| 1:b:33:LEU:HD21   | 1:b:119:ALA:HB3   | 1.96                     | 0.48              |
| 9:j:91:LYS:O      | 9:j:95:THR:N      | 2.46                     | 0.48              |
| 11:n:32:CYS:HA    | 11:n:165:GLY:HA3  | 1.96                     | 0.48              |
| 15:H:86:GLY:HA2   | 15:H:90:ARG:HH11  | 1.79                     | 0.48              |
| 19:L:290:ARG:HE   | 19:L:302:GLN:HG2  | 1.79                     | 0.48              |
| 22:O:114:GLN:C    | 22:O:116:ASN:H    | 2.21                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:S:269:GLU:HB3  | 26:S:299:LYS:HB3  | 1.94                     | 0.48              |
| 29:V:173:THR:HB   | 29:V:200:ASN:ND2  | 2.28                     | 0.48              |
| 1:b:22:ILE:HD12   | 1:b:63:CYS:HB3    | 1.95                     | 0.48              |
| 11:n:161:ALA:HB3  | 12:m:58:LEU:HD13  | 1.94                     | 0.48              |
| 15:H:86:GLY:HA2   | 15:H:90:ARG:HD2   | 1.96                     | 0.48              |
| 20:M:197:ILE:HD13 | 20:M:324:LEU:HD11 | 1.96                     | 0.48              |
| 21:N:360:GLN:HG2  | 21:N:362:TRP:H    | 1.76                     | 0.48              |
| 29:V:173:THR:HG22 | 29:V:174:THR:HG23 | 1.94                     | 0.48              |
| 29:V:237:ASN:O    | 29:V:241:THR:N    | 2.26                     | 0.48              |
| 6:e:155:CYS:HB3   | 6:e:169:LEU:HD13  | 1.96                     | 0.48              |
| 8:A:20:SER:HB2    | 8:A:21:PRO:HD2    | 1.95                     | 0.48              |
| 8:A:43:LEU:HD13   | 8:A:210:MET:HB2   | 1.95                     | 0.48              |
| 11:D:68:ASP:HB3   | 11:D:71:VAL:HB    | 1.96                     | 0.48              |
| 14:G:21:ASN:OD1   | 14:G:22:PHE:N     | 2.47                     | 0.48              |
| 15:H:434:ARG:HH11 | 33:Z:955:VAL:HB   | 1.79                     | 0.48              |
| 17:J:375:ILE:HD11 | 25:R:205:GLU:HB2  | 1.96                     | 0.48              |
| 18:K:92:VAL:O     | 18:K:94:LEU:N     | 2.47                     | 0.48              |
| 25:R:365:ASP:OD1  | 26:S:399:TYR:OH   | 2.24                     | 0.48              |
| 33:Z:133:ASP:OD1  | 33:Z:136:ARG:NH2  | 2.44                     | 0.48              |
| 4:4:4:ILE:HD11    | 4:4:133:HIS:HD2   | 1.78                     | 0.48              |
| 8:A:141:LEU:HB2   | 8:A:157:THR:HB    | 1.95                     | 0.48              |
| 11:D:64:VAL:HG11  | 11:D:213:THR:HG21 | 1.95                     | 0.48              |
| 11:D:68:ASP:OD1   | 11:D:69:SER:N     | 2.43                     | 0.48              |
| 12:E:222:ILE:HG13 | 12:E:228:PHE:HD1  | 1.77                     | 0.48              |
| 10:d:6:TYR:HD2    | 10:d:9:ARG:HD2    | 1.78                     | 0.48              |
| 13:l:13:PHE:N     | 14:k:23:GLN:OE1   | 2.46                     | 0.48              |
| 17:J:251:ASP:OD1  | 17:J:252:SER:N    | 2.46                     | 0.48              |
| 21:N:349:ILE:HA   | 21:N:356:LEU:HD11 | 1.95                     | 0.48              |
| 21:N:589:ILE:HA   | 21:N:624:ALA:HB2  | 1.94                     | 0.48              |
| 26:S:425:ARG:HD2  | 26:S:428:ARG:HG3  | 1.94                     | 0.48              |
| 28:U:259:ASN:N    | 29:V:304:ALA:HB1  | 2.28                     | 0.48              |
| 33:Z:593:HIS:HB2  | 33:Z:596:THR:HG23 | 1.95                     | 0.48              |
| 5:5:120:MET:HE3   | 5:5:128:GLN:HB2   | 1.94                     | 0.48              |
| 7:7:48:LYS:HD2    | 7:7:173:PRO:HA    | 1.96                     | 0.48              |
| 6:e:50:THR:OG1    | 6:e:55:ASN:ND2    | 2.41                     | 0.48              |
| 15:H:163:VAL:HG21 | 15:H:183:ILE:HG22 | 1.96                     | 0.48              |
| 23:P:43:GLU:HB3   | 23:P:47:ARG:NE    | 2.28                     | 0.48              |
| 25:R:79:LEU:HG    | 25:R:93:LYS:HB2   | 1.96                     | 0.48              |
| 26:S:357:LEU:HB3  | 26:S:384:ARG:HH22 | 1.79                     | 0.48              |
| 5:5:116:LEU:HD23  | 5:5:178:GLY:HA3   | 1.96                     | 0.48              |
| 20:M:187:ASP:HA   | 20:M:190:ILE:HB   | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:N:668:THR:OG1  | 21:N:711:ARG:NH2  | 2.47                     | 0.48              |
| 26:S:119:TYR:CE2  | 26:S:121:VAL:HB   | 2.49                     | 0.48              |
| 26:S:129:GLU:OE2  | 26:S:132:ALA:N    | 2.46                     | 0.48              |
| 33:Z:599:ILE:O    | 33:Z:603:VAL:HG13 | 2.14                     | 0.48              |
| 3:3:124:PHE:HB3   | 3:3:128:GLY:HA2   | 1.95                     | 0.47              |
| 8:c:113:CYS:HB2   | 8:c:144:SER:HB3   | 1.96                     | 0.47              |
| 15:H:202:GLU:HG2  | 15:H:203:LYS:HG3  | 1.96                     | 0.47              |
| 23:P:346:ILE:HG23 | 23:P:369:LEU:HD22 | 1.96                     | 0.47              |
| 25:R:261:LEU:HD11 | 25:R:265:ASP:HB2  | 1.96                     | 0.47              |
| 26:S:424:SER:O    | 27:T:192:ASN:ND2  | 2.47                     | 0.47              |
| 30:W:185:ILE:O    | 30:W:188:SER:OG   | 2.31                     | 0.47              |
| 33:Z:427:GLN:HG3  | 33:Z:458:SER:HA   | 1.95                     | 0.47              |
| 6:6:214:HIS:HE1   | 2:i:53:PRO:HB2    | 1.79                     | 0.47              |
| 16:I:259:ASP:OD1  | 16:I:262:ARG:NH2  | 2.47                     | 0.47              |
| 21:N:214:LEU:HD22 | 21:N:220:CYS:HB3  | 1.96                     | 0.47              |
| 33:Z:213:LYS:NZ   | 33:Z:239:GLU:OE2  | 2.40                     | 0.47              |
| 33:Z:256:LEU:HB3  | 33:Z:257:PRO:HD3  | 1.95                     | 0.47              |
| 3:h:53:ILE:HG22   | 3:h:60:VAL:HG22   | 1.95                     | 0.47              |
| 10:C:50:ARG:HH21  | 10:C:212:GLU:HG2  | 1.79                     | 0.47              |
| 13:F:74:LEU:HD13  | 13:F:81:ALA:HB2   | 1.96                     | 0.47              |
| 11:n:117:GLN:HE21 | 11:n:129:PHE:HB2  | 1.80                     | 0.47              |
| 12:m:71:ASP:HB3   | 12:m:74:ILE:HB    | 1.95                     | 0.47              |
| 14:k:73:HIS:CD2   | 14:k:74:ILE:HG13  | 2.49                     | 0.47              |
| 19:L:84:LEU:HD23  | 19:L:87:LEU:HD12  | 1.95                     | 0.47              |
| 20:M:248:ALA:HB1  | 20:M:286:ILE:HG12 | 1.96                     | 0.47              |
| 21:N:250:ASP:OD2  | 21:N:906:ARG:NH2  | 2.47                     | 0.47              |
| 24:Q:117:VAL:O    | 24:Q:121:SER:OG   | 2.30                     | 0.47              |
| 33:Z:359:LYS:NZ   | 33:Z:425:ILE:O    | 2.44                     | 0.47              |
| 33:Z:916:LEU:HB3  | 33:Z:920:GLY:HA2  | 1.97                     | 0.47              |
| 2:2:201:ASN:ND2   | 2:2:218:ASN:OD1   | 2.42                     | 0.47              |
| 5:5:134:LEU:HD22  | 5:5:158:LEU:HD22  | 1.95                     | 0.47              |
| 5:f:191:ASP:HB3   | 5:f:195:THR:HB    | 1.94                     | 0.47              |
| 10:C:18:ARG:HD2   | 10:C:18:ARG:O     | 2.14                     | 0.47              |
| 11:D:216:LYS:HB2  | 11:D:220:ASP:HB3  | 1.95                     | 0.47              |
| 17:J:96:VAL:HG11  | 17:J:115:LEU:HD11 | 1.95                     | 0.47              |
| 19:L:360:ILE:HA   | 19:L:363:ILE:HD12 | 1.97                     | 0.47              |
| 6:e:45:ASP:OD1    | 6:e:61:LYS:NZ     | 2.33                     | 0.47              |
| 9:B:239:THR:HG22  | 9:B:241:GLN:H     | 1.79                     | 0.47              |
| 11:D:118:GLN:OE1  | 12:E:86:ARG:NH2   | 2.38                     | 0.47              |
| 10:d:177:GLN:HE22 | 11:n:54:LEU:HB2   | 1.80                     | 0.47              |
| 16:I:181:TYR:HD1  | 16:I:184:ILE:HD11 | 1.78                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:K:236:ARG:HG3  | 18:K:270:PHE:HD2  | 1.80                     | 0.47              |
| 21:N:364:LYS:HB3  | 21:N:400:ILE:HD12 | 1.97                     | 0.47              |
| 24:Q:158:ILE:HD13 | 24:Q:161:LEU:HD12 | 1.96                     | 0.47              |
| 24:Q:382:LEU:HB3  | 25:R:263:ARG:HH22 | 1.80                     | 0.47              |
| 29:V:26:THR:HB    | 29:V:172:GLN:HE22 | 1.78                     | 0.47              |
| 30:W:125:LEU:HB3  | 30:W:157:PHE:HD1  | 1.79                     | 0.47              |
| 31:X:17:TYR:HH    | 31:X:97:TYR:HH    | 1.61                     | 0.47              |
| 5:5:243:ASP:OD1   | 3:h:33:SER:OG     | 2.32                     | 0.47              |
| 7:7:256:LYS:HB3   | 1:b:206:ILE:HG21  | 1.97                     | 0.47              |
| 7:a:183:MET:O     | 7:a:186:PRO:HD2   | 2.13                     | 0.47              |
| 13:F:190:ILE:HG23 | 13:F:213:ILE:HD13 | 1.97                     | 0.47              |
| 8:c:34:THR:HG21   | 8:c:139:ILE:HD12  | 1.97                     | 0.47              |
| 8:c:36:GLN:HG3    | 14:k:19:GLY:HA3   | 1.95                     | 0.47              |
| 10:d:4:ARG:C      | 10:d:6:TYR:H      | 2.23                     | 0.47              |
| 10:d:65:LYS:HA    | 10:d:77:VAL:HB    | 1.96                     | 0.47              |
| 21:N:902:VAL:O    | 21:N:903:VAL:HG22 | 2.15                     | 0.47              |
| 4:4:29:LYS:HD3    | 4:4:32:ASP:HB2    | 1.96                     | 0.47              |
| 1:b:195:VAL:HG22  | 1:b:204:ARG:HA    | 1.97                     | 0.47              |
| 7:a:78:VAL:HG21   | 7:a:100:LEU:HB3   | 1.97                     | 0.47              |
| 8:A:69:VAL:HG22   | 14:G:158:TRP:CD1  | 2.49                     | 0.47              |
| 9:B:50:LYS:HE2    | 9:B:52:SER:HB2    | 1.96                     | 0.47              |
| 9:B:118:MET:HE2   | 9:B:132:VAL:HG23  | 1.96                     | 0.47              |
| 10:C:115:LEU:HD23 | 10:C:118:ILE:HD12 | 1.97                     | 0.47              |
| 13:F:50:LYS:HB3   | 13:F:59:TYR:HB3   | 1.97                     | 0.47              |
| 8:c:87:PRO:HB3    | 14:k:156:SER:HB3  | 1.96                     | 0.47              |
| 11:n:158:SER:OG   | 12:m:60:GLU:OE1   | 2.32                     | 0.47              |
| 13:l:70:MET:HE1   | 13:l:103:LEU:HD23 | 1.96                     | 0.47              |
| 16:I:107:GLY:HA2  | 16:I:122:SER:HA   | 1.95                     | 0.47              |
| 16:I:253:ILE:HG21 | 16:I:286:ALA:HA   | 1.97                     | 0.47              |
| 17:J:193:THR:HA   | 17:J:355:GLY:H    | 1.78                     | 0.47              |
| 18:K:129:GLU:OE1  | 29:V:278:LYS:NZ   | 2.45                     | 0.47              |
| 19:L:432:ILE:HG23 | 19:L:435:GLN:OE1  | 2.15                     | 0.47              |
| 21:N:70:TYR:HE1   | 21:N:100:THR:HG21 | 1.80                     | 0.47              |
| 21:N:475:ALA:HB1  | 29:V:61:TYR:OH    | 2.14                     | 0.47              |
| 23:P:283:LYS:HE2  | 23:P:286:ASN:HB2  | 1.97                     | 0.47              |
| 23:P:351:ARG:HA   | 23:P:389:ILE:HD13 | 1.96                     | 0.47              |
| 24:Q:47:ASP:OD1   | 24:Q:48:ASP:N     | 2.47                     | 0.47              |
| 24:Q:113:ASP:O    | 24:Q:117:VAL:HG23 | 2.14                     | 0.47              |
| 33:Z:602:LEU:HB2  | 33:Z:738:TYR:HE2  | 1.79                     | 0.47              |
| 6:6:47:ARG:CZ     | 6:6:218:GLY:HA3   | 2.44                     | 0.47              |
| 9:B:38:LYS:HG3    | 9:B:43:VAL:HG22   | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:Q:59:LEU:HB3   | 24:Q:103:LYS:HE3  | 1.97                     | 0.47              |
| 28:U:265:LEU:HD22 | 28:U:268:LYS:HD3  | 1.95                     | 0.47              |
| 30:W:3:LEU:HD22   | 30:W:46:GLU:HB2   | 1.96                     | 0.47              |
| 13:F:67:ASP:HB3   | 13:F:70:MET:HB2   | 1.97                     | 0.47              |
| 14:G:205:GLU:HA   | 14:G:208:LYS:HE3  | 1.96                     | 0.47              |
| 8:c:53:ILE:HG12   | 8:c:224:VAL:HG22  | 1.96                     | 0.47              |
| 13:l:54:ASP:OD1   | 13:l:55:GLU:N     | 2.45                     | 0.47              |
| 16:I:243:THR:HB   | 16:I:276:PRO:HB3  | 1.96                     | 0.47              |
| 21:N:498:ILE:HG23 | 21:N:535:LEU:HD22 | 1.97                     | 0.47              |
| 22:O:289:GLN:HG2  | 22:O:293:LEU:HG   | 1.96                     | 0.47              |
| 27:T:85:LEU:HA    | 27:T:88:TYR:HD2   | 1.79                     | 0.47              |
| 27:T:111:LEU:HD22 | 27:T:181:LEU:HD11 | 1.95                     | 0.47              |
| 14:G:120:VAL:HG21 | 14:G:151:LEU:HD21 | 1.97                     | 0.47              |
| 15:H:454:TYR:OH   | 16:I:345:ASP:O    | 2.22                     | 0.47              |
| 17:J:98:VAL:HA    | 17:J:122:LEU:HB3  | 1.97                     | 0.47              |
| 21:N:912:GLU:O    | 21:N:914:VAL:N    | 2.48                     | 0.47              |
| 24:Q:161:LEU:HB3  | 24:Q:165:PHE:CE2  | 2.50                     | 0.47              |
| 24:Q:262:LEU:HD23 | 24:Q:296:ILE:HD13 | 1.96                     | 0.47              |
| 33:Z:827:LEU:O    | 33:Z:831:LEU:N    | 2.43                     | 0.47              |
| 9:B:106:PRO:HG2   | 9:B:109:LEU:HB3   | 1.95                     | 0.46              |
| 10:C:135:PHE:HB2  | 10:C:151:SER:HB3  | 1.96                     | 0.46              |
| 12:m:14:THR:HG22  | 12:m:22:PHE:HE2   | 1.79                     | 0.46              |
| 14:k:21:ASN:OD1   | 14:k:22:PHE:N     | 2.48                     | 0.46              |
| 21:N:341:ALA:HA   | 21:N:374:ILE:HA   | 1.97                     | 0.46              |
| 23:P:395:ARG:HD2  | 24:Q:358:GLU:H    | 1.79                     | 0.46              |
| 24:Q:65:TYR:HD2   | 24:Q:74:LEU:HD13  | 1.81                     | 0.46              |
| 24:Q:81:SER:HA    | 24:Q:84:TYR:HD2   | 1.79                     | 0.46              |
| 29:V:113:GLY:HA2  | 29:V:144:ILE:HD11 | 1.97                     | 0.46              |
| 33:Z:197:LYS:HG3  | 33:Z:199:ASP:H    | 1.81                     | 0.46              |
| 33:Z:237:VAL:HB   | 33:Z:271:ILE:HG12 | 1.97                     | 0.46              |
| 2:2:74:GLY:HA3    | 2:2:81:THR:HG21   | 1.97                     | 0.46              |
| 3:3:56:LEU:HD11   | 4:4:122:LEU:HD13  | 1.98                     | 0.46              |
| 3:h:104:PHE:HD1   | 3:h:126:LEU:HD13  | 1.80                     | 0.46              |
| 17:J:228:ARG:NE   | 17:J:232:GLU:OE1  | 2.46                     | 0.46              |
| 19:L:144:VAL:HA   | 19:L:161:ARG:HD3  | 1.96                     | 0.46              |
| 22:O:277:ILE:HG22 | 22:O:279:ILE:H    | 1.80                     | 0.46              |
| 3:h:63:LEU:HD11   | 3:h:105:VAL:HG21  | 1.96                     | 0.46              |
| 17:J:241:ALA:O    | 17:J:243:SER:N    | 2.47                     | 0.46              |
| 19:L:392:ARG:NE   | 20:M:340:SER:OG   | 2.41                     | 0.46              |
| 23:P:125:VAL:O    | 23:P:136:ARG:NE   | 2.47                     | 0.46              |
| 26:S:479:MET:O    | 26:S:482:PRO:HD2  | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:Z:345:GLU:O    | 33:Z:349:THR:OG1  | 2.33                     | 0.46              |
| 5:5:131:GLU:OE2   | 5:5:174:THR:OG1   | 2.30                     | 0.46              |
| 6:6:84:VAL:HG12   | 6:6:88:LYS:HE3    | 1.96                     | 0.46              |
| 10:C:18:ARG:HE    | 10:C:23:GLU:CG    | 2.22                     | 0.46              |
| 11:n:103:PRO:HG2  | 11:n:140:PRO:HG2  | 1.97                     | 0.46              |
| 16:I:219:VAL:HG12 | 16:I:346:ARG:HB3  | 1.96                     | 0.46              |
| 17:J:113:VAL:HG12 | 17:J:125:VAL:HA   | 1.97                     | 0.46              |
| 18:K:166:LYS:O    | 18:K:168:ASP:N    | 2.48                     | 0.46              |
| 22:O:72:LYS:HG2   | 22:O:73:ILE:HG12  | 1.98                     | 0.46              |
| 23:P:94:GLN:HA    | 23:P:97:ILE:HD12  | 1.96                     | 0.46              |
| 24:Q:344:GLU:HG2  | 24:Q:386:PHE:HE2  | 1.80                     | 0.46              |
| 25:R:79:LEU:HD11  | 25:R:93:LYS:HD2   | 1.97                     | 0.46              |
| 27:T:226:TRP:HE1  | 27:T:235:PHE:CB   | 2.28                     | 0.46              |
| 30:W:9:VAL:HB     | 30:W:112:ALA:HA   | 1.97                     | 0.46              |
| 1:b:20:THR:N      | 1:b:148:SER:OG    | 2.46                     | 0.46              |
| 5:f:234:ARG:HA    | 5:f:237:LEU:HB3   | 1.97                     | 0.46              |
| 6:e:219:ASP:HA    | 6:e:240:ARG:HG2   | 1.98                     | 0.46              |
| 10:C:206:LEU:HD23 | 10:C:244:ILE:HG21 | 1.97                     | 0.46              |
| 11:D:10:ILE:C     | 11:D:12:SER:H     | 2.22                     | 0.46              |
| 8:c:155:LYS:HE3   | 8:c:165:TYR:HE2   | 1.80                     | 0.46              |
| 10:d:76:ALA:HB3   | 10:d:136:ILE:HB   | 1.97                     | 0.46              |
| 19:L:280:MET:HB2  | 19:L:325:MET:HA   | 1.98                     | 0.46              |
| 20:M:129:LEU:HD22 | 20:M:154:LEU:HA   | 1.97                     | 0.46              |
| 20:M:189:GLN:HE21 | 20:M:350:PRO:HD2  | 1.80                     | 0.46              |
| 22:O:189:TYR:HE2  | 22:O:227:ILE:HB   | 1.79                     | 0.46              |
| 23:P:361:THR:HG22 | 23:P:363:LEU:H    | 1.80                     | 0.46              |
| 24:Q:391:ASP:HB3  | 24:Q:396:TRP:H    | 1.79                     | 0.46              |
| 28:U:192:ASN:O    | 29:V:230:TYR:OH   | 2.29                     | 0.46              |
| 1:b:152:PHE:CE2   | 1:b:185:ASP:HB2   | 2.50                     | 0.46              |
| 14:k:121:GLN:O    | 14:k:124:THR:OG1  | 2.32                     | 0.46              |
| 15:H:370:ARG:HG3  | 15:H:371:ILE:H    | 1.81                     | 0.46              |
| 17:J:79:VAL:HG23  | 17:J:81:ASP:H     | 1.80                     | 0.46              |
| 17:J:126:LEU:HD22 | 18:K:103:ILE:HG21 | 1.98                     | 0.46              |
| 21:N:386:MET:HB3  | 21:N:404:SER:HB2  | 1.97                     | 0.46              |
| 21:N:742:TRP:HE3  | 21:N:743:PHE:CD1  | 2.32                     | 0.46              |
| 21:N:783:SER:O    | 21:N:873:ARG:NH1  | 2.48                     | 0.46              |
| 25:R:222:ARG:HG2  | 25:R:325:HIS:CE1  | 2.50                     | 0.46              |
| 27:T:112:ASN:O    | 27:T:115:SER:OG   | 2.31                     | 0.46              |
| 33:Z:374:LEU:HD11 | 33:Z:849:ARG:HH12 | 1.81                     | 0.46              |
| 33:Z:812:ILE:HD13 | 33:Z:848:THR:HA   | 1.98                     | 0.46              |
| 4:4:101:ASN:HB3   | 4:4:133:HIS:CD2   | 2.51                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:e:128:THR:HB    | 6:e:144:PHE:HB2   | 1.97                     | 0.46              |
| 9:j:8:SER:H       | 9:j:125:GLY:N     | 2.13                     | 0.46              |
| 10:d:184:MET:HE1  | 10:d:192:LEU:HD22 | 1.97                     | 0.46              |
| 12:m:42:THR:OG1   | 12:m:45:GLY:O     | 2.31                     | 0.46              |
| 13:l:157:TYR:CE2  | 14:k:60:VAL:HG22  | 2.51                     | 0.46              |
| 17:J:132:PRO:HA   | 17:J:137:MET:HB3  | 1.96                     | 0.46              |
| 20:M:288:THR:OG1  | 20:M:290:ARG:HG2  | 2.16                     | 0.46              |
| 21:N:718:GLU:HG3  | 21:N:725:LEU:HD12 | 1.96                     | 0.46              |
| 24:Q:374:GLU:O    | 25:R:345:TYR:OH   | 2.32                     | 0.46              |
| 25:R:251:THR:OG1  | 25:R:319:CYS:SG   | 2.72                     | 0.46              |
| 3:3:28:ARG:HD2    | 3:3:183:TRP:HD1   | 1.81                     | 0.46              |
| 4:4:13:VAL:HG23   | 4:4:114:PRO:HB2   | 1.98                     | 0.46              |
| 5:5:242:ARG:HH22  | 5:5:284:ASN:HD22  | 1.63                     | 0.46              |
| 7:7:53:VAL:HG21   | 7:7:150:ALA:HB1   | 1.98                     | 0.46              |
| 15:H:430:ALA:HA   | 15:H:435:ARG:HB2  | 1.97                     | 0.46              |
| 18:K:267:SER:H    | 18:K:312:VAL:HG22 | 1.79                     | 0.46              |
| 19:L:387:ASN:ND2  | 19:L:390:ASP:O    | 2.49                     | 0.46              |
| 21:N:416:GLY:O    | 21:N:420:THR:N    | 2.49                     | 0.46              |
| 26:S:201:ILE:O    | 27:T:93:ASN:ND2   | 2.49                     | 0.46              |
| 33:Z:596:THR:HA   | 33:Z:599:ILE:HD12 | 1.98                     | 0.46              |
| 2:2:36:LYS:HB2    | 2:2:152:TYR:CE1   | 2.51                     | 0.46              |
| 7:7:183:MET:O     | 7:7:186:PRO:HD2   | 2.15                     | 0.46              |
| 1:b:151:THR:HA    | 1:b:154:TYR:CE2   | 2.51                     | 0.46              |
| 2:i:70:ILE:HG12   | 2:i:131:GLY:HA3   | 1.96                     | 0.46              |
| 5:f:233:LYS:HB3   | 5:f:271:LEU:HD21  | 1.98                     | 0.46              |
| 18:K:183:GLU:OE1  | 18:K:336:ARG:NH1  | 2.49                     | 0.46              |
| 19:L:294:GLY:C    | 19:L:296:SER:H    | 2.24                     | 0.46              |
| 20:M:82:VAL:O     | 20:M:143:ASN:N    | 2.47                     | 0.46              |
| 21:N:742:TRP:CE3  | 21:N:743:PHE:HD1  | 2.31                     | 0.46              |
| 23:P:89:LEU:HG    | 23:P:91:LEU:H     | 1.81                     | 0.46              |
| 23:P:302:LEU:HG   | 23:P:306:ASN:HB2  | 1.97                     | 0.46              |
| 23:P:392:LYS:HD2  | 23:P:401:ASN:HB2  | 1.98                     | 0.46              |
| 26:S:333:PHE:HD1  | 26:S:342:LEU:HB3  | 1.81                     | 0.46              |
| 29:V:183:ALA:H    | 29:V:186:GLN:HA   | 1.81                     | 0.46              |
| 9:B:42:GLY:HA3    | 9:B:185:LEU:HD22  | 1.97                     | 0.46              |
| 11:D:9:SER:C      | 11:D:11:PHE:H     | 2.24                     | 0.46              |
| 14:G:8:TYR:HB2    | 14:G:22:PHE:HE2   | 1.81                     | 0.46              |
| 16:I:122:SER:H    | 16:I:126:PRO:HD2  | 1.81                     | 0.46              |
| 18:K:107:THR:HA   | 18:K:121:ARG:HA   | 1.98                     | 0.46              |
| 19:L:105:ILE:HD11 | 20:M:128:PHE:HB2  | 1.98                     | 0.46              |
| 19:L:164:ASP:N    | 19:L:269:TYR:OH   | 2.43                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:M:163:PHE:HE2  | 20:M:264:ARG:HH12 | 1.64                     | 0.46              |
| 25:R:137:LEU:HG   | 25:R:141:TYR:HE2  | 1.81                     | 0.46              |
| 25:R:213:TYR:HD1  | 25:R:216:ILE:HD12 | 1.81                     | 0.46              |
| 2:2:215:TYR:HB3   | 9:B:226:GLY:HA3   | 1.98                     | 0.45              |
| 6:6:83:LEU:HD11   | 6:6:112:ILE:HG23  | 1.97                     | 0.45              |
| 8:A:86:PRO:HB2    | 8:A:89:ASP:HB2    | 1.96                     | 0.45              |
| 11:D:202:VAL:HG23 | 11:D:203:VAL:H    | 1.81                     | 0.45              |
| 14:G:88:LEU:HD21  | 14:G:151:LEU:HD23 | 1.98                     | 0.45              |
| 20:M:223:PRO:HG2  | 20:M:226:THR:HG23 | 1.98                     | 0.45              |
| 21:N:145:LEU:O    | 21:N:173:LYS:NZ   | 2.44                     | 0.45              |
| 21:N:327:LEU:HD11 | 29:V:170:PRO:HB2  | 1.98                     | 0.45              |
| 22:O:127:LEU:HD22 | 22:O:167:ILE:HG12 | 1.97                     | 0.45              |
| 23:P:271:SER:HB3  | 23:P:277:GLN:HE21 | 1.80                     | 0.45              |
| 23:P:350:LEU:HD23 | 23:P:383:LEU:HD12 | 1.98                     | 0.45              |
| 33:Z:347:ASN:HB3  | 33:Z:353:VAL:HG23 | 1.98                     | 0.45              |
| 10:C:172:ALA:HB2  | 10:C:200:THR:HG21 | 1.98                     | 0.45              |
| 8:c:16:THR:OG1    | 8:c:130:ARG:O     | 2.29                     | 0.45              |
| 9:j:222:LEU:HD13  | 9:j:232:GLY:HA2   | 1.97                     | 0.45              |
| 19:L:295:THR:HG22 | 19:L:298:ASP:HB2  | 1.97                     | 0.45              |
| 23:P:325:ASP:OD1  | 23:P:326:ASP:N    | 2.47                     | 0.45              |
| 25:R:141:TYR:HA   | 25:R:144:ILE:HD12 | 1.99                     | 0.45              |
| 33:Z:525:MET:O    | 33:Z:529:ALA:N    | 2.48                     | 0.45              |
| 3:3:65:GLU:HB3    | 10:C:100:LYS:HG3  | 1.98                     | 0.45              |
| 9:B:111:VAL:HG21  | 9:B:148:TYR:HD2   | 1.82                     | 0.45              |
| 16:I:247:ILE:HB   | 16:I:281:ILE:HG12 | 1.97                     | 0.45              |
| 21:N:376:LYS:HA   | 21:N:411:ILE:HA   | 1.98                     | 0.45              |
| 33:Z:781:GLY:HA3  | 33:Z:818:CYS:HA   | 1.98                     | 0.45              |
| 33:Z:958:ASN:H    | 33:Z:961:GLU:HB2  | 1.82                     | 0.45              |
| 9:B:94:HIS:O      | 9:B:99:ARG:N      | 2.46                     | 0.45              |
| 10:C:168:ASN:HB3  | 10:C:171:ALA:HB3  | 1.98                     | 0.45              |
| 11:D:78:LEU:HB2   | 16:I:436:TYR:CZ   | 2.51                     | 0.45              |
| 12:E:119:LEU:HD12 | 12:E:122:ARG:HE   | 1.82                     | 0.45              |
| 14:G:73:HIS:CD2   | 14:G:74:ILE:HG13  | 2.51                     | 0.45              |
| 9:j:5:TYR:HD2     | 11:n:4:TYR:HB3    | 1.82                     | 0.45              |
| 16:I:436:TYR:N    | 16:I:436:TYR:CD1  | 2.83                     | 0.45              |
| 18:K:127:ASP:OD1  | 18:K:128:ARG:N    | 2.50                     | 0.45              |
| 26:S:395:ILE:HD12 | 26:S:410:LYS:HD3  | 1.98                     | 0.45              |
| 27:T:221:ALA:HA   | 27:T:226:TRP:CD1  | 2.51                     | 0.45              |
| 30:W:107:HIS:HD2  | 30:W:197:SER:HB3  | 1.82                     | 0.45              |
| 33:Z:453:LEU:HB2  | 33:Z:488:ALA:HB1  | 1.97                     | 0.45              |
| 33:Z:491:LEU:HD11 | 33:Z:903:MET:HG2  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:5:82:ARG:HG2    | 5:5:87:ILE:HG12   | 1.98                     | 0.45              |
| 7:7:61:GLY:N      | 7:7:69:PHE:O      | 2.45                     | 0.45              |
| 9:j:5:TYR:HB2     | 11:n:4:TYR:HB3    | 1.98                     | 0.45              |
| 11:n:157:SER:OG   | 11:n:159:TRP:NE1  | 2.49                     | 0.45              |
| 15:H:240:ILE:HG22 | 20:M:368:MET:HG2  | 1.99                     | 0.45              |
| 18:K:261:ALA:HB1  | 18:K:267:SER:HB3  | 1.97                     | 0.45              |
| 19:L:168:TYR:HD2  | 20:M:143:ASN:HD22 | 1.64                     | 0.45              |
| 21:N:163:LEU:HB3  | 21:N:209:LYS:HE3  | 1.98                     | 0.45              |
| 1:1:27:PHE:HE2    | 1:1:32:ILE:HG13   | 1.80                     | 0.45              |
| 7:7:172:SER:OG    | 7:7:174:THR:O     | 2.32                     | 0.45              |
| 12:m:23:GLN:HB3   | 12:m:137:PRO:HG3  | 1.99                     | 0.45              |
| 12:m:86:ARG:HA    | 12:m:89:ILE:HD12  | 1.97                     | 0.45              |
| 15:H:105:ILE:HG23 | 15:H:145:TYR:CE1  | 2.51                     | 0.45              |
| 17:J:334:LYS:HB3  | 18:K:202:GLY:HA3  | 1.99                     | 0.45              |
| 18:K:327:ALA:O    | 18:K:333:ARG:NH1  | 2.50                     | 0.45              |
| 20:M:246:LEU:HD21 | 20:M:251:LEU:HD21 | 1.98                     | 0.45              |
| 21:N:9:LEU:HD23   | 21:N:12:LEU:HD12  | 1.97                     | 0.45              |
| 27:T:28:PRO:HA    | 27:T:31:LYS:HE2   | 1.98                     | 0.45              |
| 33:Z:204:CYS:HA   | 33:Z:232:LYS:HG2  | 1.99                     | 0.45              |
| 5:5:94:ARG:NH1    | 5:5:244:ALA:O     | 2.49                     | 0.45              |
| 10:C:124:GLN:HA   | 11:D:127:ARG:HG2  | 1.99                     | 0.45              |
| 13:l:34:VAL:HG22  | 13:l:162:GLY:HA3  | 1.99                     | 0.45              |
| 17:J:192:GLY:N    | 17:J:252:SER:O    | 2.50                     | 0.45              |
| 17:J:361:VAL:HG22 | 17:J:389:VAL:HG21 | 1.98                     | 0.45              |
| 19:L:164:ASP:O    | 19:L:166:LEU:N    | 2.49                     | 0.45              |
| 23:P:268:LEU:HD13 | 23:P:280:LEU:HD12 | 1.98                     | 0.45              |
| 24:Q:223:GLY:HA2  | 24:Q:226:HIS:HD2  | 1.82                     | 0.45              |
| 29:V:51:GLY:HA3   | 29:V:108:TYR:CZ   | 2.52                     | 0.45              |
| 3:h:72:ASN:ND2    | 10:d:96:GLN:OE1   | 2.47                     | 0.45              |
| 10:d:63:THR:HG21  | 10:d:212:GLU:HG2  | 1.98                     | 0.45              |
| 15:H:320:ASP:OD1  | 20:M:290:ARG:NH2  | 2.50                     | 0.45              |
| 22:O:352:TRP:CZ2  | 22:O:355:PRO:HA   | 2.52                     | 0.45              |
| 33:Z:321:PHE:HB3  | 33:Z:326:VAL:HG21 | 1.98                     | 0.45              |
| 33:Z:538:CYS:HA   | 33:Z:577:GLN:HE22 | 1.82                     | 0.45              |
| 6:6:183:THR:HB    | 6:6:186:LYS:HB3   | 1.98                     | 0.45              |
| 5:f:96:THR:HG22   | 5:f:101:VAL:HA    | 1.99                     | 0.45              |
| 6:e:76:PHE:HE2    | 6:e:78:ALA:HB3    | 1.82                     | 0.45              |
| 9:B:48:GLU:O      | 9:B:63:LYS:NZ     | 2.37                     | 0.45              |
| 13:F:9:ASP:OD1    | 13:F:10:THR:N     | 2.50                     | 0.45              |
| 13:l:50:LYS:HB3   | 13:l:59:TYR:HB3   | 1.99                     | 0.45              |
| 15:H:100:ALA:HB2  | 15:H:149:LEU:HD23 | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:N:875:LEU:HD12 | 21:N:876:PRO:HD2  | 1.99                     | 0.45              |
| 23:P:261:LEU:HD21 | 23:P:293:LEU:HD22 | 1.99                     | 0.45              |
| 26:S:111:ARG:HA   | 26:S:117:SER:HB3  | 1.98                     | 0.45              |
| 26:S:330:LEU:HB2  | 32:Y:64:TRP:HD1   | 1.82                     | 0.45              |
| 31:X:7:VAL:HG12   | 31:X:8:ILE:HG13   | 1.99                     | 0.45              |
| 33:Z:576:GLY:H    | 33:Z:606:CYS:HB3  | 1.81                     | 0.45              |
| 8:A:126:GLN:HE22  | 9:B:81:ASP:HA     | 1.83                     | 0.45              |
| 10:C:156:ASN:HA   | 11:D:83:ARG:HH12  | 1.82                     | 0.45              |
| 11:D:12:SER:HB2   | 11:D:17:ILE:HA    | 1.98                     | 0.45              |
| 13:l:117:GLN:HE22 | 14:k:84:ASP:HA    | 1.81                     | 0.45              |
| 14:k:50:VAL:HG21  | 14:k:66:LYS:HB2   | 1.99                     | 0.45              |
| 15:H:311:ILE:O    | 15:H:315:GLY:N    | 2.49                     | 0.45              |
| 19:L:229:THR:HG21 | 20:M:313:ASP:HB3  | 1.98                     | 0.45              |
| 20:M:214:ALA:N    | 20:M:319:ASP:OD2  | 2.50                     | 0.45              |
| 23:P:335:LYS:HE3  | 23:P:336:HIS:CE1  | 2.52                     | 0.45              |
| 25:R:325:HIS:O    | 25:R:328:PHE:HD2  | 2.00                     | 0.45              |
| 26:S:217:PHE:HD2  | 26:S:233:LEU:HD11 | 1.82                     | 0.45              |
| 27:T:131:LYS:HB3  | 27:T:134:LYS:HB2  | 1.98                     | 0.45              |
| 28:U:259:ASN:HA   | 29:V:306:LYS:N    | 2.32                     | 0.45              |
| 4:4:3:ILE:HG23    | 4:4:18:SER:HB3    | 1.98                     | 0.44              |
| 7:7:215:ARG:HH12  | 7:7:249:ASN:HD22  | 1.65                     | 0.44              |
| 1:b:167:LYS:HE3   | 1:b:196:VAL:HG11  | 1.99                     | 0.44              |
| 6:e:90:SER:OG     | 6:e:111:ASN:ND2   | 2.50                     | 0.44              |
| 8:A:156:LYS:HD3   | 8:A:166:TYR:HE2   | 1.82                     | 0.44              |
| 11:D:138:PHE:HE1  | 11:D:145:PRO:HB3  | 1.81                     | 0.44              |
| 11:n:72:VAL:HG13  | 11:n:221:ILE:HD13 | 1.99                     | 0.44              |
| 13:l:81:ALA:HB2   | 13:l:130:VAL:HG21 | 1.97                     | 0.44              |
| 17:J:147:TYR:OH   | 17:J:165:GLU:OE1  | 2.33                     | 0.44              |
| 23:P:126:THR:O    | 23:P:136:ARG:NH2  | 2.50                     | 0.44              |
| 2:i:81:THR:HG23   | 2:i:127:LEU:HD21  | 1.98                     | 0.44              |
| 3:h:12:VAL:HB     | 3:h:108:VAL:HG21  | 1.98                     | 0.44              |
| 8:c:155:LYS:HE3   | 8:c:165:TYR:CE2   | 2.52                     | 0.44              |
| 10:d:175:LEU:HD12 | 10:d:196:THR:HG23 | 2.00                     | 0.44              |
| 11:n:115:GLY:O    | 11:n:119:ARG:N    | 2.44                     | 0.44              |
| 16:I:106:ILE:HD11 | 17:J:93:LYS:HB2   | 1.99                     | 0.44              |
| 17:J:328:LEU:O    | 17:J:332:SER:N    | 2.51                     | 0.44              |
| 19:L:123:SER:C    | 19:L:125:PRO:HD2  | 2.43                     | 0.44              |
| 24:Q:117:VAL:O    | 24:Q:117:VAL:HG12 | 2.17                     | 0.44              |
| 24:Q:422:VAL:O    | 28:U:295:LYS:NZ   | 2.49                     | 0.44              |
| 29:V:26:THR:HB    | 29:V:172:GLN:NE2  | 2.32                     | 0.44              |
| 29:V:27:VAL:HG22  | 29:V:63:VAL:HG11  | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:3:63:LEU:HD11   | 3:3:105:VAL:HG21  | 2.00                     | 0.44              |
| 5:5:82:ARG:HD2    | 5:5:185:PRO:HB2   | 1.99                     | 0.44              |
| 1:b:40:THR:HG21   | 1:b:187:SER:HA    | 1.98                     | 0.44              |
| 2:i:244:GLU:HG2   | 3:h:198:ARG:HG2   | 1.99                     | 0.44              |
| 3:h:10:GLY:HA3    | 3:h:42:LYS:NZ     | 2.32                     | 0.44              |
| 11:n:68:ASP:OD1   | 11:n:69:SER:N     | 2.45                     | 0.44              |
| 12:m:35:SER:OG    | 12:m:51:GLU:O     | 2.26                     | 0.44              |
| 15:H:279:LEU:HB3  | 15:H:332:THR:HG21 | 2.00                     | 0.44              |
| 18:K:395:VAL:HG21 | 19:L:207:PHE:HE1  | 1.81                     | 0.44              |
| 21:N:750:SER:HA   | 21:N:753:PHE:HD2  | 1.82                     | 0.44              |
| 26:S:247:VAL:O    | 26:S:251:SER:N    | 2.47                     | 0.44              |
| 28:U:27:THR:HG23  | 28:U:31:LYS:HB2   | 2.00                     | 0.44              |
| 1:1:182:ILE:HG12  | 1:1:189:GLY:HA2   | 1.99                     | 0.44              |
| 2:2:123:ILE:HG22  | 2:2:125:ALA:H     | 1.83                     | 0.44              |
| 6:e:35:ALA:HB3    | 6:e:154:GLN:HA    | 1.99                     | 0.44              |
| 13:F:95:SER:O     | 13:F:100:ASN:N    | 2.50                     | 0.44              |
| 14:G:78:TYR:HE2   | 14:G:82:ILE:HA    | 1.83                     | 0.44              |
| 10:d:15:PRO:HA    | 11:n:22:TYR:CZ    | 2.52                     | 0.44              |
| 11:n:122:GLN:HG3  | 12:m:138:PHE:HE1  | 1.82                     | 0.44              |
| 18:K:360:MET:HE1  | 19:L:212:ILE:HA   | 1.99                     | 0.44              |
| 19:L:137:ARG:HA   | 19:L:140:LEU:HD12 | 2.00                     | 0.44              |
| 21:N:176:GLN:HG3  | 21:N:182:ASN:HD22 | 1.83                     | 0.44              |
| 31:X:37:PRO:HB3   | 31:X:46:TRP:HD1   | 1.83                     | 0.44              |
| 1:b:181:ALA:O     | 1:b:185:ASP:HB3   | 2.17                     | 0.44              |
| 6:e:157:ALA:N     | 6:e:166:MET:SD    | 2.91                     | 0.44              |
| 10:C:232:PRO:HA   | 10:C:235:ILE:HD12 | 1.99                     | 0.44              |
| 11:D:196:VAL:HG13 | 11:D:210:ILE:HD13 | 1.99                     | 0.44              |
| 15:H:311:ILE:HG22 | 15:H:355:THR:HB   | 1.99                     | 0.44              |
| 21:N:245:LEU:HD11 | 21:N:257:ILE:HD12 | 1.98                     | 0.44              |
| 28:U:210:TYR:HE2  | 28:U:229:LEU:HD11 | 1.83                     | 0.44              |
| 29:V:168:LEU:HD12 | 29:V:170:PRO:HD2  | 1.98                     | 0.44              |
| 30:W:110:ILE:HB   | 30:W:139:VAL:HA   | 2.00                     | 0.44              |
| 33:Z:930:GLY:HA2  | 33:Z:966:GLU:HG3  | 1.99                     | 0.44              |
| 5:f:91:VAL:HG11   | 5:f:109:VAL:HG23  | 2.00                     | 0.44              |
| 8:A:88:PRO:HB3    | 14:G:156:SER:HB3  | 1.99                     | 0.44              |
| 12:E:169:ALA:HB1  | 12:E:183:LEU:HD22 | 1.98                     | 0.44              |
| 10:d:120:GLN:HE22 | 11:n:83:ARG:HB2   | 1.82                     | 0.44              |
| 12:m:21:LEU:HB3   | 12:m:24:VAL:HG23  | 1.99                     | 0.44              |
| 18:K:291:GLU:C    | 18:K:293:GLN:H    | 2.24                     | 0.44              |
| 24:Q:377:LEU:HD23 | 24:Q:390:LEU:HD21 | 2.00                     | 0.44              |
| 26:S:226:ASP:OD2  | 26:S:229:THR:OG1  | 2.31                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 33:Z:352:LYS:HB3  | 33:Z:466:GLU:HG3  | 2.00                     | 0.44              |
| 10:C:91:ALA:HB2   | 10:C:115:LEU:HD21 | 1.99                     | 0.44              |
| 12:m:21:LEU:HG    | 12:m:23:GLN:H     | 1.83                     | 0.44              |
| 20:M:340:SER:HA   | 20:M:344:ASP:OD1  | 2.17                     | 0.44              |
| 21:N:375:HIS:CD2  | 21:N:385:VAL:HG21 | 2.52                     | 0.44              |
| 21:N:773:MET:HG3  | 21:N:869:ASP:OD2  | 2.18                     | 0.44              |
| 23:P:358:SER:O    | 23:P:402:PHE:N    | 2.51                     | 0.44              |
| 26:S:82:TYR:CD2   | 26:S:86:SER:HB3   | 2.52                     | 0.44              |
| 28:U:74:GLU:OE2   | 28:U:113:TYR:OH   | 2.28                     | 0.44              |
| 33:Z:812:ILE:HD12 | 33:Z:847:ILE:HG22 | 2.00                     | 0.44              |
| 33:Z:821:GLY:HA3  | 33:Z:862:MET:HB2  | 1.98                     | 0.44              |
| 2:2:244:GLU:HG3   | 3:3:198:ARG:HG2   | 2.00                     | 0.44              |
| 4:4:7:ILE:HD12    | 4:4:144:LEU:HD22  | 2.00                     | 0.44              |
| 5:5:186:THR:HG23  | 5:5:198:LYS:HE3   | 2.00                     | 0.44              |
| 13:F:132:LEU:HB2  | 13:F:147:PHE:HB3  | 2.00                     | 0.44              |
| 9:j:66:LEU:HD13   | 9:j:69:PRO:HB3    | 2.00                     | 0.44              |
| 14:k:95:GLU:HB3   | 14:k:115:ARG:HE   | 1.82                     | 0.44              |
| 17:J:48:ARG:HD3   | 18:K:72:GLN:HB2   | 2.00                     | 0.44              |
| 21:N:778:LYS:HD3  | 21:N:878:GLN:HB2  | 2.00                     | 0.44              |
| 30:W:109:ARG:HH22 | 30:W:195:GLY:HA3  | 1.83                     | 0.44              |
| 2:2:30:THR:OG1    | 2:2:62:LYS:NZ     | 2.50                     | 0.44              |
| 7:7:108:ALA:HA    | 7:7:112:PRO:HB3   | 2.00                     | 0.44              |
| 6:e:107:SER:HB3   | 12:m:103:TYR:HD1  | 1.83                     | 0.44              |
| 7:a:162:TYR:HE1   | 7:a:177:THR:HG22  | 1.83                     | 0.44              |
| 10:C:52:VAL:HG23  | 10:C:59:GLN:HE21  | 1.83                     | 0.44              |
| 14:G:150:MET:HB3  | 14:G:160:TYR:CE2  | 2.53                     | 0.44              |
| 8:c:95:ARG:HE     | 8:c:123:LEU:HD13  | 1.83                     | 0.44              |
| 14:k:70:VAL:HB    | 14:k:74:ILE:HB    | 2.00                     | 0.44              |
| 21:N:596:LEU:HD23 | 21:N:628:ALA:HB2  | 1.98                     | 0.44              |
| 21:N:724:THR:HG23 | 21:N:725:LEU:H    | 1.83                     | 0.44              |
| 28:U:263:LYS:HE2  | 29:V:306:LYS:NZ   | 2.32                     | 0.44              |
| 29:V:202:ASP:OD1  | 29:V:203:TYR:N    | 2.51                     | 0.44              |
| 33:Z:309:GLN:HA   | 33:Z:312:TYR:HD2  | 1.83                     | 0.44              |
| 33:Z:374:LEU:HB3  | 33:Z:379:GLN:NE2  | 2.33                     | 0.44              |
| 5:f:112:ILE:HG23  | 5:f:135:GLY:HA2   | 2.00                     | 0.43              |
| 14:G:204:HIS:CE1  | 14:G:208:LYS:HA   | 2.53                     | 0.43              |
| 11:n:65:SER:O     | 11:n:73:LEU:N     | 2.51                     | 0.43              |
| 24:Q:124:PHE:O    | 24:Q:126:LYS:N    | 2.50                     | 0.43              |
| 3:3:4:PRO:HA      | 3:3:7:ILE:HD12    | 1.98                     | 0.43              |
| 3:3:53:ILE:HG22   | 3:3:60:VAL:HG22   | 2.00                     | 0.43              |
| 6:6:74:ASN:HB3    | 6:6:127:HIS:HB3   | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:f:253:TYR:HE1   | 5:f:262:TYR:HD1   | 1.66                     | 0.43              |
| 8:A:114:CYS:HB2   | 8:A:145:SER:OG    | 2.18                     | 0.43              |
| 8:c:125:GLN:NE2   | 9:j:81:ASP:OD1    | 2.51                     | 0.43              |
| 9:j:38:LYS:HG3    | 9:j:43:VAL:HG22   | 1.99                     | 0.43              |
| 12:m:78:MET:HA    | 12:m:142:LEU:HD23 | 2.00                     | 0.43              |
| 20:M:178:GLU:HB3  | 20:M:233:ARG:HG2  | 2.00                     | 0.43              |
| 21:N:58:ARG:HA    | 21:N:61:ALA:HB3   | 2.00                     | 0.43              |
| 21:N:625:LEU:HD21 | 21:N:637:ALA:HB1  | 1.99                     | 0.43              |
| 25:R:191:LEU:HD13 | 25:R:213:TYR:HB3  | 2.00                     | 0.43              |
| 28:U:94:HIS:CE1   | 28:U:122:ILE:HG12 | 2.53                     | 0.43              |
| 33:Z:307:HIS:CE1  | 33:Z:340:LEU:HD12 | 2.53                     | 0.43              |
| 33:Z:572:ILE:HD11 | 33:Z:882:LEU:HB2  | 2.00                     | 0.43              |
| 1:1:145:ILE:HD11  | 1:1:154:TYR:CD1   | 2.50                     | 0.43              |
| 3:3:8:ASN:OD1     | 3:3:57:ALA:N      | 2.37                     | 0.43              |
| 3:3:29:LEU:HB3    | 3:3:37:SER:HB3    | 2.00                     | 0.43              |
| 4:g:41:HIS:HB2    | 4:g:107:TYR:HB3   | 2.00                     | 0.43              |
| 5:f:203:CYS:HB2   | 5:f:212:TYR:CE1   | 2.53                     | 0.43              |
| 6:e:41:VAL:HG12   | 6:e:225:ILE:HG12  | 2.00                     | 0.43              |
| 8:A:77:ARG:O      | 8:A:78:THR:OG1    | 2.30                     | 0.43              |
| 12:E:45:GLY:HA2   | 12:E:153:TYR:CD1  | 2.53                     | 0.43              |
| 11:n:167:ASN:HD22 | 11:n:202:VAL:HG12 | 1.83                     | 0.43              |
| 13:l:39:ARG:HD3   | 13:l:144:LEU:HB2  | 2.00                     | 0.43              |
| 15:H:177:ASP:OD1  | 15:H:178:ARG:N    | 2.51                     | 0.43              |
| 22:O:76:LEU:HA    | 22:O:79:VAL:HG22  | 2.00                     | 0.43              |
| 23:P:76:ASN:HB3   | 23:P:121:THR:HG21 | 2.01                     | 0.43              |
| 25:R:63:TYR:HE1   | 25:R:92:ILE:HD12  | 1.83                     | 0.43              |
| 25:R:240:SER:C    | 25:R:242:GLU:H    | 2.25                     | 0.43              |
| 29:V:159:ILE:HD11 | 29:V:197:TYR:HA   | 2.00                     | 0.43              |
| 30:W:4:GLU:CD     | 30:W:109:ARG:HE   | 2.26                     | 0.43              |
| 7:7:114:ALA:HB1   | 7:7:117:GLU:HB2   | 2.00                     | 0.43              |
| 3:h:113:ASN:OD1   | 3:h:114:SER:N     | 2.52                     | 0.43              |
| 6:e:98:HIS:HD2    | 12:m:108:ASN:HD22 | 1.64                     | 0.43              |
| 10:C:45:VAL:HG22  | 10:C:215:THR:HG23 | 2.00                     | 0.43              |
| 10:C:83:ASP:HB3   | 10:C:131:PHE:CG   | 2.53                     | 0.43              |
| 13:F:77:LEU:N     | 13:F:130:VAL:HG12 | 2.33                     | 0.43              |
| 8:c:24:LEU:HD23   | 8:c:27:VAL:HG23   | 2.01                     | 0.43              |
| 8:c:90:ARG:NH2    | 14:k:114:ASP:OD1  | 2.51                     | 0.43              |
| 11:n:11:PHE:HB2   | 12:m:23:GLN:HE22  | 1.84                     | 0.43              |
| 11:n:105:THR:HG22 | 11:n:107:GLU:H    | 1.83                     | 0.43              |
| 18:K:48:TYR:HB3   | 21:N:151:LYS:HD3  | 2.00                     | 0.43              |
| 22:O:132:GLU:OE2  | 22:O:135:ARG:NH1  | 2.51                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:Q:390:LEU:HB2  | 25:R:345:TYR:HD1  | 1.84                     | 0.43              |
| 27:T:202:LEU:HD23 | 27:T:205:ILE:HD12 | 1.99                     | 0.43              |
| 3:3:16:THR:O      | 3:3:154:TYR:OH    | 2.27                     | 0.43              |
| 7:7:185:ASN:HB3   | 7:7:186:PRO:HD3   | 1.98                     | 0.43              |
| 7:a:47:MET:HG2    | 7:a:210:ILE:HD11  | 2.00                     | 0.43              |
| 8:A:78:THR:HA     | 8:A:233:PHE:HB2   | 2.01                     | 0.43              |
| 14:G:54:ILE:HB    | 14:G:211:ASP:HB2  | 1.99                     | 0.43              |
| 8:c:86:ILE:N      | 8:c:87:PRO:HD2    | 2.34                     | 0.43              |
| 18:K:186:GLU:HA   | 18:K:190:LEU:HD12 | 1.99                     | 0.43              |
| 20:M:50:ARG:HG2   | 30:W:73:LEU:HD12  | 2.01                     | 0.43              |
| 22:O:157:LEU:HD21 | 22:O:168:THR:HG23 | 2.01                     | 0.43              |
| 28:U:12:PRO:HD2   | 28:U:163:ALA:HB2  | 2.01                     | 0.43              |
| 28:U:14:VAL:HG13  | 28:U:51:SER:HB3   | 2.00                     | 0.43              |
| 29:V:274:GLN:O    | 29:V:278:LYS:HG3  | 2.18                     | 0.43              |
| 30:W:98:LEU:HD13  | 30:W:108:GLN:HB3  | 2.01                     | 0.43              |
| 31:X:85:ARG:HH22  | 31:X:104:LYS:HG3  | 1.82                     | 0.43              |
| 33:Z:76:LYS:HE2   | 33:Z:150:GLY:HA2  | 2.01                     | 0.43              |
| 2:i:206:VAL:HB    | 2:i:214:GLU:HB2   | 2.01                     | 0.43              |
| 3:h:34:LEU:HD11   | 4:g:141:PHE:HE2   | 1.84                     | 0.43              |
| 7:a:49:TYR:HE2    | 7:a:54:ILE:HG13   | 1.83                     | 0.43              |
| 10:C:12:ILE:HA    | 11:D:19:GLN:NE2   | 2.34                     | 0.43              |
| 11:n:35:GLY:HA3   | 11:n:44:LEU:HD23  | 2.01                     | 0.43              |
| 20:M:186:LEU:HD13 | 20:M:231:LEU:HD11 | 2.00                     | 0.43              |
| 21:N:230:VAL:CG1  | 21:N:723:GLY:HA3  | 2.49                     | 0.43              |
| 21:N:681:ASN:HA   | 21:N:684:SER:HB3  | 2.00                     | 0.43              |
| 25:R:235:LEU:HD12 | 25:R:253:ALA:HB2  | 2.01                     | 0.43              |
| 26:S:427:ILE:HG22 | 26:S:432:ILE:HB   | 2.01                     | 0.43              |
| 4:4:38:LEU:O      | 4:4:65:GLN:NE2    | 2.51                     | 0.43              |
| 2:i:92:ILE:HG23   | 2:i:103:PRO:HG2   | 2.00                     | 0.43              |
| 2:i:206:VAL:O     | 2:i:214:GLU:N     | 2.48                     | 0.43              |
| 7:a:87:SER:OG     | 7:a:146:ALA:HB3   | 2.19                     | 0.43              |
| 7:a:176:ALA:HB3   | 7:a:181:ALA:HA    | 1.99                     | 0.43              |
| 8:A:218:PHE:HB3   | 8:A:222:ASP:HB2   | 2.01                     | 0.43              |
| 9:B:94:HIS:HA     | 9:B:98:LYS:HB3    | 1.99                     | 0.43              |
| 9:B:139:HIS:O     | 9:B:234:ARG:NH1   | 2.52                     | 0.43              |
| 13:F:43:HIS:CD2   | 13:F:217:GLY:HA3  | 2.54                     | 0.43              |
| 13:F:157:TYR:CE2  | 14:G:60:VAL:HG22  | 2.54                     | 0.43              |
| 9:j:45:ILE:HD12   | 9:j:74:VAL:HB     | 1.99                     | 0.43              |
| 16:I:171:MET:O    | 17:J:278:GLN:NE2  | 2.48                     | 0.43              |
| 22:O:308:LEU:HB3  | 22:O:348:VAL:HB   | 2.00                     | 0.43              |
| 23:P:144:VAL:HG13 | 23:P:156:ALA:HB1  | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:Q:189:ARG:HB3  | 25:R:277:LEU:HD13 | 2.00                     | 0.43              |
| 28:U:263:LYS:HE2  | 29:V:306:LYS:HZ2  | 1.83                     | 0.43              |
| 29:V:287:THR:O    | 29:V:291:ASN:ND2  | 2.49                     | 0.43              |
| 2:2:242:LEU:N     | 3:3:199:TYR:O     | 2.49                     | 0.43              |
| 6:6:89:ASN:HA     | 6:6:92:LYS:HB2    | 2.00                     | 0.43              |
| 6:e:114:HIS:NE2   | 12:m:101:LEU:O    | 2.52                     | 0.43              |
| 9:B:78:MET:HB2    | 9:B:81:ASP:HB2    | 2.00                     | 0.43              |
| 10:C:19:LEU:HG    | 10:C:21:GLN:H     | 1.83                     | 0.43              |
| 10:C:194:LEU:HD13 | 10:C:239:LEU:HD23 | 2.00                     | 0.43              |
| 14:k:218:TRP:CH2  | 14:k:224:THR:HG23 | 2.54                     | 0.43              |
| 16:I:96:LEU:O     | 16:I:100:ARG:N    | 2.51                     | 0.43              |
| 17:J:25:GLN:HE22  | 21:N:99:GLU:HB3   | 1.84                     | 0.43              |
| 20:M:69:ILE:HA    | 20:M:72:ASN:HB2   | 2.01                     | 0.43              |
| 21:N:83:LEU:HD13  | 21:N:132:LYS:HB3  | 2.00                     | 0.43              |
| 21:N:585:ARG:HB2  | 21:N:616:HIS:HB3  | 2.01                     | 0.43              |
| 22:O:196:LEU:HD13 | 22:O:203:THR:HB   | 2.00                     | 0.43              |
| 22:O:222:LEU:HB3  | 22:O:280:LEU:HD13 | 2.00                     | 0.43              |
| 23:P:55:SER:HA    | 23:P:59:LEU:HB3   | 2.00                     | 0.43              |
| 23:P:392:LYS:NZ   | 23:P:401:ASN:HD22 | 2.16                     | 0.43              |
| 23:P:408:SER:HB2  | 23:P:413:ASN:HB3  | 2.01                     | 0.43              |
| 24:Q:378:SER:HA   | 24:Q:381:ILE:HD12 | 2.01                     | 0.43              |
| 26:S:486:LYS:HE2  | 28:U:308:ASP:HB3  | 2.00                     | 0.43              |
| 2:2:126:TYR:HE1   | 2:2:144:ALA:H     | 1.67                     | 0.43              |
| 8:A:87:ILE:N      | 8:A:88:PRO:HD2    | 2.34                     | 0.43              |
| 9:j:32:VAL:O      | 9:j:76:SER:OG     | 2.27                     | 0.43              |
| 9:j:92:VAL:O      | 9:j:96:SER:OG     | 2.32                     | 0.43              |
| 15:H:362:ASP:HB3  | 15:H:365:LEU:HB2  | 1.99                     | 0.43              |
| 17:J:64:LEU:HB3   | 18:K:121:ARG:HD2  | 2.01                     | 0.43              |
| 18:K:426:PHE:HD1  | 18:K:427:TYR:H    | 1.67                     | 0.43              |
| 19:L:107:GLU:OE2  | 19:L:145:ARG:NH2  | 2.52                     | 0.43              |
| 25:R:72:VAL:O     | 25:R:72:VAL:HG12  | 2.19                     | 0.43              |
| 27:T:88:TYR:C     | 27:T:90:PHE:H     | 2.25                     | 0.43              |
| 28:U:24:ARG:HH11  | 29:V:100:ARG:HG2  | 1.84                     | 0.43              |
| 29:V:23:THR:OG1   | 29:V:24:LYS:N     | 2.47                     | 0.43              |
| 33:Z:312:TYR:CD1  | 33:Z:349:THR:HA   | 2.54                     | 0.43              |
| 3:h:18:LYS:HB2    | 3:h:157:ASN:HA    | 2.01                     | 0.43              |
| 6:e:21:PHE:CZ     | 7:a:142:PRO:HG2   | 2.53                     | 0.43              |
| 6:e:203:VAL:HG12  | 6:e:221:LEU:HD21  | 2.00                     | 0.43              |
| 14:G:54:ILE:HG12  | 14:G:59:LEU:HD23  | 2.00                     | 0.43              |
| 14:G:119:TYR:O    | 14:G:123:HIS:ND1  | 2.47                     | 0.43              |
| 15:H:170:GLU:HB3  | 20:M:166:ARG:HH22 | 1.84                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:I:229:LYS:HD2  | 16:I:327:ALA:HB1  | 2.01                     | 0.43              |
| 17:J:48:ARG:HD2   | 18:K:75:LEU:HD23  | 2.01                     | 0.43              |
| 19:L:255:TYR:HB2  | 19:L:258:GLU:HB3  | 1.99                     | 0.43              |
| 25:R:352:SER:O    | 25:R:356:ALA:HB3  | 2.19                     | 0.43              |
| 27:T:238:GLN:HG3  | 27:T:239:SER:N    | 2.34                     | 0.43              |
| 8:A:183:GLU:HG2   | 8:A:187:LYS:HE3   | 2.00                     | 0.42              |
| 8:c:193:ILE:HG22  | 8:c:195:GLU:H     | 1.84                     | 0.42              |
| 19:L:421:LYS:O    | 19:L:425:VAL:HG23 | 2.19                     | 0.42              |
| 21:N:286:LEU:HD23 | 21:N:289:ILE:HD12 | 2.00                     | 0.42              |
| 21:N:724:THR:HG23 | 21:N:725:LEU:N    | 2.34                     | 0.42              |
| 28:U:226:LEU:HD23 | 28:U:229:LEU:HD12 | 2.00                     | 0.42              |
| 1:1:122:ASP:OD1   | 1:1:123:ASP:N     | 2.51                     | 0.42              |
| 4:4:30:ASP:HB2    | 4:4:177:LYS:HB3   | 2.01                     | 0.42              |
| 18:K:198:TYR:HA   | 18:K:201:ILE:HG12 | 2.01                     | 0.42              |
| 21:N:227:LYS:O    | 21:N:231:ASN:HB2  | 2.20                     | 0.42              |
| 22:O:306:ARG:NH1  | 22:O:349:THR:HB   | 2.31                     | 0.42              |
| 24:Q:358:GLU:HG2  | 24:Q:360:SER:H    | 1.83                     | 0.42              |
| 29:V:53:MET:HG3   | 29:V:108:TYR:HD1  | 1.84                     | 0.42              |
| 2:2:36:LYS:HA     | 2:2:41:VAL:HA     | 2.01                     | 0.42              |
| 3:h:69:TYR:HB2    | 10:d:100:LYS:HD2  | 2.01                     | 0.42              |
| 15:H:304:CYS:SG   | 15:H:349:ILE:HG21 | 2.59                     | 0.42              |
| 16:I:435:LEU:O    | 16:I:436:TYR:HB3  | 2.19                     | 0.42              |
| 18:K:148:ASP:OD1  | 18:K:149:ILE:N    | 2.52                     | 0.42              |
| 18:K:420:THR:C    | 18:K:422:ASP:H    | 2.27                     | 0.42              |
| 22:O:308:LEU:O    | 22:O:348:VAL:N    | 2.47                     | 0.42              |
| 25:R:313:ALA:HA   | 25:R:317:ILE:HD12 | 2.00                     | 0.42              |
| 27:T:151:TRP:HE3  | 27:T:156:SER:HB3  | 1.83                     | 0.42              |
| 27:T:227:PRO:O    | 27:T:229:VAL:N    | 2.52                     | 0.42              |
| 2:i:239:THR:HG21  | 3:h:168:SER:HB3   | 2.01                     | 0.42              |
| 6:e:43:ALA:HB1    | 6:e:221:LEU:HD11  | 2.00                     | 0.42              |
| 8:A:24:ARG:HB3    | 18:K:427:TYR:HE1  | 1.84                     | 0.42              |
| 12:E:21:LEU:HD12  | 20:M:432:PHE:CE2  | 2.54                     | 0.42              |
| 11:n:11:PHE:CE2   | 12:m:26:TYR:HB2   | 2.54                     | 0.42              |
| 17:J:156:GLN:NE2  | 17:J:315:GLU:O    | 2.51                     | 0.42              |
| 22:O:289:GLN:HG3  | 22:O:313:ILE:HD11 | 2.00                     | 0.42              |
| 23:P:54:SER:O     | 23:P:58:VAL:N     | 2.52                     | 0.42              |
| 23:P:90:LYS:HD3   | 23:P:93:ILE:HD12  | 2.01                     | 0.42              |
| 23:P:224:LEU:HD13 | 23:P:240:TYR:CG   | 2.55                     | 0.42              |
| 26:S:327:ILE:HD11 | 26:S:390:THR:HG21 | 2.02                     | 0.42              |
| 27:T:226:TRP:HA   | 27:T:232:LYS:HB3  | 2.01                     | 0.42              |
| 33:Z:571:GLY:HA2  | 33:Z:574:TYR:CE2  | 2.54                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:4:149:ARG:HG2   | 4:4:152:MET:HG3   | 2.01                     | 0.42              |
| 12:E:103:TYR:HB3  | 12:E:105:GLU:HG2  | 2.02                     | 0.42              |
| 11:n:89:ALA:HB1   | 11:n:109:LEU:HD11 | 2.00                     | 0.42              |
| 13:l:20:PHE:HA    | 13:l:23:GLU:HG2   | 2.01                     | 0.42              |
| 16:I:435:LEU:C    | 16:I:436:TYR:HD1  | 2.28                     | 0.42              |
| 17:J:41:VAL:O     | 17:J:45:GLU:HG2   | 2.19                     | 0.42              |
| 18:K:180:GLN:HE22 | 18:K:219:LYS:NZ   | 2.17                     | 0.42              |
| 21:N:207:LEU:HD22 | 21:N:228:VAL:HG22 | 2.01                     | 0.42              |
| 26:S:26:ALA:HB2   | 26:S:68:LEU:HD12  | 2.02                     | 0.42              |
| 29:V:60:ASP:HB3   | 29:V:61:TYR:CD2   | 2.55                     | 0.42              |
| 7:7:94:GLN:HA     | 7:7:97:GLU:HB3    | 2.02                     | 0.42              |
| 11:D:100:LEU:C    | 11:D:102:ASP:H    | 2.27                     | 0.42              |
| 14:G:152:GLU:OE1  | 14:G:156:SER:OG   | 2.37                     | 0.42              |
| 15:H:177:ASP:HB3  | 15:H:180:LYS:O    | 2.19                     | 0.42              |
| 16:I:219:VAL:HA   | 16:I:344:ILE:HG23 | 2.02                     | 0.42              |
| 21:N:668:THR:HG22 | 21:N:675:VAL:HB   | 2.02                     | 0.42              |
| 24:Q:356:CYS:HA   | 24:Q:397:LEU:HB3  | 2.02                     | 0.42              |
| 26:S:452:TYR:HE2  | 28:U:274:MET:HG3  | 1.84                     | 0.42              |
| 6:6:214:HIS:ND1   | 2:i:54:ILE:HD13   | 2.35                     | 0.42              |
| 6:e:46:THR:HB     | 6:e:58:TYR:HA     | 2.02                     | 0.42              |
| 7:a:48:LYS:HG2    | 7:a:53:VAL:HG12   | 2.01                     | 0.42              |
| 7:a:60:LEU:HD21   | 7:a:67:LEU:HD13   | 2.00                     | 0.42              |
| 7:a:151:GLY:HA2   | 7:a:233:ILE:HG21  | 2.00                     | 0.42              |
| 7:a:234:ASP:OD1   | 7:a:235:LYS:N     | 2.53                     | 0.42              |
| 12:E:52:LYS:NZ    | 12:E:61:SER:HB3   | 2.35                     | 0.42              |
| 14:G:62:GLN:HE22  | 14:G:236:LEU:HD21 | 1.85                     | 0.42              |
| 14:G:67:ILE:HA    | 14:G:77:VAL:HG12  | 2.01                     | 0.42              |
| 8:c:76:ARG:C      | 8:c:78:ILE:H      | 2.28                     | 0.42              |
| 15:H:402:ILE:HD12 | 15:H:440:GLU:HB2  | 2.00                     | 0.42              |
| 18:K:209:VAL:N    | 18:K:314:VAL:O    | 2.52                     | 0.42              |
| 19:L:74:LEU:HD21  | 20:M:49:GLN:HB2   | 2.01                     | 0.42              |
| 19:L:124:GLY:N    | 19:L:125:PRO:HD2  | 2.35                     | 0.42              |
| 20:M:144:ASP:OD1  | 20:M:145:LEU:N    | 2.53                     | 0.42              |
| 22:O:325:GLU:OE1  | 23:P:364:ARG:NH1  | 2.53                     | 0.42              |
| 24:Q:359:ILE:HD12 | 24:Q:395:GLY:HA2  | 2.01                     | 0.42              |
| 31:X:17:TYR:OH    | 31:X:97:TYR:OH    | 2.32                     | 0.42              |
| 33:Z:284:LEU:HB3  | 33:Z:293:MET:HB3  | 2.01                     | 0.42              |
| 33:Z:767:TYR:O    | 33:Z:773:ARG:NH2  | 2.52                     | 0.42              |
| 2:2:50:THR:HG22   | 2:2:55:VAL:HG13   | 2.02                     | 0.42              |
| 3:3:78:GLU:HB3    | 3:3:80:ARG:NH1    | 2.35                     | 0.42              |
| 1:b:152:PHE:HE2   | 1:b:185:ASP:HB2   | 1.85                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:B:72:GLY:N      | 9:B:137:ALA:O     | 2.42                     | 0.42              |
| 10:C:77:VAL:HG13  | 10:C:133:VAL:HG13 | 2.01                     | 0.42              |
| 11:D:139:ASP:HB2  | 11:D:142:ASP:HB3  | 2.02                     | 0.42              |
| 20:M:81:ASN:O     | 20:M:120:LYS:N    | 2.32                     | 0.42              |
| 21:N:606:VAL:HB   | 21:N:621:THR:HB   | 2.01                     | 0.42              |
| 21:N:781:ALA:HB1  | 21:N:868:VAL:HG11 | 2.01                     | 0.42              |
| 23:P:393:VAL:H    | 24:Q:354:PHE:HB3  | 1.85                     | 0.42              |
| 27:T:233:VAL:CG1  | 27:T:234:TYR:H    | 2.25                     | 0.42              |
| 27:T:238:GLN:HG3  | 27:T:239:SER:H    | 1.85                     | 0.42              |
| 6:6:62:VAL:HG22   | 6:6:72:SER:HB2    | 2.02                     | 0.42              |
| 7:7:124:TYR:HD1   | 13:F:100:ASN:HB3  | 1.85                     | 0.42              |
| 3:h:178:ASP:OD1   | 3:h:179:ALA:N     | 2.53                     | 0.42              |
| 7:a:60:LEU:HB2    | 7:a:225:SER:HB3   | 2.02                     | 0.42              |
| 23:P:425:HIS:NE2  | 28:U:203:LYS:HG3  | 2.35                     | 0.42              |
| 33:Z:182:SER:H    | 33:Z:267:THR:HG22 | 1.84                     | 0.42              |
| 3:3:30:GLY:HA3    | 3:3:35:GLY:HA2    | 2.02                     | 0.42              |
| 5:5:265:ASN:OD1   | 5:5:266:HIS:N     | 2.53                     | 0.42              |
| 7:7:60:LEU:HD11   | 7:7:62:SER:HB2    | 2.02                     | 0.42              |
| 7:7:115:ASP:OD1   | 7:7:116:ALA:N     | 2.52                     | 0.42              |
| 6:e:116:LEU:HD13  | 6:e:148:GLY:HA2   | 2.02                     | 0.42              |
| 9:B:9:LEU:HD11    | 9:B:123:GLN:O     | 2.20                     | 0.42              |
| 8:c:155:LYS:HB3   | 8:c:165:TYR:HE2   | 1.84                     | 0.42              |
| 10:d:52:VAL:HG11  | 10:d:57:LEU:HD13  | 2.02                     | 0.42              |
| 18:K:94:LEU:HB3   | 18:K:138:ALA:HB1  | 2.01                     | 0.42              |
| 19:L:435:GLN:OE1  | 19:L:435:GLN:N    | 2.53                     | 0.42              |
| 21:N:322:ASP:HB2  | 21:N:358:LYS:HE3  | 2.01                     | 0.42              |
| 21:N:335:ALA:HB2  | 21:N:701:VAL:HA   | 2.01                     | 0.42              |
| 22:O:56:PRO:HG2   | 22:O:59:LEU:HB2   | 2.02                     | 0.42              |
| 26:S:352:VAL:HG22 | 26:S:387:VAL:HG22 | 2.02                     | 0.42              |
| 28:U:13:LEU:HD13  | 29:V:35:LEU:HB2   | 2.01                     | 0.42              |
| 29:V:67:ASP:OD1   | 29:V:68:VAL:N     | 2.52                     | 0.42              |
| 1:1:139:HIS:HB2   | 7:7:69:PHE:CE1    | 2.55                     | 0.41              |
| 2:2:217:ARG:HG2   | 2:2:218:ASN:HD22  | 1.84                     | 0.41              |
| 3:3:109:VAL:HB    | 3:3:122:ALA:HB3   | 2.01                     | 0.41              |
| 6:6:21:PHE:CZ     | 7:7:142:PRO:HG2   | 2.55                     | 0.41              |
| 7:7:150:ALA:HB2   | 7:7:160:LEU:HD13  | 2.02                     | 0.41              |
| 1:b:79:GLN:NE2    | 8:c:104:ARG:HE    | 2.18                     | 0.41              |
| 2:i:47:THR:HB     | 2:i:59:ASN:HA     | 2.00                     | 0.41              |
| 8:A:47:GLY:O      | 8:A:193:HIS:ND1   | 2.41                     | 0.41              |
| 8:A:196:GLU:HG2   | 8:A:201:LYS:HB2   | 2.02                     | 0.41              |
| 13:F:168:ALA:N    | 13:F:200:SER:OG   | 2.53                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:c:134:ARG:NE    | 14:k:13:SER:O     | 2.53                     | 0.41              |
| 11:n:31:THR:O     | 11:n:76:SER:OG    | 2.31                     | 0.41              |
| 15:H:292:ARG:HH21 | 20:M:168:LYS:NZ   | 2.18                     | 0.41              |
| 17:J:43:ARG:HD2   | 26:S:477:VAL:HG12 | 2.02                     | 0.41              |
| 17:J:231:ARG:HG2  | 17:J:275:LEU:HD11 | 2.01                     | 0.41              |
| 22:O:47:LYS:NZ    | 22:O:52:ALA:H     | 2.18                     | 0.41              |
| 22:O:124:ASP:OD1  | 22:O:125:GLY:N    | 2.53                     | 0.41              |
| 22:O:186:ASN:HB3  | 22:O:226:LYS:HD2  | 2.02                     | 0.41              |
| 25:R:36:SER:H     | 25:R:43:ARG:HH21  | 1.67                     | 0.41              |
| 27:T:132:HIS:O    | 27:T:136:LEU:HB3  | 2.20                     | 0.41              |
| 29:V:26:THR:HG23  | 29:V:200:ASN:O    | 2.20                     | 0.41              |
| 3:3:8:ASN:OD1     | 3:3:56:LEU:HD12   | 2.21                     | 0.41              |
| 5:5:218:ASN:HB2   | 5:5:231:LEU:HD13  | 2.03                     | 0.41              |
| 4:g:29:LYS:HE2    | 4:g:31:SER:O      | 2.20                     | 0.41              |
| 10:C:46:LEU:HD11  | 10:C:76:ALA:HB2   | 2.01                     | 0.41              |
| 12:E:214:GLU:HG3  | 12:E:233:ASN:HB3  | 2.02                     | 0.41              |
| 9:j:44:VAL:HG23   | 9:j:213:ILE:HG22  | 2.03                     | 0.41              |
| 9:j:194:LEU:HG    | 9:j:250:LEU:HD11  | 2.01                     | 0.41              |
| 15:H:100:ALA:O    | 15:H:174:VAL:N    | 2.37                     | 0.41              |
| 15:H:422:VAL:HA   | 15:H:450:VAL:HG21 | 2.02                     | 0.41              |
| 19:L:167:VAL:O    | 19:L:171:THR:HG22 | 2.19                     | 0.41              |
| 21:N:760:GLY:H    | 21:N:769:PRO:HD2  | 1.85                     | 0.41              |
| 25:R:62:TYR:HB2   | 25:R:180:PHE:CZ   | 2.55                     | 0.41              |
| 26:S:424:SER:HB3  | 27:T:192:ASN:HD22 | 1.85                     | 0.41              |
| 33:Z:462:VAL:HG22 | 33:Z:465:GLY:H    | 1.86                     | 0.41              |
| 33:Z:804:ASP:OD1  | 33:Z:805:LEU:N    | 2.53                     | 0.41              |
| 2:2:55:VAL:HB     | 6:e:213:ARG:HA    | 2.02                     | 0.41              |
| 2:2:128:ILE:HD11  | 2:2:156:LEU:HB2   | 2.02                     | 0.41              |
| 2:2:192:ILE:HG23  | 2:2:199:GLY:HA2   | 2.03                     | 0.41              |
| 3:3:110:ALA:HA    | 3:3:121:ILE:HG22  | 2.01                     | 0.41              |
| 4:4:130:TYR:HB2   | 4:4:144:LEU:HD13  | 2.03                     | 0.41              |
| 1:b:20:THR:O      | 1:b:148:SER:N     | 2.48                     | 0.41              |
| 4:g:1:MET:HA      | 4:g:176:PHE:HZ    | 1.85                     | 0.41              |
| 8:A:24:ARG:HH11   | 18:K:424:PHE:HE2  | 1.67                     | 0.41              |
| 8:A:30:TYR:HA     | 8:A:33:LYS:HG2    | 2.03                     | 0.41              |
| 9:B:10:THR:O      | 9:B:12:PHE:HD2    | 1.96                     | 0.41              |
| 15:H:247:LEU:HD13 | 15:H:374:LYS:HG2  | 2.02                     | 0.41              |
| 15:H:396:MET:HB2  | 16:I:213:ILE:HG22 | 2.01                     | 0.41              |
| 17:J:48:ARG:NH2   | 21:N:608:LEU:HB3  | 2.34                     | 0.41              |
| 19:L:96:LYS:HG2   | 28:U:85:ALA:HB1   | 2.01                     | 0.41              |
| 21:N:402:GLY:HA3  | 21:N:441:VAL:HG12 | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:T:233:VAL:O    | 27:T:234:TYR:HB2  | 2.21                     | 0.41              |
| 4:4:70:ARG:HA     | 11:D:90:ARG:NH1   | 2.35                     | 0.41              |
| 5:5:177:CYS:HA    | 5:5:187:ILE:HG12  | 2.02                     | 0.41              |
| 4:g:100:VAL:HG12  | 4:g:102:VAL:HG13  | 2.02                     | 0.41              |
| 8:A:133:TYR:O     | 8:A:135:ARG:NH1   | 2.53                     | 0.41              |
| 9:B:9:LEU:CD2     | 9:B:125:GLY:HA2   | 2.44                     | 0.41              |
| 11:D:196:VAL:HG11 | 11:D:233:VAL:HG22 | 2.03                     | 0.41              |
| 10:d:120:GLN:HE21 | 11:n:80:ALA:HA    | 1.86                     | 0.41              |
| 11:n:118:GLN:NE2  | 12:m:83:ALA:O     | 2.54                     | 0.41              |
| 21:N:875:LEU:HG   | 21:N:877:GLN:H    | 1.85                     | 0.41              |
| 22:O:292:CYS:O    | 22:O:295:THR:OG1  | 2.31                     | 0.41              |
| 27:T:227:PRO:N    | 27:T:232:LYS:HG3  | 2.36                     | 0.41              |
| 27:T:234:TYR:O    | 27:T:239:SER:HA   | 2.19                     | 0.41              |
| 28:U:16:LEU:HB3   | 29:V:32:ILE:HD11  | 2.02                     | 0.41              |
| 28:U:135:ASP:HB3  | 28:U:156:HIS:CD2  | 2.55                     | 0.41              |
| 28:U:291:LEU:HA   | 28:U:294:ASN:HB3  | 2.01                     | 0.41              |
| 33:Z:841:GLU:H    | 33:Z:844:ALA:HB3  | 1.84                     | 0.41              |
| 3:3:12:VAL:HG22   | 3:3:25:CYS:HB3    | 2.02                     | 0.41              |
| 6:6:47:ARG:NH2    | 6:6:218:GLY:HA3   | 2.35                     | 0.41              |
| 7:7:144:TRP:HE3   | 7:7:165:LEU:HD21  | 1.84                     | 0.41              |
| 4:g:84:VAL:HG11   | 4:g:102:VAL:HG21  | 2.03                     | 0.41              |
| 6:e:214:HIS:CE1   | 6:e:216:GLN:HB2   | 2.55                     | 0.41              |
| 12:E:208:MET:SD   | 12:E:216:ASN:ND2  | 2.93                     | 0.41              |
| 9:j:86:VAL:O      | 9:j:90:ARG:N      | 2.53                     | 0.41              |
| 10:d:125:HIS:HE1  | 11:n:120:TYR:CZ   | 2.38                     | 0.41              |
| 16:I:248:VAL:HG12 | 16:I:250:SER:H    | 1.86                     | 0.41              |
| 18:K:151:PRO:O    | 18:K:153:ASP:N    | 2.52                     | 0.41              |
| 25:R:305:PHE:N    | 25:R:306:PRO:HD2  | 2.36                     | 0.41              |
| 28:U:222:ASN:CG   | 28:U:223:HIS:H    | 2.29                     | 0.41              |
| 33:Z:172:ASP:HB3  | 33:Z:193:PHE:HB3  | 2.02                     | 0.41              |
| 2:2:141:SER:HB3   | 2:2:154:LEU:HD13  | 2.03                     | 0.41              |
| 3:3:89:GLN:HE22   | 3:3:130:ILE:HD13  | 1.85                     | 0.41              |
| 1:b:57:HIS:HB3    | 1:b:60:ILE:HB     | 2.01                     | 0.41              |
| 4:g:91:SER:HB3    | 4:g:98:TYR:HB2    | 2.03                     | 0.41              |
| 5:f:134:LEU:HD21  | 5:f:154:ALA:HB1   | 2.02                     | 0.41              |
| 10:C:9:ARG:HD2    | 11:D:4:TYR:HE2    | 1.86                     | 0.41              |
| 12:m:47:VAL:HG11  | 12:m:197:GLU:HA   | 2.03                     | 0.41              |
| 14:k:52:LYS:NZ    | 14:k:64:ASN:O     | 2.39                     | 0.41              |
| 14:k:71:ASP:CG    | 14:k:72:ARG:H     | 2.27                     | 0.41              |
| 18:K:136:SER:HB3  | 18:K:150:LEU:HD12 | 2.03                     | 0.41              |
| 19:L:120:LYS:HA   | 19:L:126:ARG:HG2  | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:M:223:PRO:HA   | 20:M:224:PRO:HD3  | 1.95                     | 0.41              |
| 20:M:287:GLY:O    | 20:M:288:THR:HB   | 2.21                     | 0.41              |
| 21:N:269:LEU:HD12 | 21:N:272:ILE:HD12 | 2.03                     | 0.41              |
| 21:N:773:MET:HE2  | 21:N:869:ASP:OD1  | 2.21                     | 0.41              |
| 22:O:287:LEU:HD23 | 22:O:290:LYS:HD3  | 2.03                     | 0.41              |
| 23:P:116:ILE:HD11 | 23:P:146:ILE:HG21 | 2.01                     | 0.41              |
| 23:P:319:GLU:OE1  | 23:P:323:ASN:HB3  | 2.21                     | 0.41              |
| 28:U:157:LEU:O    | 28:U:159:CYS:N    | 2.53                     | 0.41              |
| 29:V:169:GLU:O    | 29:V:171:ARG:N    | 2.50                     | 0.41              |
| 1:1:209:PRO:HG2   | 7:a:252:TRP:CE2   | 2.55                     | 0.41              |
| 6:6:55:ASN:O      | 7:7:189:ARG:NH2   | 2.54                     | 0.41              |
| 6:6:203:VAL:HG12  | 6:6:221:LEU:HD21  | 2.02                     | 0.41              |
| 7:7:77:PRO:HA     | 7:7:83:VAL:HA     | 2.03                     | 0.41              |
| 7:7:123:SER:HB3   | 7:7:153:GLN:HE21  | 1.85                     | 0.41              |
| 7:7:186:PRO:HG2   | 2:i:162:ALA:HB1   | 2.02                     | 0.41              |
| 3:h:21:VAL:HG13   | 3:h:190:ILE:HD13  | 2.02                     | 0.41              |
| 5:f:114:PRO:HA    | 5:f:260:TRP:CD1   | 2.56                     | 0.41              |
| 6:e:35:ALA:N      | 6:e:154:GLN:O     | 2.53                     | 0.41              |
| 9:B:97:TYR:O      | 9:B:101:TYR:N     | 2.49                     | 0.41              |
| 10:C:124:GLN:HG2  | 11:D:126:VAL:HG13 | 2.03                     | 0.41              |
| 14:G:41:LYS:HE3   | 14:G:147:HIS:HA   | 2.03                     | 0.41              |
| 14:G:137:ILE:HD13 | 14:G:163:ALA:HB1  | 2.02                     | 0.41              |
| 8:c:91:ASN:OD1    | 14:k:118:GLN:NE2  | 2.53                     | 0.41              |
| 17:J:34:ILE:HD11  | 18:K:58:TYR:HB3   | 2.02                     | 0.41              |
| 18:K:87:LYS:HE2   | 18:K:125:THR:HG21 | 2.03                     | 0.41              |
| 18:K:206:PRO:HB3  | 18:K:335:ASP:HB3  | 2.03                     | 0.41              |
| 21:N:873:ARG:CG   | 21:N:874:ILE:H    | 2.29                     | 0.41              |
| 22:O:360:GLY:HA2  | 22:O:363:ILE:HD12 | 2.03                     | 0.41              |
| 27:T:227:PRO:C    | 27:T:229:VAL:H    | 2.29                     | 0.41              |
| 27:T:239:SER:OG   | 27:T:240:LYS:N    | 2.49                     | 0.41              |
| 29:V:58:VAL:HG12  | 29:V:59:ASP:O     | 2.21                     | 0.41              |
| 30:W:186:ALA:HA   | 30:W:191:ILE:HD12 | 2.02                     | 0.41              |
| 3:3:150:CYS:O     | 3:3:154:TYR:HB3   | 2.21                     | 0.41              |
| 4:4:110:LYS:NZ    | 10:C:142:ASP:OD2  | 2.49                     | 0.41              |
| 4:4:164:CYS:O     | 4:4:168:LEU:HG    | 2.20                     | 0.41              |
| 2:i:143:HIS:HD2   | 2:i:147:SER:HB3   | 1.85                     | 0.41              |
| 4:g:152:MET:HE1   | 4:g:160:LEU:HD22  | 2.03                     | 0.41              |
| 5:f:94:ARG:CZ     | 5:f:247:GLY:HA3   | 2.51                     | 0.41              |
| 6:e:183:THR:HB    | 6:e:186:LYS:HB2   | 2.02                     | 0.41              |
| 10:C:8:SER:HB3    | 10:C:12:ILE:HD12  | 2.02                     | 0.41              |
| 11:D:7:ALA:HB3    | 12:E:136:ARG:HB3  | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:E:50:VAL:HG21  | 12:E:66:LYS:HB2   | 2.02                     | 0.41              |
| 12:E:54:ALA:HA    | 12:E:59:LEU:HD23  | 2.03                     | 0.41              |
| 14:G:65:VAL:HG12  | 14:G:67:ILE:H     | 1.84                     | 0.41              |
| 13:l:46:LEU:HG    | 13:l:135:ILE:HD13 | 2.03                     | 0.41              |
| 23:P:122:ILE:HG22 | 23:P:124:VAL:H    | 1.86                     | 0.41              |
| 23:P:384:VAL:HG12 | 24:Q:352:GLU:HG3  | 2.02                     | 0.41              |
| 28:U:261:LEU:HD12 | 29:V:305:ILE:HB   | 2.02                     | 0.41              |
| 29:V:57:PHE:CE1   | 29:V:135:ARG:HD3  | 2.56                     | 0.41              |
| 30:W:20:ASP:HA    | 30:W:24:THR:C     | 2.46                     | 0.41              |
| 31:X:66:LEU:HD11  | 31:X:91:PHE:HE2   | 1.86                     | 0.41              |
| 31:X:91:PHE:HB3   | 31:X:94:ASN:ND2   | 2.35                     | 0.41              |
| 1:l:47:ASN:HA     | 7:a:220:ARG:HH12  | 1.86                     | 0.41              |
| 3:3:124:PHE:HA    | 3:3:129:CYS:O     | 2.21                     | 0.41              |
| 3:3:176:ASP:O     | 5:f:104:GLN:NE2   | 2.54                     | 0.41              |
| 6:6:43:ALA:HB2    | 6:6:223:ILE:HG12  | 2.03                     | 0.41              |
| 6:6:84:VAL:O      | 6:6:88:LYS:N      | 2.48                     | 0.41              |
| 3:h:34:LEU:HD11   | 4:g:141:PHE:CE2   | 2.56                     | 0.41              |
| 5:f:109:VAL:HG21  | 5:f:253:TYR:HE2   | 1.85                     | 0.41              |
| 5:f:196:ARG:NH1   | 11:n:101:GLU:OE2  | 2.54                     | 0.41              |
| 6:e:83:LEU:HB3    | 6:e:87:PHE:CE2    | 2.56                     | 0.41              |
| 11:n:11:PHE:CZ    | 12:m:26:TYR:HB2   | 2.56                     | 0.41              |
| 11:n:48:ARG:HB2   | 11:n:209:ASN:HA   | 2.02                     | 0.41              |
| 11:n:122:GLN:HG3  | 12:m:138:PHE:CE1  | 2.56                     | 0.41              |
| 17:J:283:GLU:O    | 17:J:284:THR:OG1  | 2.37                     | 0.41              |
| 18:K:99:PHE:HD2   | 18:K:133:PRO:HA   | 1.86                     | 0.41              |
| 18:K:285:GLN:CD   | 19:L:302:GLN:HE22 | 2.29                     | 0.41              |
| 19:L:97:ALA:HB1   | 20:M:132:VAL:HA   | 2.02                     | 0.41              |
| 19:L:407:ARG:HH12 | 19:L:411:ASN:ND2  | 2.19                     | 0.41              |
| 21:N:593:PHE:HA   | 21:N:596:LEU:HG   | 2.02                     | 0.41              |
| 24:Q:378:SER:HB2  | 25:R:344:SER:HB2  | 2.03                     | 0.41              |
| 24:Q:412:ALA:O    | 24:Q:416:VAL:HG22 | 2.20                     | 0.41              |
| 27:T:29:PRO:HA    | 27:T:32:ILE:HD12  | 2.03                     | 0.41              |
| 28:U:62:ASN:ND2   | 30:W:92:GLN:OE1   | 2.53                     | 0.41              |
| 29:V:52:LEU:HD23  | 29:V:69:PHE:CZ    | 2.56                     | 0.41              |
| 29:V:245:VAL:O    | 29:V:249:GLU:HB2  | 2.21                     | 0.41              |
| 33:Z:72:LYS:HG3   | 33:Z:121:ILE:HD11 | 2.03                     | 0.41              |
| 33:Z:217:GLU:O    | 33:Z:221:VAL:HG23 | 2.21                     | 0.41              |
| 2:2:47:THR:O      | 2:2:60:CYS:N      | 2.37                     | 0.41              |
| 8:A:16:ILE:HD12   | 8:A:18:ILE:HG13   | 2.03                     | 0.41              |
| 8:A:160:ALA:HB3   | 18:K:426:PHE:CZ   | 2.56                     | 0.41              |
| 9:B:177:LYS:HE2   | 24:Q:132:PHE:HE1  | 1.86                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:D:163:THR:HG21 | 11:D:171:VAL:HB   | 2.02                     | 0.41              |
| 12:E:74:ILE:HG21  | 12:E:112:LEU:HD23 | 2.03                     | 0.41              |
| 19:L:277:ILE:HG12 | 19:L:322:LYS:HB2  | 2.03                     | 0.41              |
| 22:O:79:VAL:HG12  | 22:O:128:LEU:HG   | 2.03                     | 0.41              |
| 26:S:22:GLU:HB3   | 26:S:68:LEU:HD22  | 2.03                     | 0.41              |
| 26:S:49:ASP:HB2   | 26:S:50:PRO:HD3   | 2.03                     | 0.41              |
| 27:T:191:LYS:HA   | 27:T:237:ASN:HB3  | 2.02                     | 0.41              |
| 7:7:90:ILE:HG23   | 7:7:93:MET:HE2    | 2.02                     | 0.40              |
| 7:a:49:TYR:CE2    | 7:a:54:ILE:HG13   | 2.55                     | 0.40              |
| 7:a:162:TYR:HB2   | 7:a:175:LEU:HD13  | 2.03                     | 0.40              |
| 11:D:17:ILE:HG22  | 11:D:19:GLN:H     | 1.84                     | 0.40              |
| 11:D:118:GLN:HE21 | 11:D:122:GLN:NE2  | 2.19                     | 0.40              |
| 12:E:119:LEU:HD13 | 12:E:122:ARG:HH21 | 1.86                     | 0.40              |
| 14:G:53:LEU:HD21  | 14:G:207:ASN:HD21 | 1.86                     | 0.40              |
| 17:J:153:LEU:HD13 | 17:J:198:LEU:HD11 | 2.03                     | 0.40              |
| 20:M:157:ASP:OD1  | 20:M:158:THR:N    | 2.54                     | 0.40              |
| 22:O:370:LEU:HA   | 22:O:373:TRP:HD1  | 1.86                     | 0.40              |
| 24:Q:65:TYR:HA    | 24:Q:70:ALA:HB3   | 2.02                     | 0.40              |
| 29:V:54:LEU:HB3   | 29:V:102:GLN:HB2  | 2.02                     | 0.40              |
| 1:1:32:ILE:HG12   | 1:1:196:VAL:HA    | 2.03                     | 0.40              |
| 4:4:3:ILE:HD12    | 4:4:136:SER:HB2   | 2.03                     | 0.40              |
| 1:b:35:ALA:HB1    | 1:b:52:LYS:HB2    | 2.03                     | 0.40              |
| 2:i:50:THR:HG22   | 2:i:55:VAL:HG22   | 2.03                     | 0.40              |
| 8:A:23:GLY:HA2    | 9:B:23:TYR:HB3    | 2.02                     | 0.40              |
| 10:C:26:LEU:HD12  | 16:I:432:LEU:HD12 | 2.03                     | 0.40              |
| 16:I:167:MET:HE3  | 17:J:228:ARG:HH12 | 1.86                     | 0.40              |
| 18:K:193:VAL:HG12 | 18:K:194:GLN:HG2  | 2.03                     | 0.40              |
| 18:K:209:VAL:HB   | 18:K:315:ILE:HG12 | 2.03                     | 0.40              |
| 19:L:329:ARG:HA   | 19:L:330:PRO:HD3  | 1.92                     | 0.40              |
| 22:O:218:SER:HA   | 22:O:251:LEU:HD21 | 2.04                     | 0.40              |
| 25:R:98:LEU:HA    | 25:R:101:GLU:HB2  | 2.03                     | 0.40              |
| 26:S:357:LEU:HA   | 26:S:384:ARG:HH12 | 1.85                     | 0.40              |
| 27:T:164:LEU:O    | 27:T:170:ASN:ND2  | 2.53                     | 0.40              |
| 30:W:21:PHE:HB2   | 30:W:22:PRO:HD3   | 2.03                     | 0.40              |
| 33:Z:352:LYS:O    | 33:Z:355:GLU:HG2  | 2.20                     | 0.40              |
| 33:Z:456:GLY:HA2  | 33:Z:496:ALA:HB2  | 2.03                     | 0.40              |
| 1:1:78:VAL:HG22   | 1:1:100:VAL:HG12  | 2.04                     | 0.40              |
| 3:3:101:GLY:N     | 3:3:102:PRO:HD3   | 2.36                     | 0.40              |
| 7:7:124:TYR:HE2   | 13:F:101:ARG:HH11 | 1.69                     | 0.40              |
| 4:g:8:ARG:N       | 4:g:129:PRO:O     | 2.42                     | 0.40              |
| 6:e:76:PHE:HD2    | 6:e:79:ASP:H      | 1.69                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:B:227:ILE:HG22  | 9:B:229:THR:H     | 1.86                     | 0.40              |
| 9:j:217:GLU:HG2   | 9:j:231:LYS:HB3   | 2.03                     | 0.40              |
| 15:H:272:ILE:HB   | 15:H:306:ILE:HA   | 2.03                     | 0.40              |
| 16:I:318:ASP:OD2  | 16:I:321:ASP:HB2  | 2.22                     | 0.40              |
| 18:K:346:ARG:HG2  | 18:K:349:ARG:HH22 | 1.86                     | 0.40              |
| 19:L:151:THR:HG22 | 29:V:45:VAL:HG23  | 2.02                     | 0.40              |
| 21:N:55:PHE:CZ    | 21:N:57:ASP:HB2   | 2.57                     | 0.40              |
| 21:N:339:MET:HA   | 21:N:709:GLY:H    | 1.85                     | 0.40              |
| 27:T:27:LEU:HB2   | 27:T:28:PRO:HD3   | 2.03                     | 0.40              |
| 27:T:224:ARG:NH2  | 27:T:235:PHE:O    | 2.54                     | 0.40              |
| 33:Z:528:LEU:HD13 | 33:Z:883:THR:HA   | 2.04                     | 0.40              |
| 6:6:241:ASP:OXT   | 2:i:48:ARG:NH2    | 2.54                     | 0.40              |
| 7:7:254:PHE:HB2   | 2:i:152:TYR:CE2   | 2.57                     | 0.40              |
| 4:g:101:ASN:HB3   | 4:g:133:HIS:CG    | 2.56                     | 0.40              |
| 10:C:120:GLN:HE22 | 11:D:81:ASP:HA    | 1.87                     | 0.40              |
| 10:C:186:VAL:HG11 | 10:C:217:ARG:HD2  | 2.04                     | 0.40              |
| 11:D:78:LEU:HG    | 11:D:80:ALA:H     | 1.87                     | 0.40              |
| 13:l:11:VAL:HA    | 14:k:130:ARG:HD3  | 2.02                     | 0.40              |
| 18:K:95:VAL:HB    | 18:K:139:LEU:HB2  | 2.03                     | 0.40              |
| 21:N:510:HIS:HB2  | 21:N:513:ILE:HB   | 2.02                     | 0.40              |
| 21:N:738:GLN:HG3  | 21:N:741:TYR:CD2  | 2.56                     | 0.40              |
| 23:P:392:LYS:HG3  | 24:Q:354:PHE:CE2  | 2.57                     | 0.40              |
| 24:Q:83:GLU:HA    | 24:Q:86:MET:HE2   | 2.04                     | 0.40              |
| 24:Q:302:VAL:HG11 | 24:Q:338:LEU:HD13 | 2.03                     | 0.40              |
| 24:Q:411:SER:HA   | 24:Q:414:GLU:HB3  | 2.03                     | 0.40              |
| 29:V:130:GLU:HG3  | 29:V:158:LEU:HD23 | 2.03                     | 0.40              |
| 29:V:169:GLU:HB2  | 29:V:170:PRO:HD3  | 2.04                     | 0.40              |
| 29:V:262:THR:HA   | 29:V:270:TYR:HB2  | 2.03                     | 0.40              |
| 7:7:220:ARG:HB3   | 1:b:44:TYR:CE1    | 2.57                     | 0.40              |
| 2:i:63:LEU:HD12   | 2:i:215:TYR:HE1   | 1.87                     | 0.40              |
| 7:a:53:VAL:HG21   | 7:a:150:ALA:HB1   | 2.03                     | 0.40              |
| 11:D:70:HIS:ND1   | 11:D:71:VAL:HG23  | 2.36                     | 0.40              |
| 8:c:29:TYR:HD1    | 8:c:32:LYS:HD2    | 1.87                     | 0.40              |
| 16:I:150:HIS:O    | 16:I:154:MET:HA   | 2.21                     | 0.40              |
| 18:K:383:ILE:HA   | 18:K:386:ILE:HD12 | 2.01                     | 0.40              |
| 19:L:261:ARG:O    | 19:L:265:GLU:HG3  | 2.21                     | 0.40              |
| 21:N:8:PRO:HB3    | 27:T:83:ASN:HB2   | 2.04                     | 0.40              |
| 21:N:28:ILE:O     | 21:N:32:VAL:HG13  | 2.21                     | 0.40              |
| 21:N:762:ARG:H    | 21:N:767:ALA:HB2  | 1.86                     | 0.40              |
| 22:O:299:THR:HG22 | 22:O:300:VAL:HG23 | 2.03                     | 0.40              |
| 23:P:144:VAL:HG12 | 23:P:148:LYS:HE3  | 2.04                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 25:R:246:TYR:CE2 | 25:R:279:LEU:HD13 | 2.56                     | 0.40              |
| 29:V:28:TYR:HA   | 29:V:202:ASP:O    | 2.21                     | 0.40              |
| 29:V:66:VAL:HG21 | 29:V:102:GLN:HG3  | 2.02                     | 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     | 194/215 (90%) | 188 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | b     | 194/215 (90%) | 186 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 2   | 2     | 224/261 (86%) | 214 (96%) | 10 (4%) | 0        | 100         | 100 |
| 2   | i     | 224/261 (86%) | 220 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 3   | 3     | 202/205 (98%) | 195 (96%) | 6 (3%)  | 1 (0%)   | 24          | 63  |
| 3   | h     | 202/205 (98%) | 193 (96%) | 8 (4%)  | 1 (0%)   | 24          | 63  |
| 4   | 4     | 193/198 (98%) | 189 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 4   | g     | 193/198 (98%) | 189 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 5   | 5     | 210/287 (73%) | 206 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 5   | f     | 210/287 (73%) | 204 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 6   | 6     | 220/241 (91%) | 211 (96%) | 9 (4%)  | 0        | 100         | 100 |
| 6   | e     | 220/241 (91%) | 211 (96%) | 9 (4%)  | 0        | 100         | 100 |
| 7   | 7     | 227/266 (85%) | 214 (94%) | 13 (6%) | 0        | 100         | 100 |
| 7   | a     | 230/266 (86%) | 223 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 8   | A     | 239/252 (95%) | 230 (96%) | 9 (4%)  | 0        | 100         | 100 |
| 8   | c     | 239/252 (95%) | 228 (95%) | 11 (5%) | 0        | 100         | 100 |
| 9   | B     | 248/250 (99%) | 237 (96%) | 11 (4%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 9   | j     | 248/250 (99%)     | 232 (94%)   | 16 (6%)  | 0        | 100         | 100 |
| 10  | C     | 242/258 (94%)     | 231 (96%)   | 11 (4%)  | 0        | 100         | 100 |
| 10  | d     | 242/258 (94%)     | 229 (95%)   | 13 (5%)  | 0        | 100         | 100 |
| 11  | D     | 238/254 (94%)     | 225 (94%)   | 11 (5%)  | 2 (1%)   | 16          | 53  |
| 11  | n     | 238/254 (94%)     | 227 (95%)   | 11 (5%)  | 0        | 100         | 100 |
| 12  | E     | 240/260 (92%)     | 229 (95%)   | 9 (4%)   | 2 (1%)   | 16          | 53  |
| 12  | m     | 240/260 (92%)     | 228 (95%)   | 12 (5%)  | 0        | 100         | 100 |
| 13  | F     | 231/234 (99%)     | 217 (94%)   | 14 (6%)  | 0        | 100         | 100 |
| 13  | l     | 229/234 (98%)     | 227 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 14  | G     | 241/288 (84%)     | 232 (96%)   | 9 (4%)   | 0        | 100         | 100 |
| 14  | k     | 241/288 (84%)     | 236 (98%)   | 5 (2%)   | 0        | 100         | 100 |
| 15  | H     | 351/467 (75%)     | 313 (89%)   | 38 (11%) | 0        | 100         | 100 |
| 16  | I     | 360/437 (82%)     | 324 (90%)   | 36 (10%) | 0        | 100         | 100 |
| 17  | J     | 371/405 (92%)     | 350 (94%)   | 19 (5%)  | 2 (0%)   | 24          | 63  |
| 18  | K     | 379/428 (89%)     | 336 (89%)   | 40 (11%) | 3 (1%)   | 16          | 53  |
| 19  | L     | 369/437 (84%)     | 338 (92%)   | 31 (8%)  | 0        | 100         | 100 |
| 20  | M     | 363/434 (84%)     | 329 (91%)   | 32 (9%)  | 2 (1%)   | 21          | 58  |
| 21  | N     | 843/945 (89%)     | 783 (93%)   | 56 (7%)  | 4 (0%)   | 24          | 63  |
| 22  | O     | 385/393 (98%)     | 345 (90%)   | 40 (10%) | 0        | 100         | 100 |
| 23  | P     | 430/445 (97%)     | 381 (89%)   | 49 (11%) | 0        | 100         | 100 |
| 24  | Q     | 429/434 (99%)     | 394 (92%)   | 35 (8%)  | 0        | 100         | 100 |
| 25  | R     | 398/429 (93%)     | 354 (89%)   | 41 (10%) | 3 (1%)   | 16          | 53  |
| 26  | S     | 473/523 (90%)     | 454 (96%)   | 18 (4%)  | 1 (0%)   | 43          | 77  |
| 27  | T     | 270/274 (98%)     | 228 (84%)   | 42 (16%) | 0        | 100         | 100 |
| 28  | U     | 254/338 (75%)     | 244 (96%)   | 8 (3%)   | 2 (1%)   | 16          | 53  |
| 29  | V     | 282/306 (92%)     | 239 (85%)   | 36 (13%) | 7 (2%)   | 4           | 26  |
| 30  | W     | 195/268 (73%)     | 177 (91%)   | 14 (7%)  | 4 (2%)   | 5           | 30  |
| 31  | X     | 109/156 (70%)     | 96 (88%)    | 13 (12%) | 0        | 100         | 100 |
| 32  | Y     | 25/89 (28%)       | 20 (80%)    | 5 (20%)  | 0        | 100         | 100 |
| 33  | Z     | 807/993 (81%)     | 747 (93%)   | 60 (7%)  | 0        | 100         | 100 |
| All | All   | 13392/15139 (88%) | 12503 (93%) | 855 (6%) | 34 (0%)  | 37          | 71  |

All (34) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | D     | 7   | ALA  |
| 11  | D     | 10  | ILE  |
| 18  | K     | 292 | VAL  |
| 18  | K     | 421 | VAL  |
| 21  | N     | 903 | VAL  |
| 25  | R     | 241 | ILE  |
| 18  | K     | 188 | VAL  |
| 21  | N     | 724 | THR  |
| 21  | N     | 874 | ILE  |
| 29  | V     | 60  | ASP  |
| 29  | V     | 61  | TYR  |
| 30  | W     | 22  | PRO  |
| 12  | E     | 134 | MET  |
| 28  | U     | 130 | VAL  |
| 3   | 3     | 105 | VAL  |
| 12  | E     | 135 | SER  |
| 17  | J     | 134 | VAL  |
| 20  | M     | 167 | VAL  |
| 25  | R     | 421 | VAL  |
| 29  | V     | 144 | ILE  |
| 29  | V     | 172 | GLN  |
| 29  | V     | 189 | ILE  |
| 30  | W     | 147 | ILE  |
| 20  | M     | 422 | VAL  |
| 3   | h     | 105 | VAL  |
| 25  | R     | 72  | VAL  |
| 21  | N     | 761 | ILE  |
| 26  | S     | 83  | PRO  |
| 29  | V     | 303 | VAL  |
| 30  | W     | 21  | PHE  |
| 17  | J     | 258 | VAL  |
| 28  | U     | 215 | ILE  |
| 29  | V     | 165 | ILE  |
| 30  | W     | 118 | 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     | 162/178 (91%)  | 162 (100%) | 0        | 100         | 100 |
| 1   | b     | 162/178 (91%)  | 162 (100%) | 0        | 100         | 100 |
| 2   | 2     | 185/214 (86%)  | 185 (100%) | 0        | 100         | 100 |
| 2   | i     | 185/214 (86%)  | 185 (100%) | 0        | 100         | 100 |
| 3   | 3     | 172/173 (99%)  | 172 (100%) | 0        | 100         | 100 |
| 3   | h     | 172/173 (99%)  | 172 (100%) | 0        | 100         | 100 |
| 4   | 4     | 173/175 (99%)  | 173 (100%) | 0        | 100         | 100 |
| 4   | g     | 173/175 (99%)  | 173 (100%) | 0        | 100         | 100 |
| 5   | 5     | 169/235 (72%)  | 169 (100%) | 0        | 100         | 100 |
| 5   | f     | 169/235 (72%)  | 169 (100%) | 0        | 100         | 100 |
| 6   | 6     | 185/201 (92%)  | 185 (100%) | 0        | 100         | 100 |
| 6   | e     | 185/201 (92%)  | 185 (100%) | 0        | 100         | 100 |
| 7   | 7     | 195/224 (87%)  | 195 (100%) | 0        | 100         | 100 |
| 7   | a     | 198/224 (88%)  | 198 (100%) | 0        | 100         | 100 |
| 8   | A     | 206/210 (98%)  | 206 (100%) | 0        | 100         | 100 |
| 8   | c     | 206/210 (98%)  | 206 (100%) | 0        | 100         | 100 |
| 9   | B     | 209/209 (100%) | 209 (100%) | 0        | 100         | 100 |
| 9   | j     | 209/209 (100%) | 209 (100%) | 0        | 100         | 100 |
| 10  | C     | 203/216 (94%)  | 202 (100%) | 1 (0%)   | 81          | 81  |
| 10  | d     | 203/216 (94%)  | 203 (100%) | 0        | 100         | 100 |
| 11  | D     | 212/226 (94%)  | 212 (100%) | 0        | 100         | 100 |
| 11  | n     | 212/226 (94%)  | 212 (100%) | 0        | 100         | 100 |
| 12  | E     | 198/215 (92%)  | 198 (100%) | 0        | 100         | 100 |
| 12  | m     | 198/215 (92%)  | 198 (100%) | 0        | 100         | 100 |
| 13  | F     | 192/193 (100%) | 192 (100%) | 0        | 100         | 100 |
| 13  | l     | 190/193 (98%)  | 190 (100%) | 0        | 100         | 100 |
| 14  | G     | 201/239 (84%)  | 201 (100%) | 0        | 100         | 100 |
| 14  | k     | 201/239 (84%)  | 201 (100%) | 0        | 100         | 100 |
| 15  | H     | 303/399 (76%)  | 303 (100%) | 0        | 100         | 100 |
| 16  | I     | 319/385 (83%)  | 317 (99%)  | 2 (1%)   | 78          | 80  |
| 17  | J     | 325/352 (92%)  | 325 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 18  | K     | 334/374 (89%)     | 334 (100%)   | 0        | 100         | 100 |
| 19  | L     | 317/377 (84%)     | 317 (100%)   | 0        | 100         | 100 |
| 20  | M     | 315/375 (84%)     | 315 (100%)   | 0        | 100         | 100 |
| 21  | N     | 713/797 (90%)     | 710 (100%)   | 3 (0%)   | 84          | 82  |
| 22  | O     | 363/368 (99%)     | 363 (100%)   | 0        | 100         | 100 |
| 23  | P     | 405/415 (98%)     | 405 (100%)   | 0        | 100         | 100 |
| 24  | Q     | 388/391 (99%)     | 388 (100%)   | 0        | 100         | 100 |
| 25  | R     | 351/379 (93%)     | 351 (100%)   | 0        | 100         | 100 |
| 26  | S     | 447/489 (91%)     | 446 (100%)   | 1 (0%)   | 87          | 85  |
| 27  | T     | 254/256 (99%)     | 254 (100%)   | 0        | 100         | 100 |
| 28  | U     | 241/308 (78%)     | 240 (100%)   | 1 (0%)   | 84          | 82  |
| 29  | V     | 249/268 (93%)     | 249 (100%)   | 0        | 100         | 100 |
| 30  | W     | 171/230 (74%)     | 171 (100%)   | 0        | 100         | 100 |
| 31  | X     | 101/144 (70%)     | 101 (100%)   | 0        | 100         | 100 |
| 32  | Y     | 26/81 (32%)       | 26 (100%)    | 0        | 100         | 100 |
| 33  | Z     | 692/850 (81%)     | 692 (100%)   | 0        | 100         | 100 |
| All | All   | 11639/13054 (89%) | 11631 (100%) | 8 (0%)   | 87          | 88  |

All (8) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | C     | 18  | ARG  |
| 16  | I     | 435 | LEU  |
| 16  | I     | 436 | TYR  |
| 21  | N     | 231 | ASN  |
| 21  | N     | 510 | HIS  |
| 21  | N     | 512 | ASN  |
| 26  | S     | 477 | VAL  |
| 28  | U     | 151 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (162) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 180 | GLN  |
| 2   | 2     | 115 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 2     | 138 | HIS  |
| 2   | 2     | 143 | HIS  |
| 3   | 3     | 89  | GLN  |
| 3   | 3     | 169 | GLN  |
| 4   | 4     | 55  | GLN  |
| 4   | 4     | 86  | GLN  |
| 4   | 4     | 112 | ASN  |
| 4   | 4     | 133 | HIS  |
| 4   | 4     | 146 | HIS  |
| 4   | 4     | 147 | HIS  |
| 5   | 5     | 104 | GLN  |
| 5   | 5     | 251 | ASN  |
| 5   | 5     | 266 | HIS  |
| 5   | 5     | 284 | ASN  |
| 6   | 6     | 127 | HIS  |
| 6   | 6     | 172 | GLN  |
| 6   | 6     | 178 | GLN  |
| 7   | 7     | 35  | GLN  |
| 7   | 7     | 153 | GLN  |
| 7   | 7     | 249 | ASN  |
| 1   | b     | 79  | GLN  |
| 2   | i     | 64  | HIS  |
| 2   | i     | 110 | GLN  |
| 2   | i     | 114 | GLN  |
| 2   | i     | 143 | HIS  |
| 2   | i     | 223 | ASN  |
| 3   | h     | 204 | GLN  |
| 4   | g     | 86  | GLN  |
| 5   | f     | 104 | GLN  |
| 5   | f     | 137 | GLN  |
| 5   | f     | 141 | HIS  |
| 6   | e     | 98  | HIS  |
| 6   | e     | 111 | ASN  |
| 6   | e     | 174 | ASN  |
| 6   | e     | 216 | GLN  |
| 7   | a     | 70  | ASN  |
| 8   | A     | 15  | HIS  |
| 8   | A     | 126 | GLN  |
| 8   | A     | 181 | ASN  |
| 9   | B     | 143 | ASN  |
| 10  | C     | 21  | GLN  |
| 10  | C     | 120 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | D     | 19  | GLN  |
| 11  | D     | 94  | GLN  |
| 11  | D     | 122 | GLN  |
| 11  | D     | 178 | ASN  |
| 12  | E     | 147 | HIS  |
| 13  | F     | 43  | HIS  |
| 13  | F     | 60  | GLN  |
| 13  | F     | 121 | GLN  |
| 14  | G     | 62  | GLN  |
| 14  | G     | 64  | ASN  |
| 14  | G     | 73  | HIS  |
| 14  | G     | 121 | GLN  |
| 14  | G     | 183 | HIS  |
| 14  | G     | 195 | GLN  |
| 14  | G     | 207 | ASN  |
| 14  | G     | 228 | HIS  |
| 14  | G     | 244 | GLN  |
| 8   | c     | 208 | HIS  |
| 9   | j     | 20  | GLN  |
| 10  | d     | 59  | GLN  |
| 10  | d     | 120 | GLN  |
| 10  | d     | 125 | HIS  |
| 10  | d     | 168 | ASN  |
| 11  | n     | 19  | GLN  |
| 11  | n     | 117 | GLN  |
| 11  | n     | 118 | GLN  |
| 11  | n     | 167 | ASN  |
| 11  | n     | 209 | ASN  |
| 12  | m     | 99  | HIS  |
| 12  | m     | 157 | HIS  |
| 13  | l     | 43  | HIS  |
| 13  | l     | 210 | ASN  |
| 14  | k     | 121 | GLN  |
| 14  | k     | 147 | HIS  |
| 15  | H     | 95  | HIS  |
| 15  | H     | 98  | GLN  |
| 15  | H     | 265 | ASN  |
| 17  | J     | 25  | GLN  |
| 17  | J     | 28  | GLN  |
| 17  | J     | 156 | GLN  |
| 17  | J     | 240 | HIS  |
| 18  | K     | 180 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | K     | 388 | GLN  |
| 19  | L     | 99  | GLN  |
| 19  | L     | 203 | ASN  |
| 19  | L     | 273 | HIS  |
| 19  | L     | 302 | GLN  |
| 19  | L     | 328 | ASN  |
| 20  | M     | 240 | ASN  |
| 20  | M     | 364 | HIS  |
| 21  | N     | 116 | GLN  |
| 21  | N     | 176 | GLN  |
| 21  | N     | 300 | ASN  |
| 21  | N     | 375 | HIS  |
| 21  | N     | 525 | ASN  |
| 22  | O     | 75  | GLN  |
| 22  | O     | 117 | ASN  |
| 22  | O     | 177 | GLN  |
| 22  | O     | 235 | HIS  |
| 22  | O     | 304 | ASN  |
| 22  | O     | 326 | HIS  |
| 22  | O     | 354 | GLN  |
| 23  | P     | 30  | ASN  |
| 23  | P     | 183 | GLN  |
| 23  | P     | 401 | ASN  |
| 24  | Q     | 19  | GLN  |
| 24  | Q     | 145 | HIS  |
| 24  | Q     | 178 | HIS  |
| 24  | Q     | 226 | HIS  |
| 24  | Q     | 379 | GLN  |
| 24  | Q     | 418 | GLN  |
| 24  | Q     | 425 | GLN  |
| 25  | R     | 325 | HIS  |
| 25  | R     | 399 | GLN  |
| 26  | S     | 19  | HIS  |
| 26  | S     | 20  | HIS  |
| 26  | S     | 32  | GLN  |
| 26  | S     | 135 | ASN  |
| 26  | S     | 191 | HIS  |
| 26  | S     | 207 | ASN  |
| 26  | S     | 235 | ASN  |
| 26  | S     | 311 | GLN  |
| 26  | S     | 314 | ASN  |
| 26  | S     | 321 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | S     | 369 | GLN  |
| 26  | S     | 437 | ASN  |
| 26  | S     | 438 | HIS  |
| 26  | S     | 450 | ASN  |
| 27  | T     | 74  | ASN  |
| 27  | T     | 93  | ASN  |
| 27  | T     | 192 | ASN  |
| 28  | U     | 71  | ASN  |
| 28  | U     | 127 | GLN  |
| 28  | U     | 128 | GLN  |
| 28  | U     | 142 | GLN  |
| 28  | U     | 173 | HIS  |
| 29  | V     | 172 | GLN  |
| 29  | V     | 186 | GLN  |
| 29  | V     | 193 | ASN  |
| 29  | V     | 195 | HIS  |
| 29  | V     | 217 | HIS  |
| 30  | W     | 29  | GLN  |
| 30  | W     | 42  | ASN  |
| 30  | W     | 106 | GLN  |
| 30  | W     | 107 | HIS  |
| 30  | W     | 136 | ASN  |
| 31  | X     | 38  | ASN  |
| 31  | X     | 94  | ASN  |
| 33  | Z     | 132 | HIS  |
| 33  | Z     | 276 | ASN  |
| 33  | Z     | 379 | GLN  |
| 33  | Z     | 577 | GLN  |
| 33  | Z     | 760 | HIS  |
| 33  | Z     | 766 | HIS  |
| 33  | Z     | 801 | HIS  |
| 33  | Z     | 810 | ASN  |
| 33  | Z     | 897 | HIS  |
| 33  | Z     | 959 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

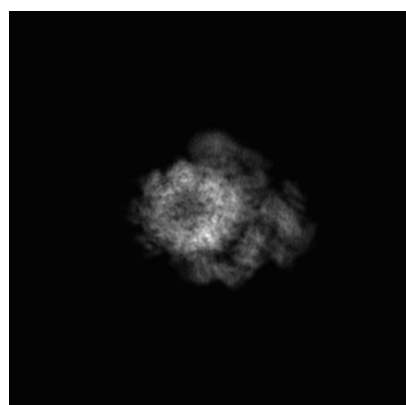
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9773. These allow visual inspection of the internal detail of the map and identification of artifacts.

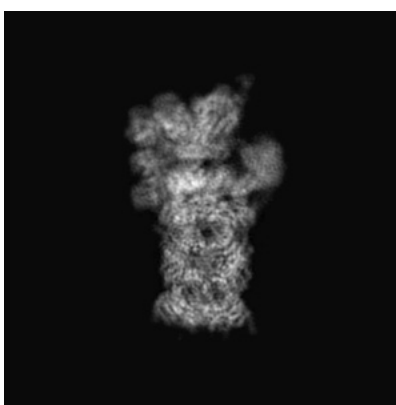
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

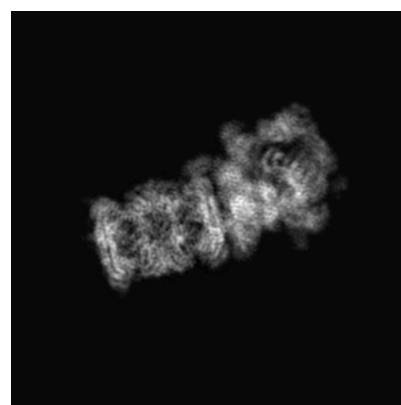
#### 6.1.1 Primary map



X



Y

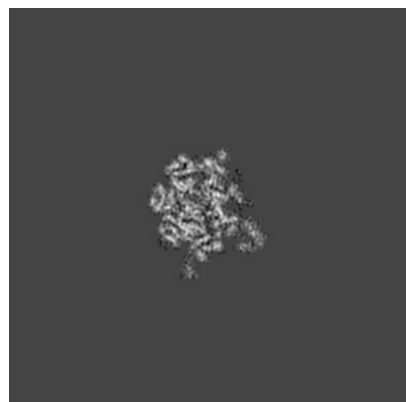


Z

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

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

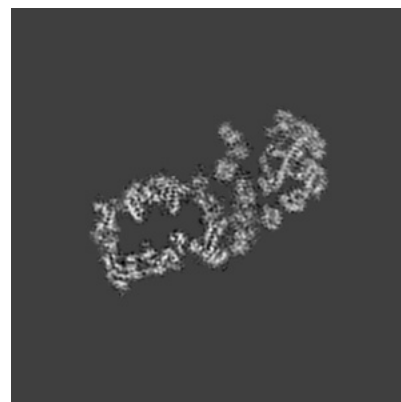
#### 6.2.1 Primary map



X Index: 180



Y Index: 180

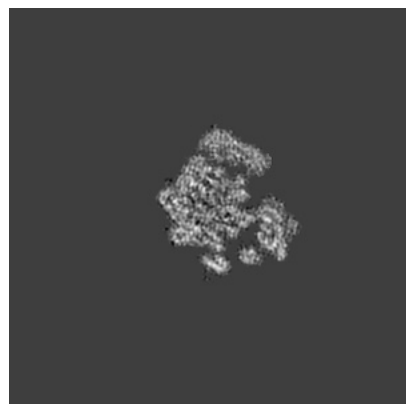


Z Index: 180

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

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

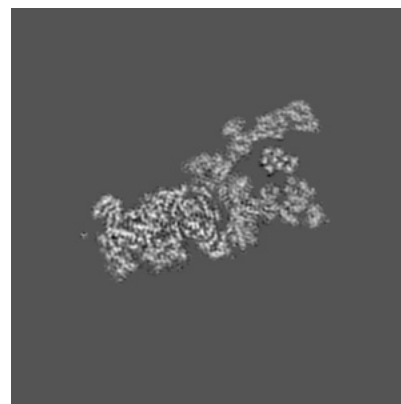
### 6.3.1 Primary map



X Index: 206



Y Index: 178

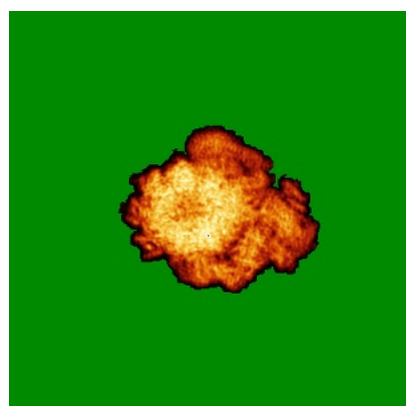


Z Index: 159

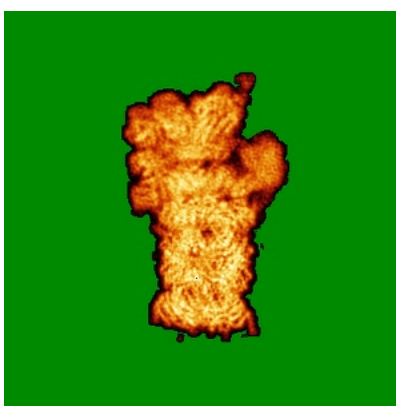
The images above show the largest variance slices of the map in three orthogonal directions.

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

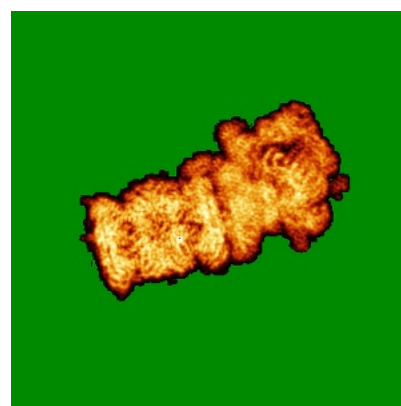
### 6.4.1 Primary map



X



Y

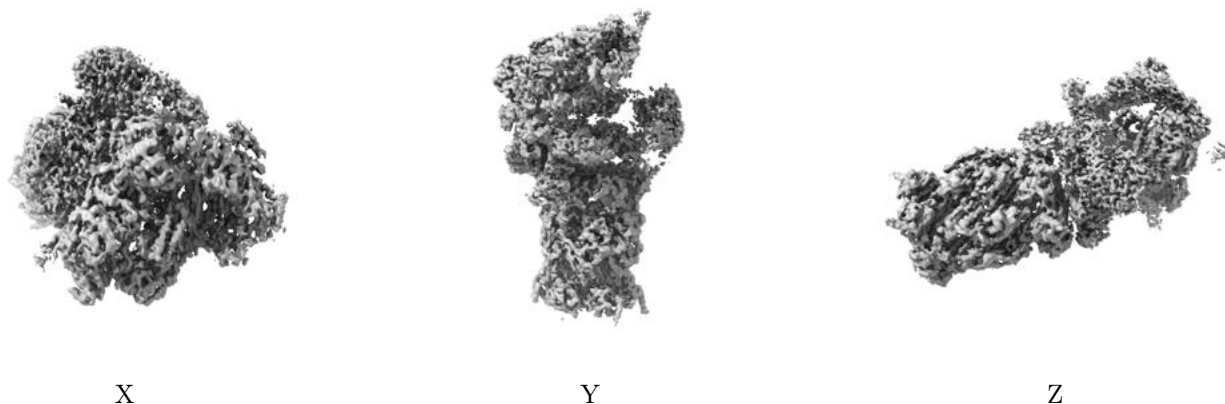


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.686. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

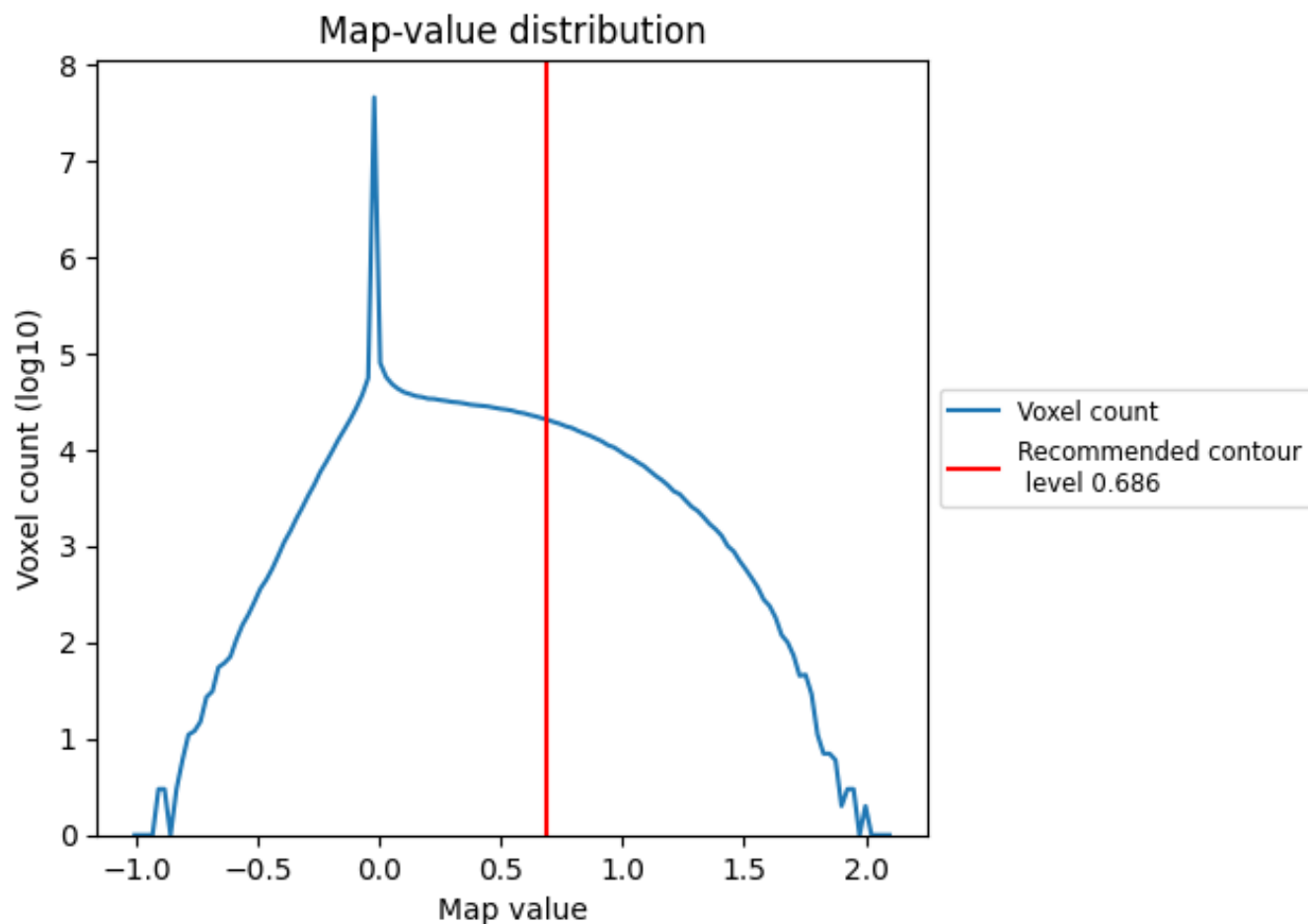
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

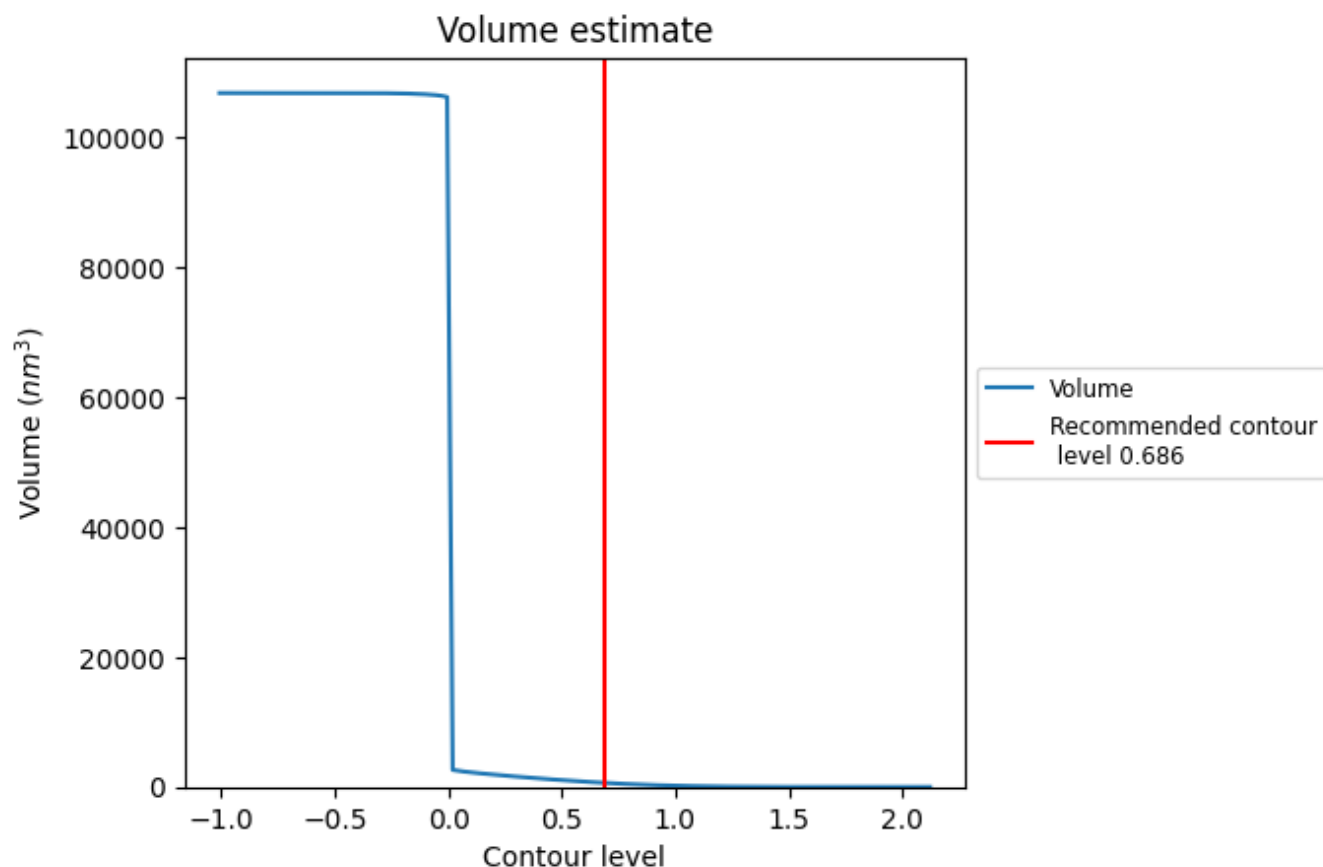
This section contains the results of statistical analysis of the map.

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



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

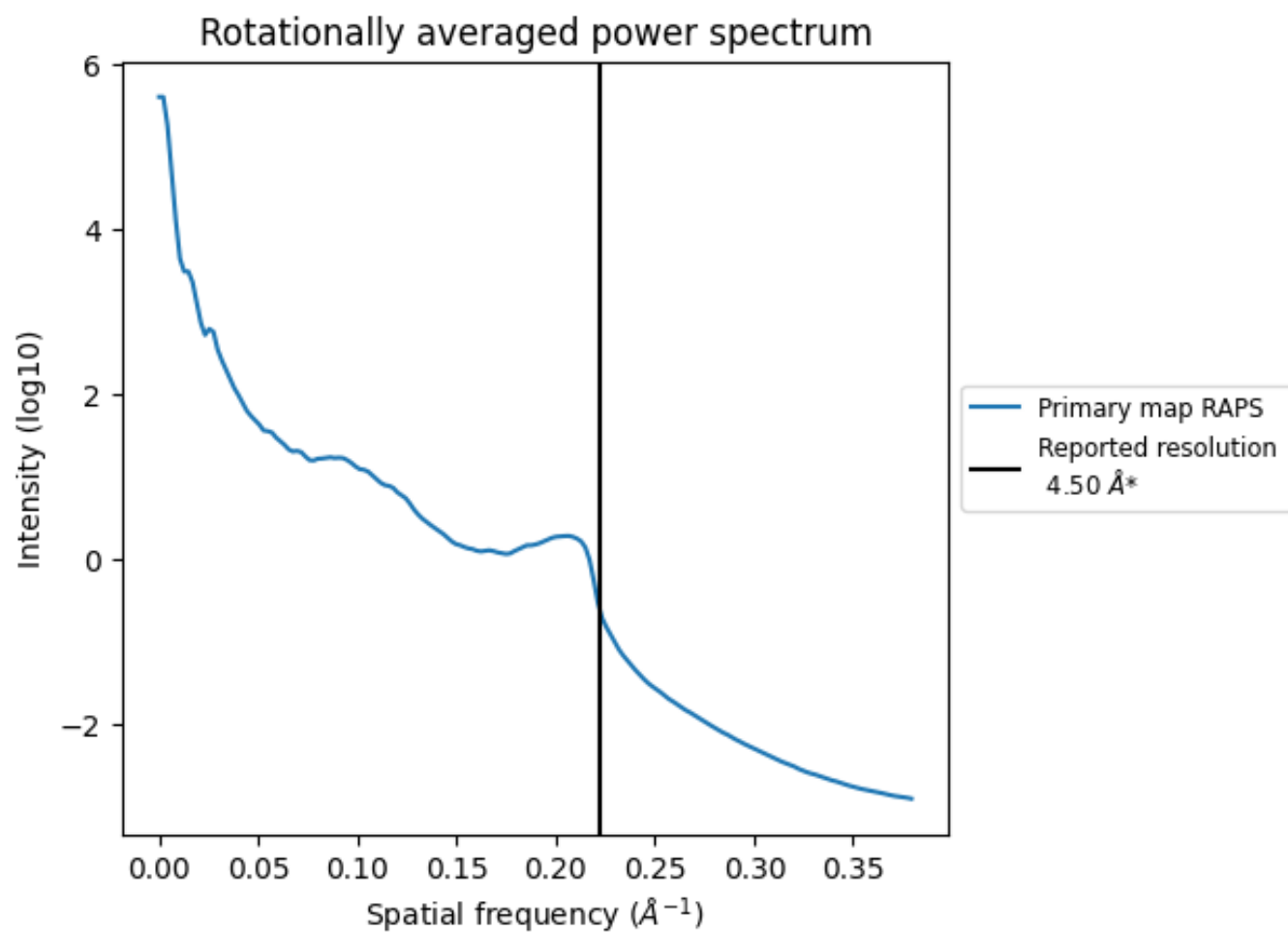
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 636  $\text{nm}^3$ ; this corresponds to an approximate mass of 574 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 0.222  $\text{\AA}^{-1}$

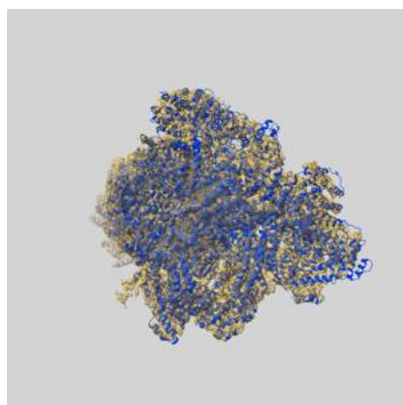
## 8 Fourier-Shell correlation ⓘ

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

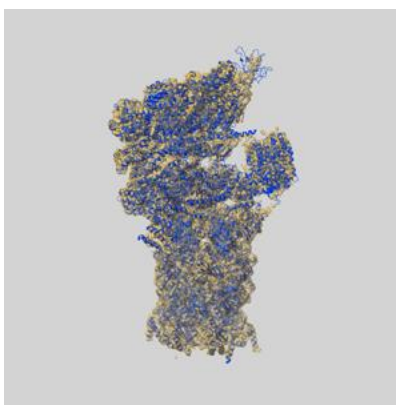
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9773 and PDB model 6J30. Per-residue inclusion information can be found in section 3 on page 11.

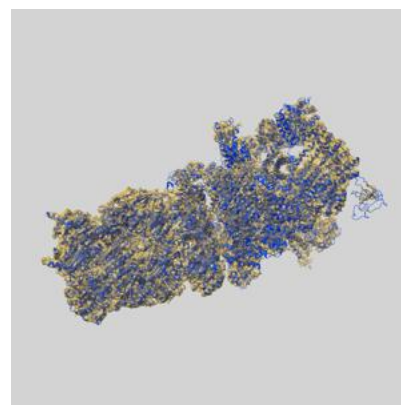
### 9.1 Map-model overlay [i](#)



X



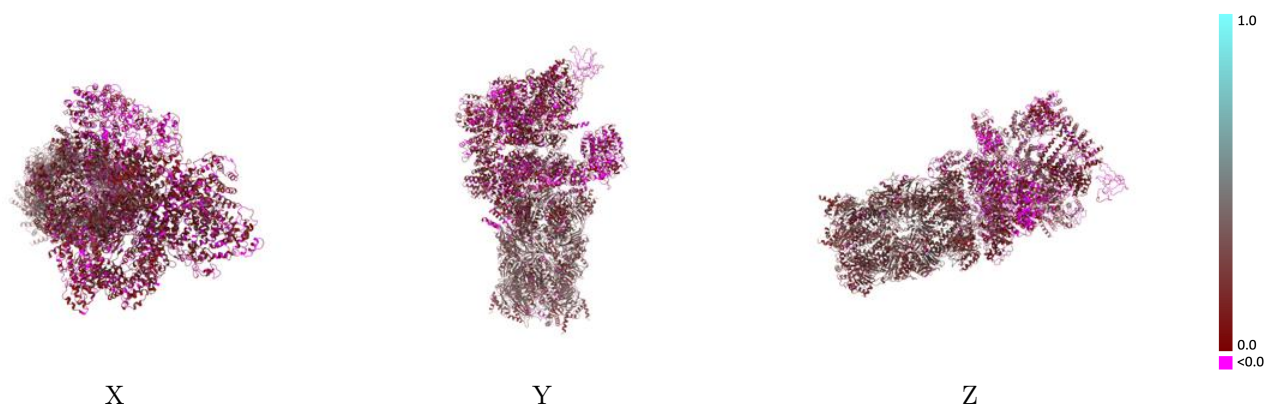
Y



Z

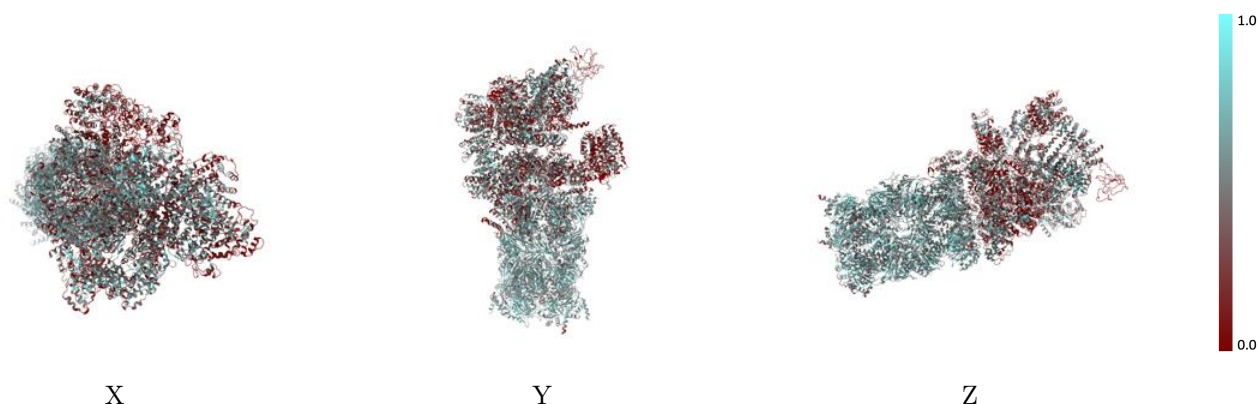
The images above show the 3D surface view of the map at the recommended contour level 0.686 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



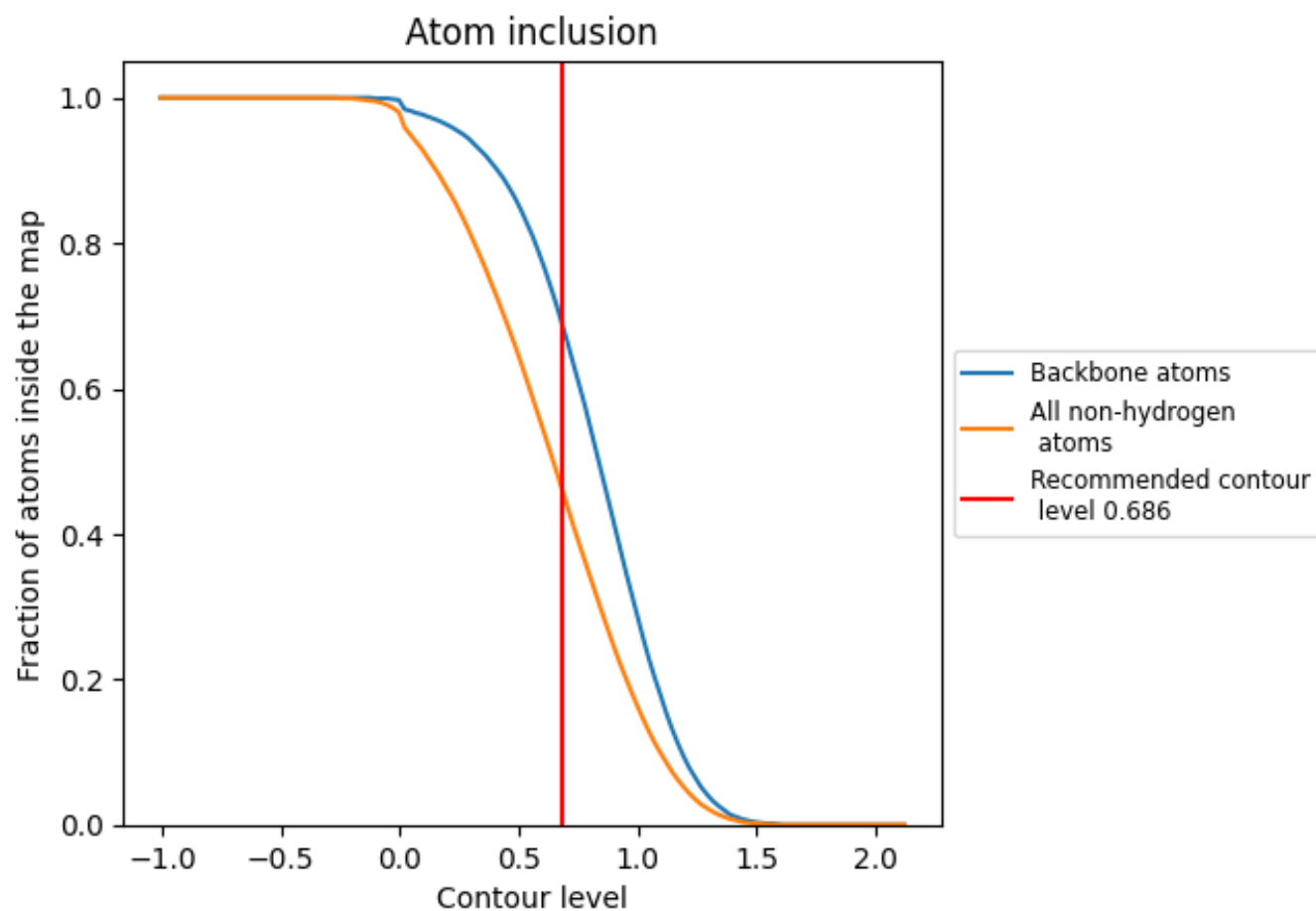
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.686).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 46% 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 (0.686) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                     |
|-------|--------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------|
| All   |  0.4570   |  0.1710    |
| 1     |  0.6120   |  0.2860    |
| 2     |  0.5980   |  0.2640    |
| 3     |  0.5810   |  0.2540    |
| 4     |  0.6020   |  0.2560    |
| 5     |  0.6020   |  0.2670    |
| 6     |  0.6060   |  0.2690    |
| 7     |  0.6100   |  0.2740    |
| A     |  0.5450   |  0.2310    |
| B     |  0.4860   |  0.2040    |
| C     |  0.5090   |  0.1880    |
| D     |  0.5520   |  0.2190    |
| E     |  0.5460   |  0.2210    |
| F     |  0.5650   |  0.2210    |
| G     |  0.5700  |  0.2380   |
| H     |  0.3540 |  0.1410  |
| I     |  0.3080 |  0.1020  |
| J     |  0.2950 |  0.1080  |
| K     |  0.3320 |  0.1150  |
| L     |  0.3820 |  0.1520  |
| M     |  0.3840 |  0.1380  |
| N     |  0.4490 |  0.1330  |
| O     |  0.4020 |  0.1020  |
| P     |  0.4490 |  0.1250  |
| Q     |  0.3680 |  0.1110  |
| R     |  0.3890 |  0.0980  |
| S     |  0.3390 |  0.1080  |
| T     |  0.2080 |  0.0490  |
| U     |  0.4530 |  0.1550  |
| V     |  0.3640 |  0.1150  |
| W     |  0.3950 |  0.0980  |
| X     |  0.0290 |  -0.0290 |
| Y     |  0.5000 |  0.1450  |
| Z     |  0.2140 |  0.0320  |
| a     |  0.6110 |  0.2860  |



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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| b     |  0.6070 |  0.2680 |
| c     |  0.5950 |  0.2280 |
| d     |  0.5640 |  0.2290 |
| e     |  0.5980 |  0.2550 |
| f     |  0.6230 |  0.2740 |
| g     |  0.6050 |  0.2700 |
| h     |  0.5840 |  0.2840 |
| i     |  0.5960 |  0.2760 |
| j     |  0.5500 |  0.2170 |
| k     |  0.5990 |  0.2380 |
| l     |  0.6180 |  0.2470 |
| m     |  0.5550 |  0.2150 |
| n     |  0.5830 |  0.2290 |