



## Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 07:51 PM UTC

PDB ID : 5WVI / pdb\_00005wvi  
EMDB ID : EMD-6693  
Title : The resting state of yeast proteasome  
Authors : Ding, Z.; Cong, Y.  
Deposited on : 2016-12-25  
Resolution : 6.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

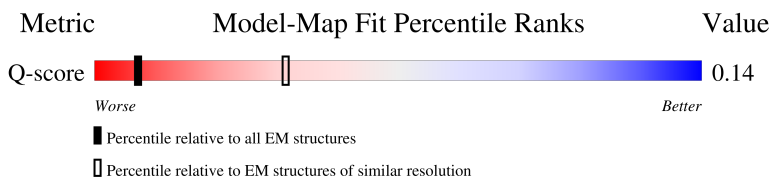
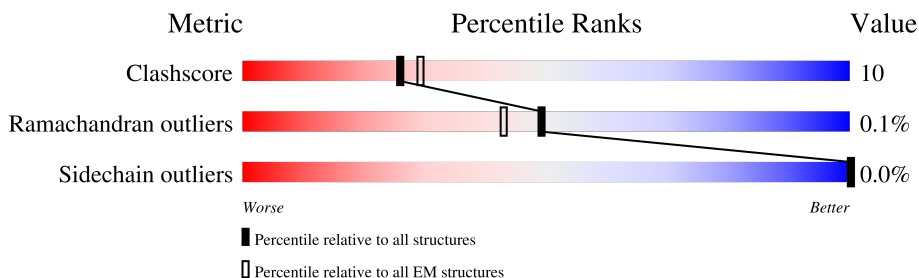
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

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

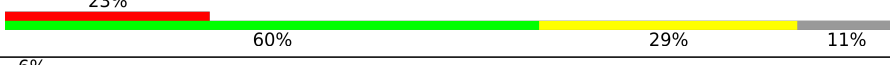
The reported resolution of this entry is 6.30 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 550 ( 5.80 - 6.80 )                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | I     | 437    |  |
| 2   | K     | 428    |  |
| 3   | 2     | 261    |  |
| 3   | i     | 261    |  |

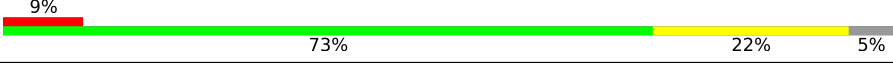
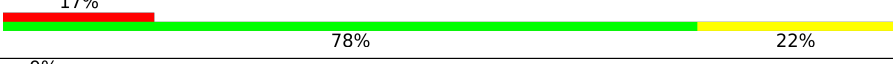
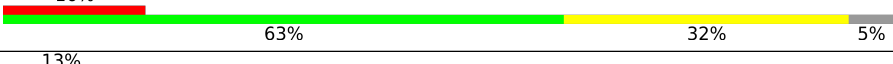
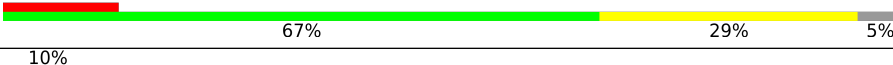
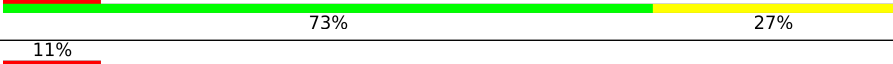
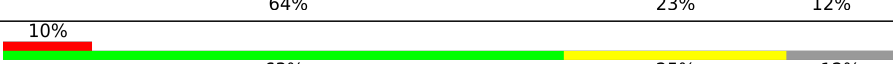
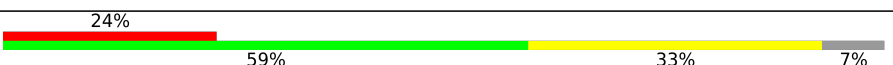
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | A     | 252    |                  |
| 4   | c     | 252    |                  |
| 5   | 3     | 205    |                  |
| 5   | h     | 205    |                  |
| 6   | G     | 288    |                  |
| 6   | k     | 288    |                  |
| 7   | F     | 234    |                  |
| 7   | l     | 234    |                  |
| 8   | E     | 260    |                  |
| 8   | m     | 260    |                  |
| 9   | D     | 254    |                  |
| 9   | n     | 254    |                  |
| 10  | Y     | 89     |                  |
| 11  | N     | 945    |                  |
| 12  | S     | 523    |                  |
| 13  | T     | 274    |                  |
| 14  | R     | 429    |                  |
| 15  | Q     | 434    |                  |
| 16  | J     | 405    |                  |
| 17  | L     | 437    |                  |
| 18  | M     | 434    |                  |
| 19  | U     | 338    |                  |
| 20  | W     | 268    |                  |
| 21  | O     | 393    |                  |
| 22  | P     | 445    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 23  | H     | 467    |    |
| 24  | C     | 258    |    |
| 24  | d     | 258    |    |
| 25  | B     | 250    |    |
| 25  | j     | 250    |    |
| 26  | 1     | 215    |    |
| 26  | b     | 215    |    |
| 27  | 4     | 198    |    |
| 27  | g     | 198    |    |
| 28  | 5     | 287    |    |
| 28  | f     | 287    |    |
| 29  | 6     | 241    |   |
| 29  | e     | 241    |  |
| 30  | 7     | 266    |  |
| 30  | a     | 266    |  |
| 31  | X     | 156    |  |
| 32  | Z     | 993    |  |
| 33  | V     | 306    |  |

## 2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 105787 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 26S protease regulatory subunit 4 homolog.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | I     | 362      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2822  | 1773 | 471 | 563 | 15 |         |       |

- Molecule 2 is a protein called 26S protease regulatory subunit 6B homolog.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | K     | 381      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3019  | 1898 | 530 | 581 | 10 |         |       |

- Molecule 3 is a protein called Proteasome subunit beta type-2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | i     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1684  | 1061 | 293 | 323 | 7 |         |       |
| 3   | 2     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1684  | 1061 | 293 | 323 | 7 |         |       |

- Molecule 4 is a protein called Proteasome subunit alpha type-1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | c     | 243      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1921  | 1221 | 322 | 370 | 8 |         |       |
| 4   | A     | 243      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1921  | 1221 | 322 | 370 | 8 |         |       |

- Molecule 5 is a protein called Proteasome subunit beta type-3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | h     | 204      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 1010 | 258 | 305 | 8 |         |       |
| 5   | 3     | 204      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1581  | 1010 | 258 | 305 | 8 |         |       |

- Molecule 6 is a protein called Probable proteasome subunit alpha type-7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | k     | 245      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1900  | 1207 | 331 | 358 | 4 |         |       |
| 6   | G     | 245      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1900  | 1207 | 331 | 358 | 4 |         |       |

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | l     | 233      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1795  | 1129 | 312 | 350 | 4 |         |       |
| 7   | F     | 233      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1795  | 1129 | 312 | 350 | 4 |         |       |

- Molecule 8 is a protein called Proteasome subunit alpha type-5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8   | m     | 243      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1867  | 1165 | 315 | 380 | 7 |         |       |
| 8   | E     | 243      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1867  | 1165 | 315 | 380 | 7 |         |       |

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9   | n     | 242      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1899  | 1186 | 333 | 376 | 4 |         |       |
| 9   | D     | 242      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1899  | 1186 | 333 | 376 | 4 |         |       |

- Molecule 10 is a protein called 26S proteasome complex subunit SEM1.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 10  | Y     | 27       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 236   | 143 | 39 | 54 |         |       |

- Molecule 11 is a protein called 26S proteasome regulatory subunit RPN2.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 11  | N     | 849      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6562  | 4174 | 1099 | 1261 | 28 |         |       |

- Molecule 12 is a protein called 26S proteasome regulatory subunit RPN3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12  | S     | 353      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2893  | 1857 | 482 | 541 | 13 |         |       |

- Molecule 13 is a protein called 26S proteasome regulatory subunit RPN12.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | T     | 272      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2235  | 1432 | 355 | 441 | 7 |         |       |

- Molecule 14 is a protein called 26S proteasome regulatory subunit RPN7.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 14  | R     | 400      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3218  | 2051 | 527 | 630 | 10 |         |       |

- Molecule 15 is a protein called 26S proteasome regulatory subunit RPN6.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 15  | Q     | 431      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3471  | 2205 | 574 | 676 | 16 |         |       |

- Molecule 16 is a protein called 26S protease regulatory subunit 8 homolog.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 16  | J     | 373      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2928  | 1837 | 527 | 547 | 17 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 17  | L     | 361      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2853  | 1798 | 507 | 536 | 12 |         |       |

- Molecule 18 is a protein called 26S protease regulatory subunit 6A.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 18  | M     | 367      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2866  | 1799 | 503 | 553 | 11 |         |       |

- Molecule 19 is a protein called 26S proteasome regulatory subunit RPN8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 19  | U     | 282      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2257  | 1429 | 387 | 435 | 6 |         |       |

- Molecule 20 is a protein called 26S proteasome regulatory subunit RPN10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | W     | 197      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1534  | 962 | 269 | 300 | 3 |         |       |

- Molecule 21 is a protein called 26S proteasome regulatory subunit RPN9.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 21  | O     | 387      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3182  | 2047 | 520 | 606 | 9 |         |       |

- Molecule 22 is a protein called 26S proteasome regulatory subunit RPN5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 22  | P     | 432      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3545  | 2260 | 592 | 684 | 9 |         |       |

- Molecule 23 is a protein called 26S protease regulatory subunit 7 homolog.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 23  | H     | 370      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2889  | 1815 | 515 | 543 | 16 |         |       |

- Molecule 24 is a protein called Proteasome subunit alpha type-3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 24  | C     | 245      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1913  | 1207 | 323 | 380 | 3 |         |       |
| 24  | d     | 245      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1913  | 1207 | 323 | 380 | 3 |         |       |

- Molecule 25 is a protein called Proteasome subunit alpha type-2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 25  | B     | 250      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1915  | 1219 | 315 | 377 | 4 |         |       |
| 25  | j     | 250      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1915  | 1219 | 315 | 377 | 4 |         |       |



- Molecule 26 is a protein called Proteasome subunit beta type-1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | 1     | 205      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1576  | 996 | 261 | 312 | 7 |         |       |
| 26  | b     | 205      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1574  | 995 | 261 | 311 | 7 |         |       |

- Molecule 27 is a protein called Proteasome subunit beta type-4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 27  | 4     | 198      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1585  | 1005 | 269 | 305 | 6 |         |       |
| 27  | g     | 198      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1585  | 1005 | 269 | 305 | 6 |         |       |

- Molecule 28 is a protein called Proteasome subunit beta type-5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 28  | 5     | 212      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1644  | 1045 | 280 | 312 | 7 |         |       |
| 28  | f     | 212      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1644  | 1045 | 280 | 312 | 7 |         |       |

- Molecule 29 is a protein called Proteasome subunit beta type-6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 29  | 6     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1757  | 1115 | 303 | 335 | 4 |         |       |
| 29  | e     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1757  | 1115 | 303 | 335 | 4 |         |       |

- Molecule 30 is a protein called Proteasome subunit beta type-7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 30  | 7     | 233      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1824  | 1154 | 312 | 351 | 7 |         |       |
| 30  | a     | 233      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1824  | 1154 | 312 | 351 | 7 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | X     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1032  | 664 | 169 | 195 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 32  | Z     | 813      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6289  | 3995 | 1029 | 1236 | 29 |         |       |

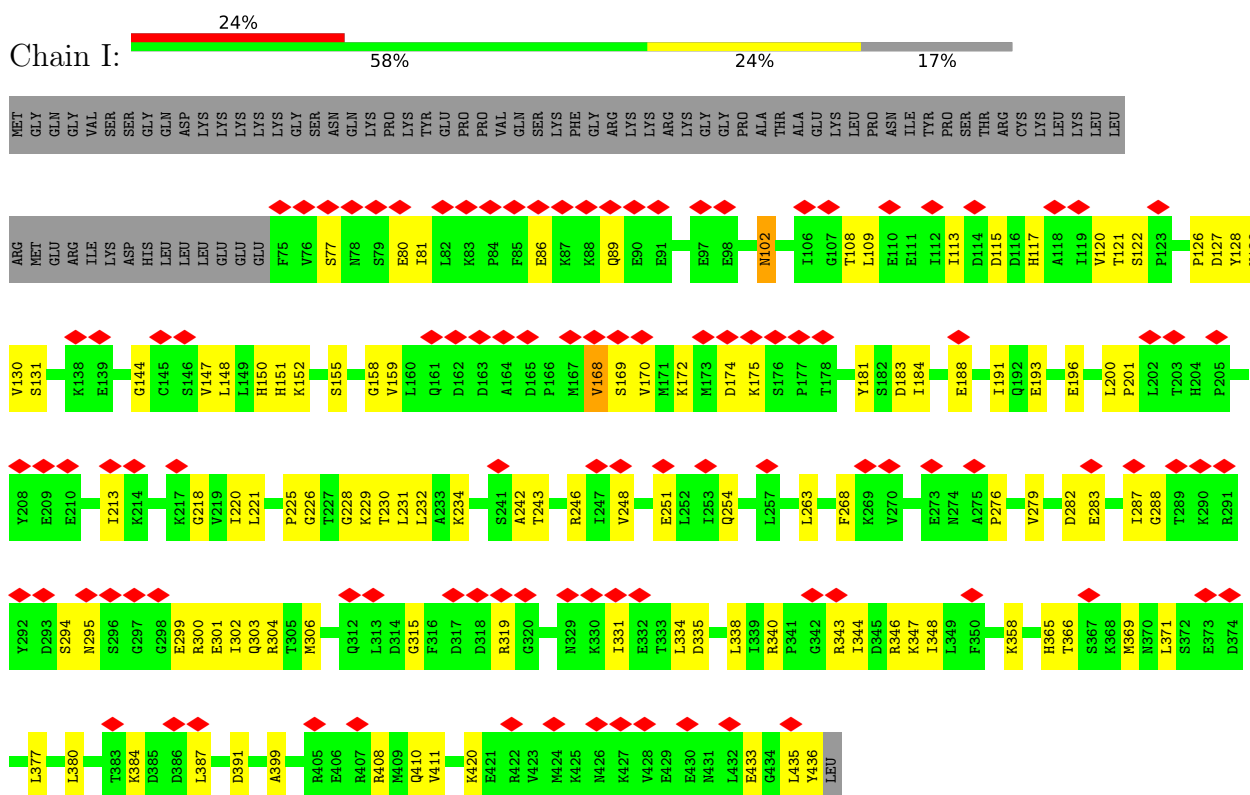
- Molecule 33 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 33  | V     | 284      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2236  | 1405 | 381 | 436 | 14 |         |       |

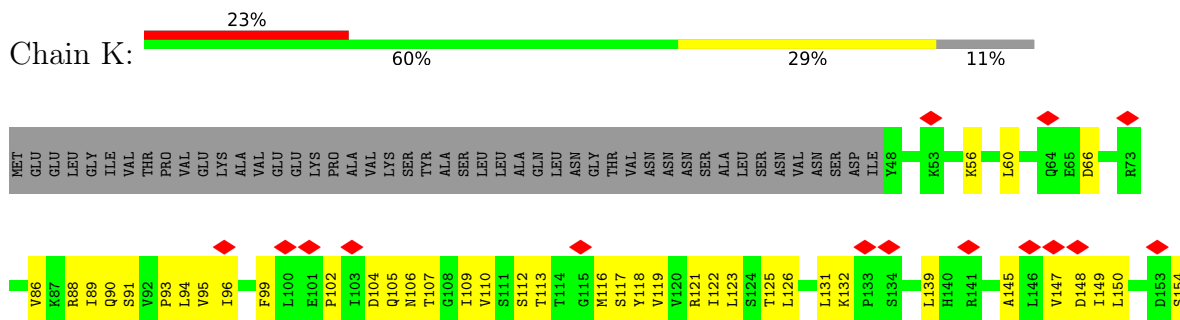
### 3 Residue-property plots

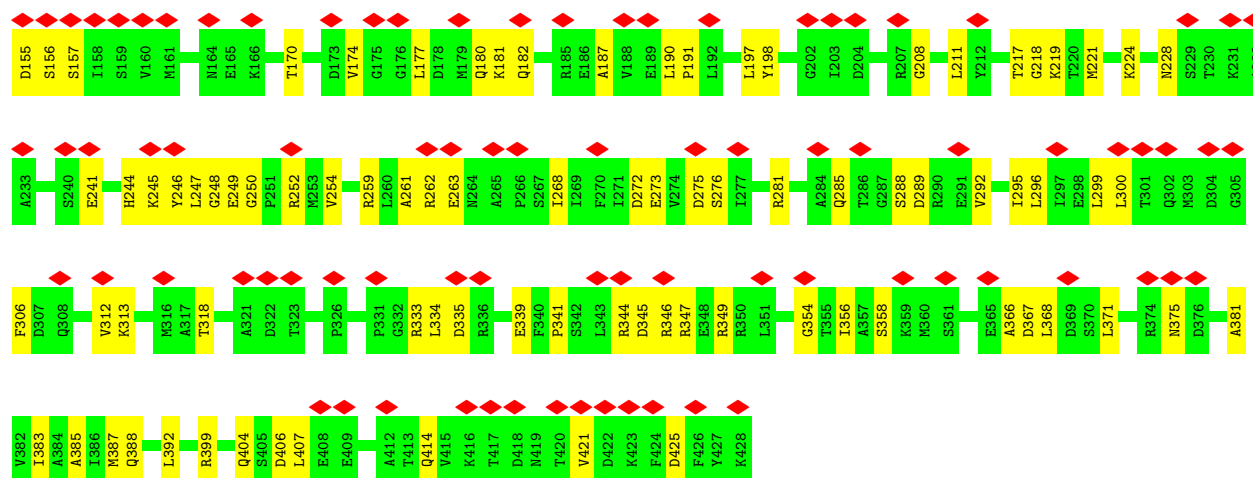
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 26S protease regulatory subunit 4 homolog

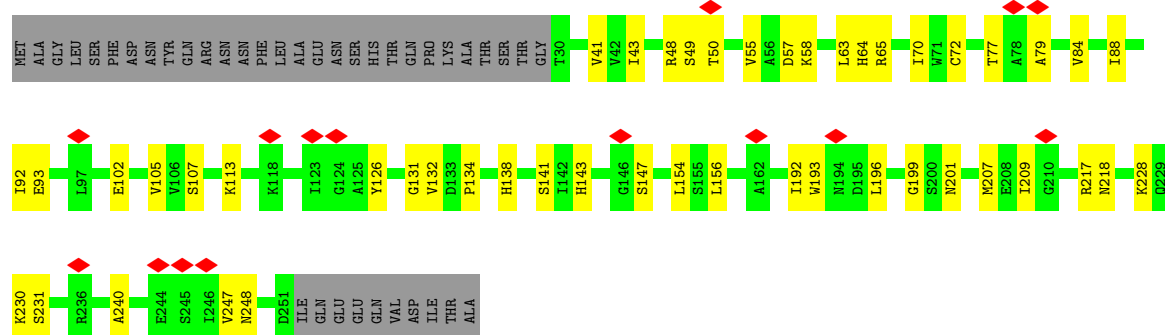


- Molecule 2: 26S protease regulatory subunit 6B homolog

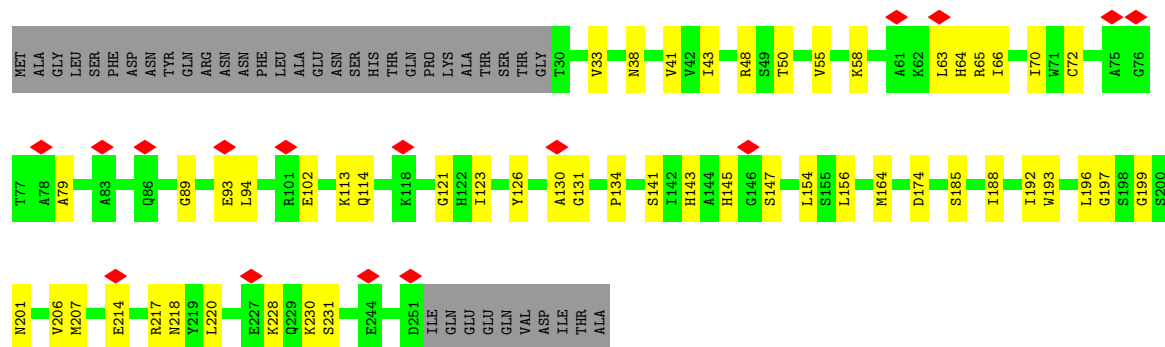




• Molecule 3: Proteasome subunit beta type-2

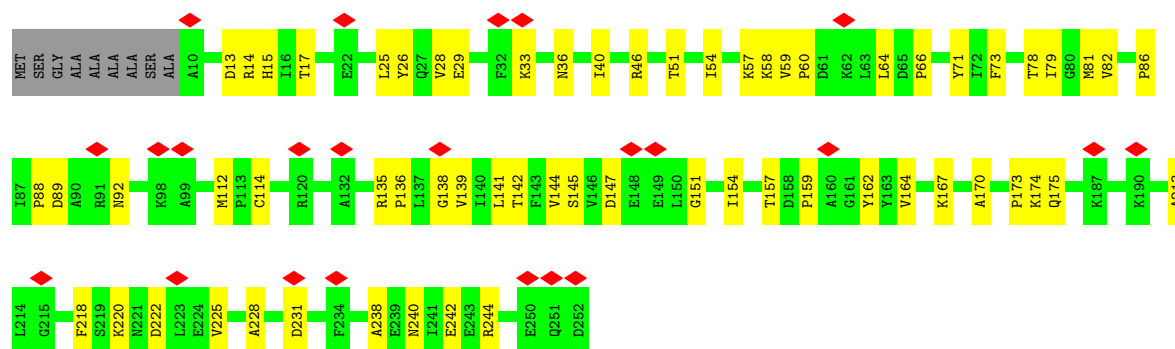


• Molecule 3: Proteasome subunit beta type-2

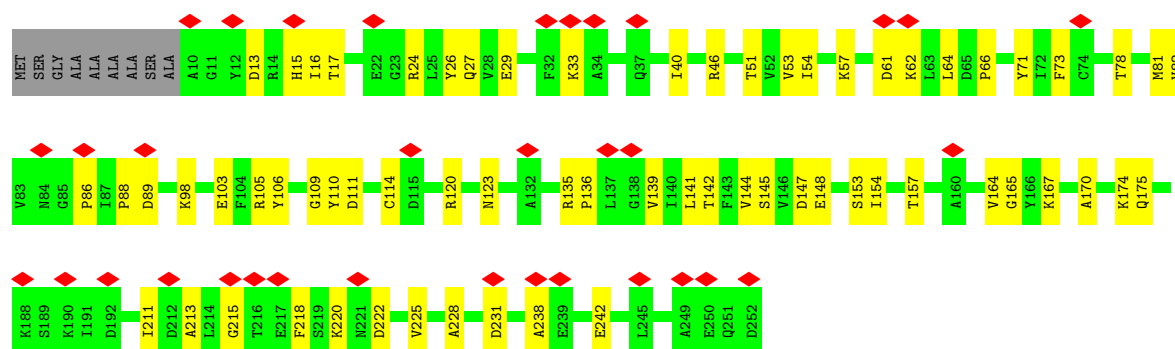


• Molecule 4: Proteasome subunit alpha type-1

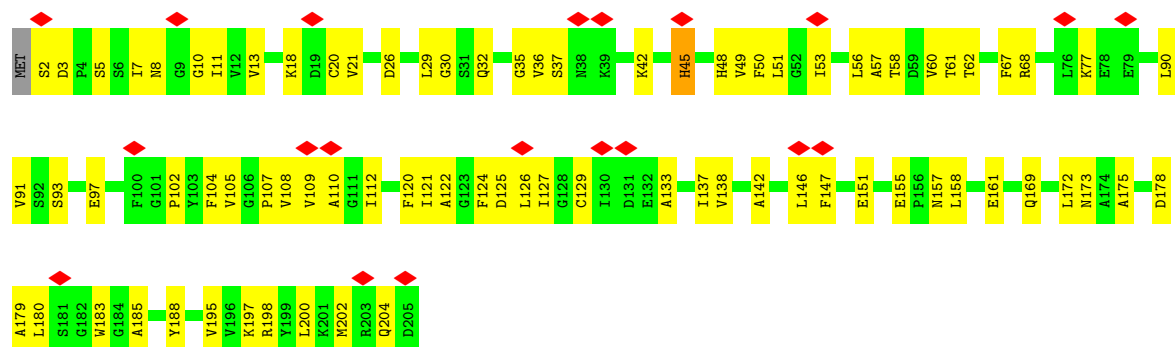




• Molecule 4: Proteasome subunit alpha type-1

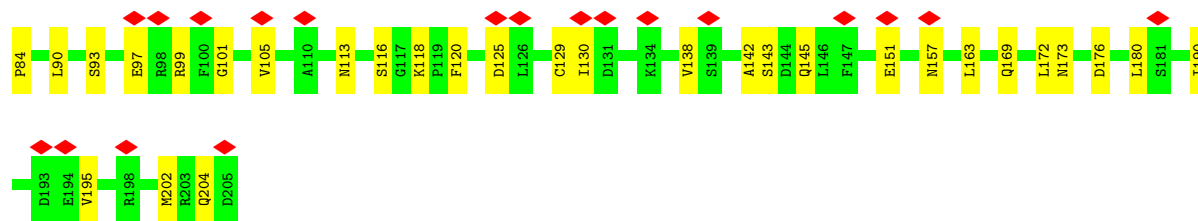


• Molecule 5: Proteasome subunit beta type-3

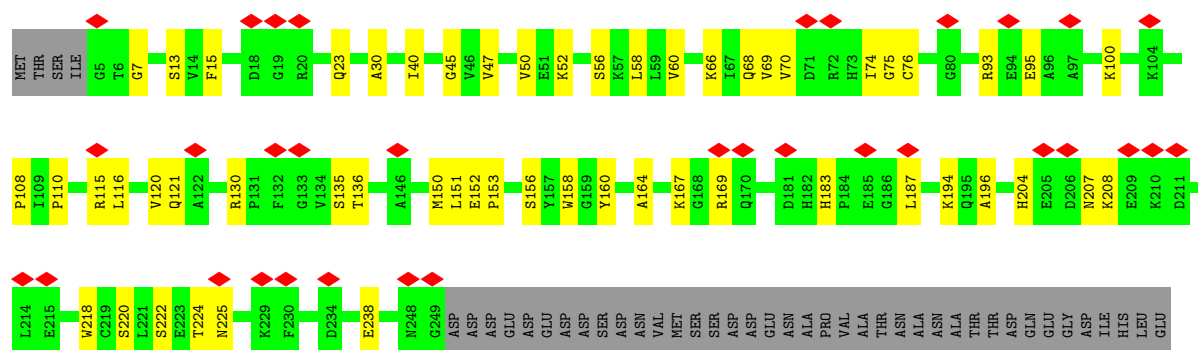


• Molecule 5: Proteasome subunit beta type-3

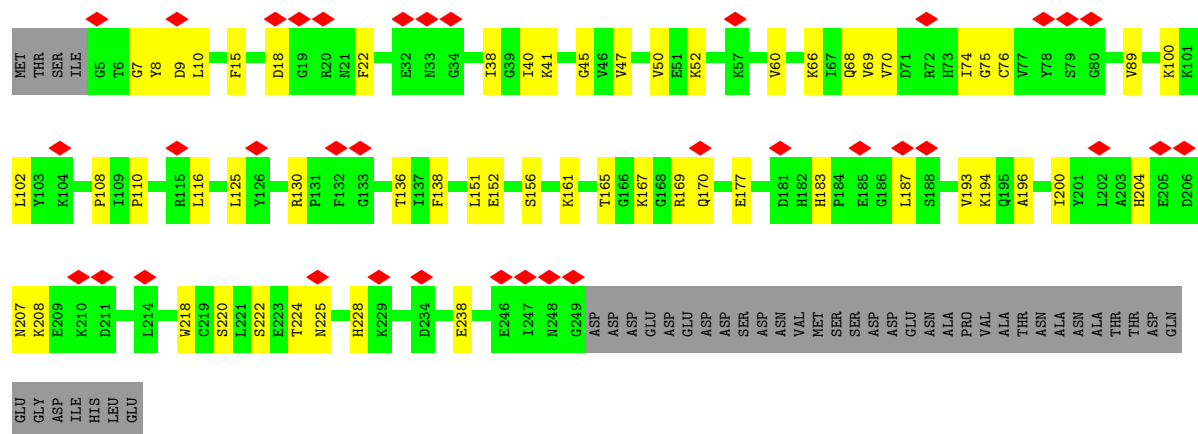




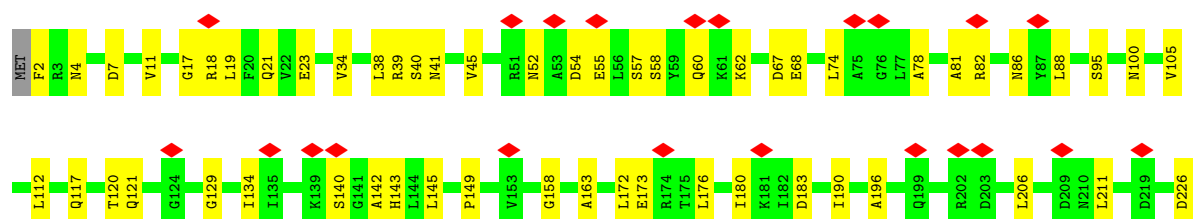
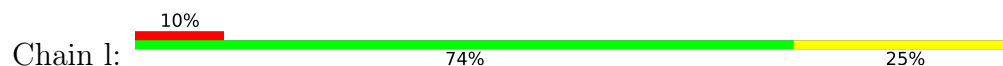
• Molecule 6: Probable proteasome subunit alpha type-7

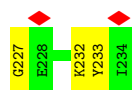


• Molecule 6: Probable proteasome subunit alpha type-7

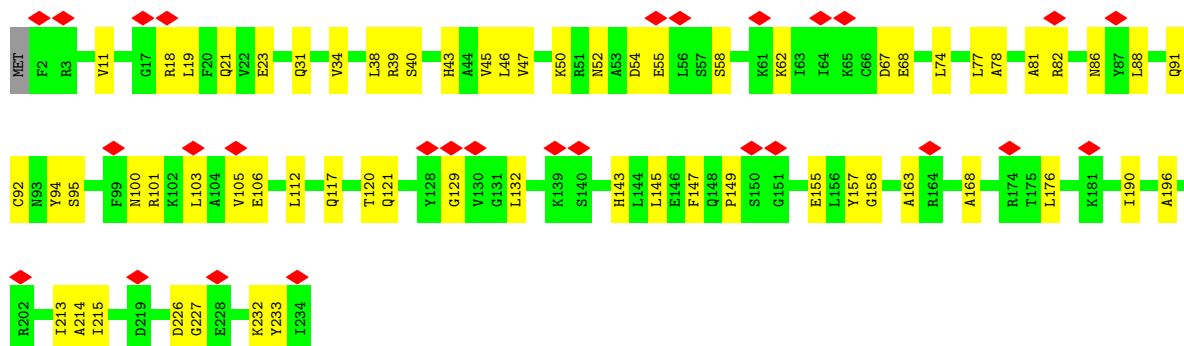
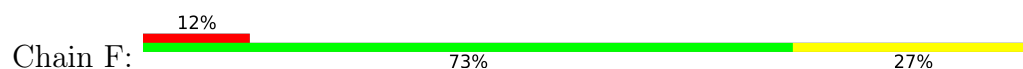


• Molecule 7: Proteasome subunit alpha type-6

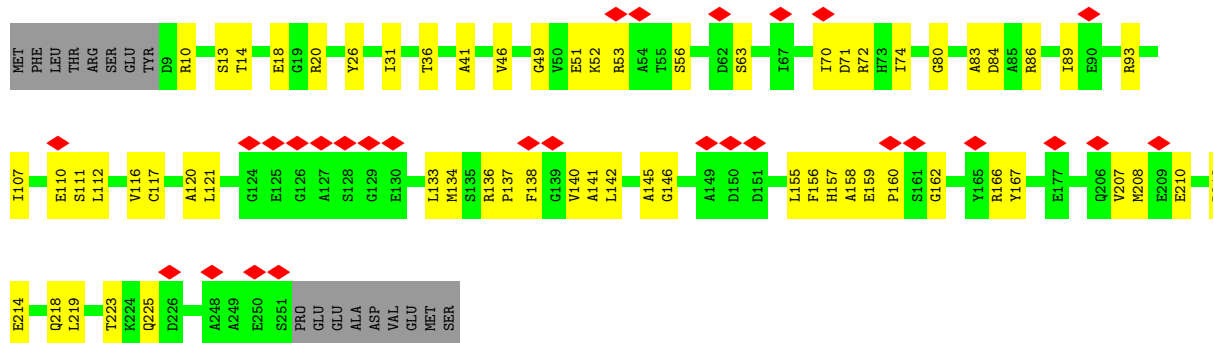




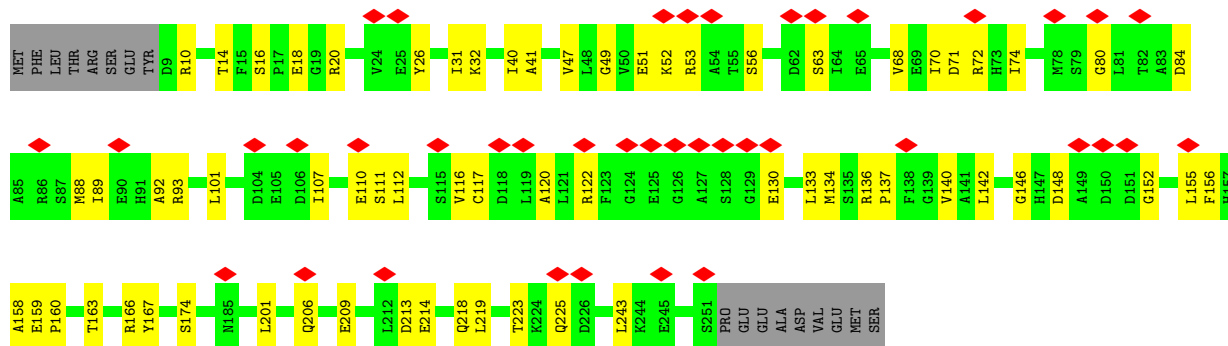
- Molecule 7: Proteasome subunit alpha type-6



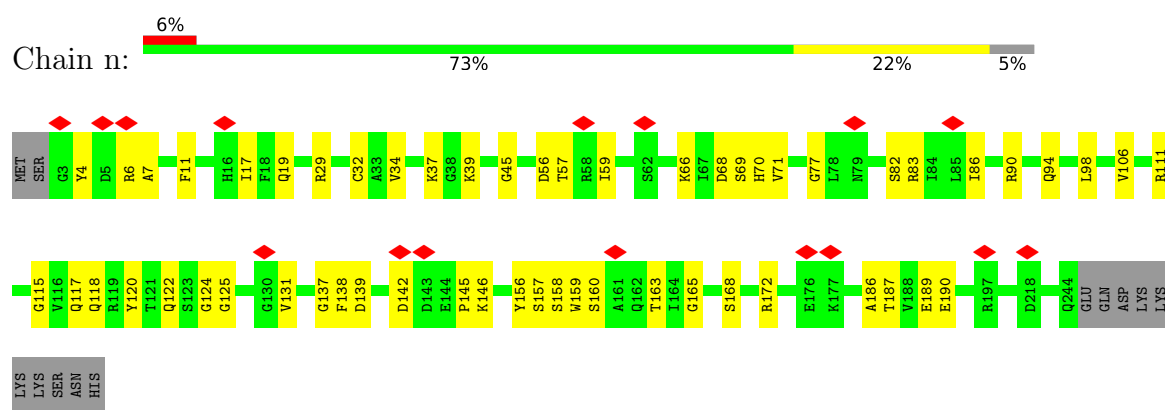
- Molecule 8: Proteasome subunit alpha type-5



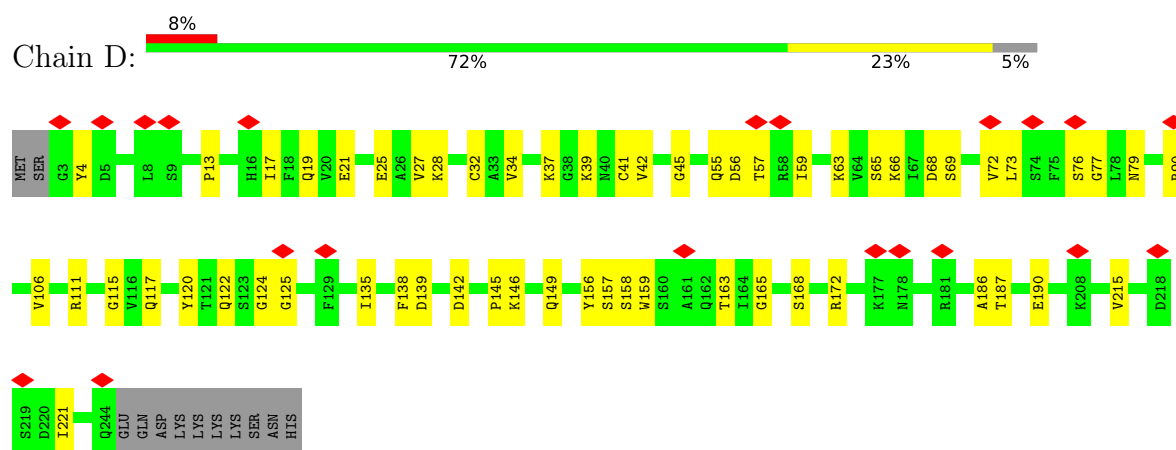
- Molecule 8: Proteasome subunit alpha type-5



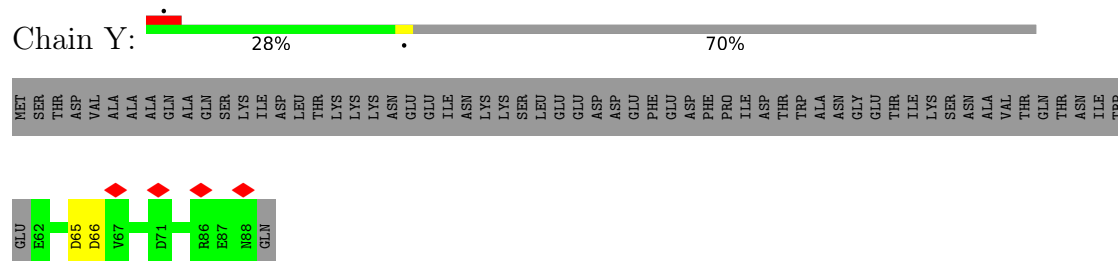
- Molecule 9: Proteasome subunit alpha type-4



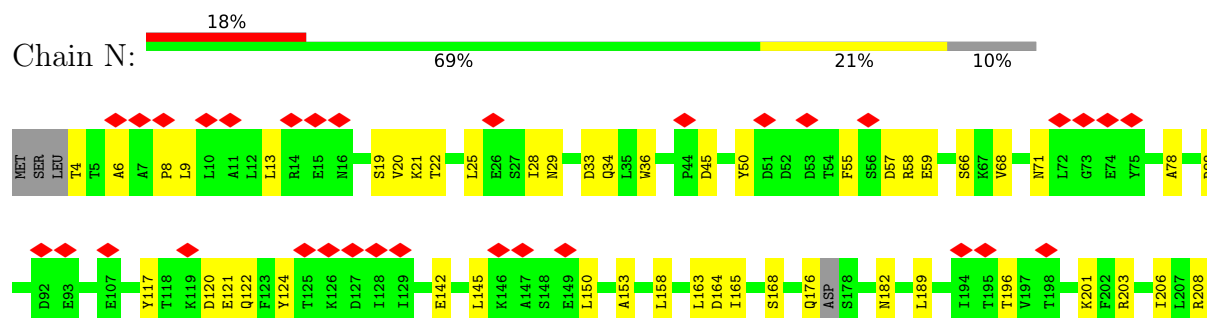
• Molecule 9: Proteasome subunit alpha type-4



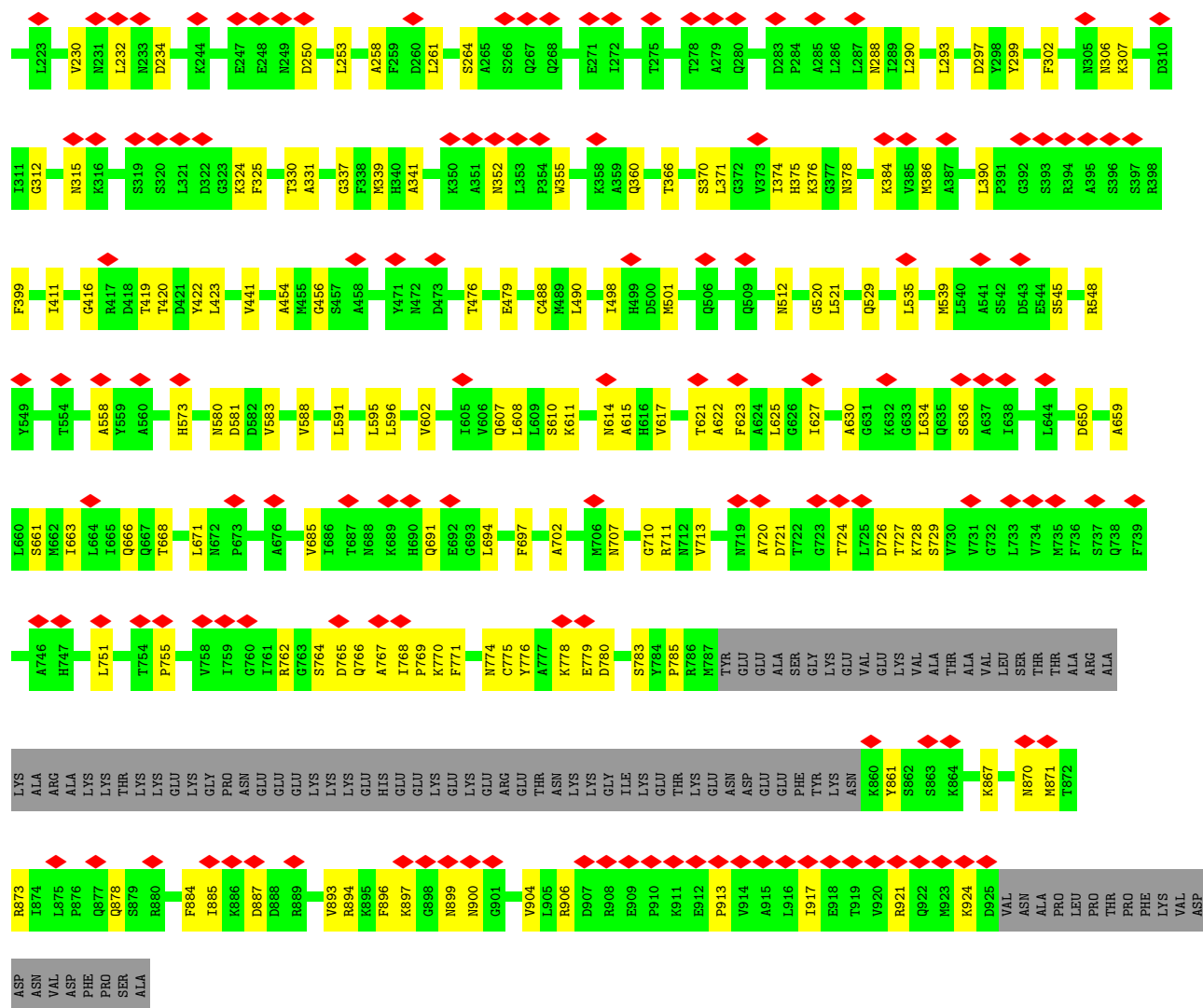
• Molecule 10: 26S proteasome complex subunit SEM1



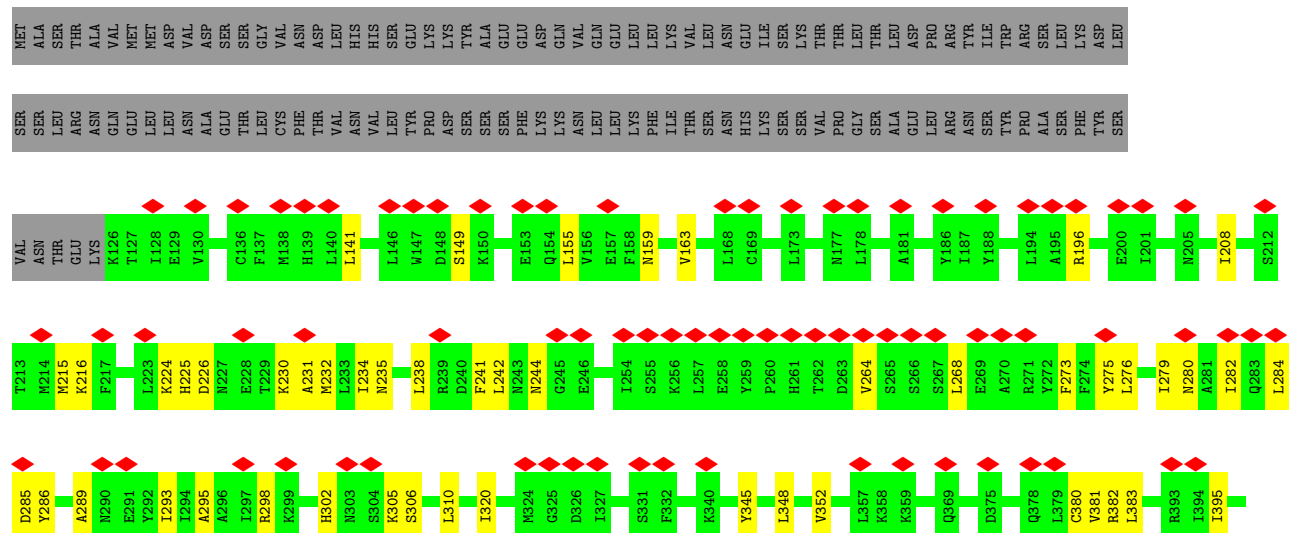
• Molecule 11: 26S proteasome regulatory subunit RPN2

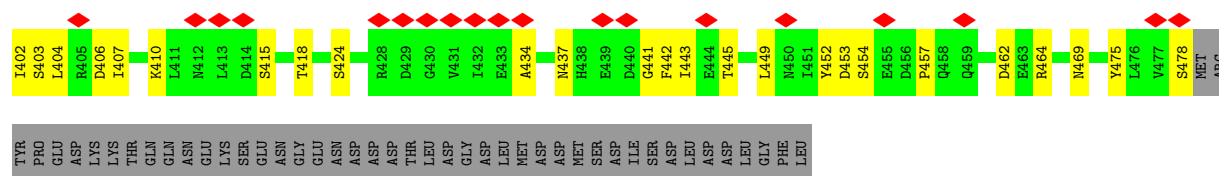






• Molecule 12: 26S proteasome regulatory subunit RPN3

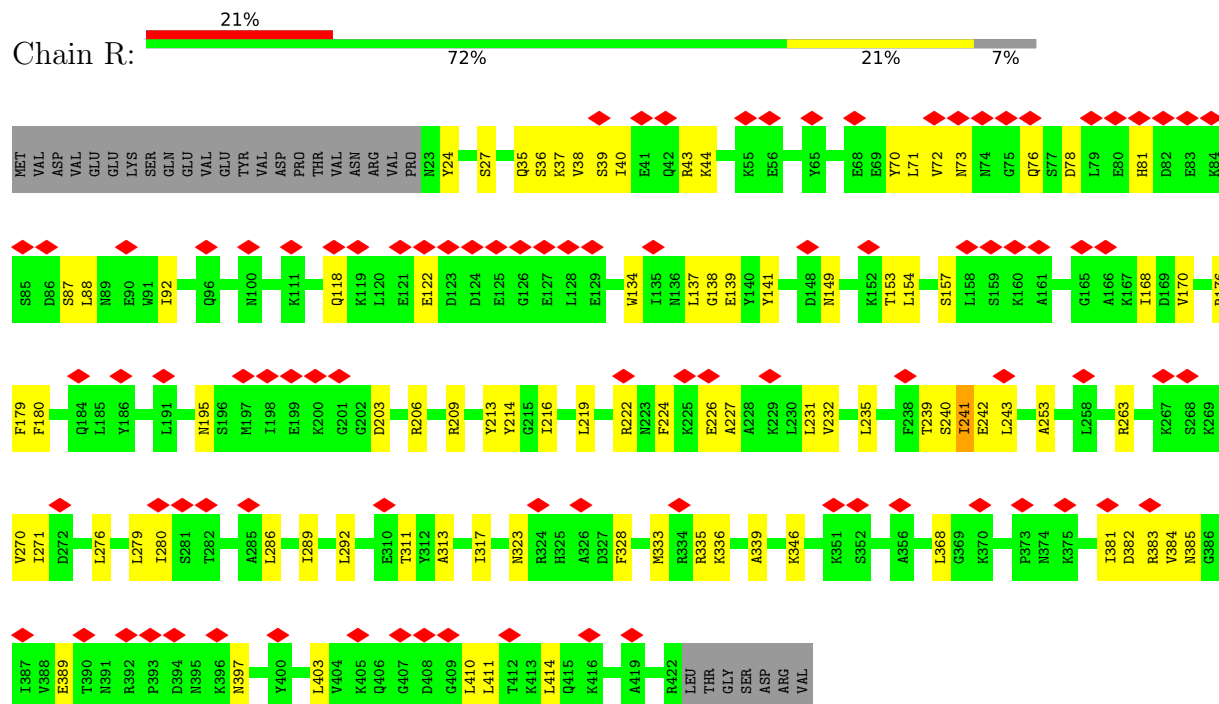




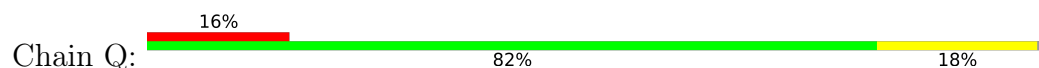
• Molecule 13: 26S proteasome regulatory subunit RPN12

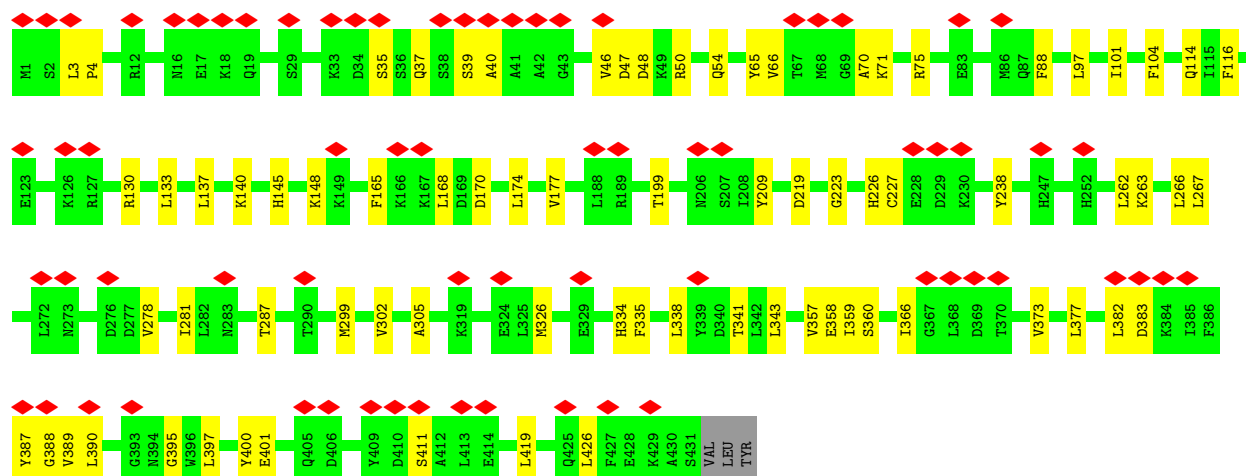


• Molecule 14: 26S proteasome regulatory subunit RPN7

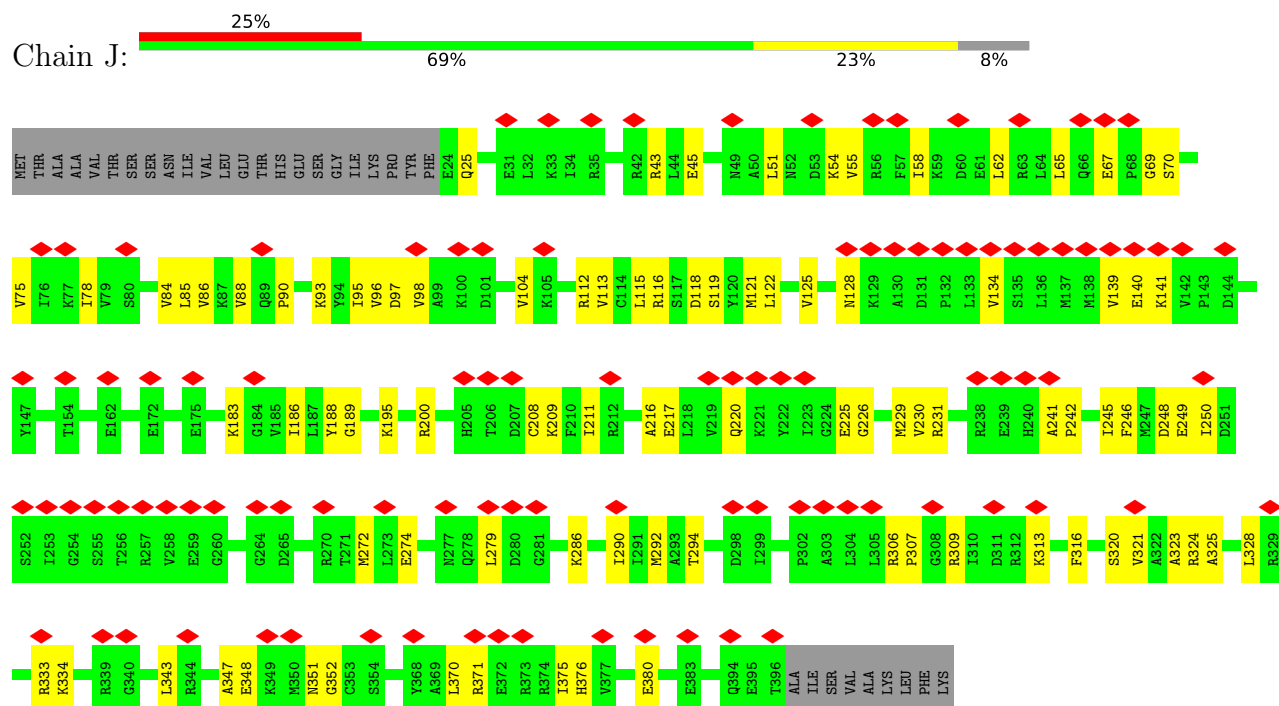


• Molecule 15: 26S proteasome regulatory subunit RPN6

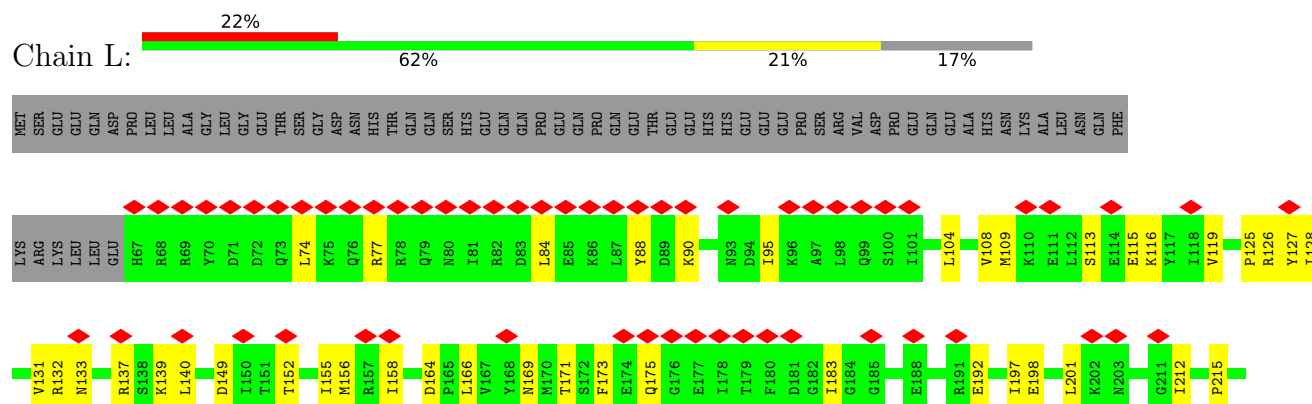


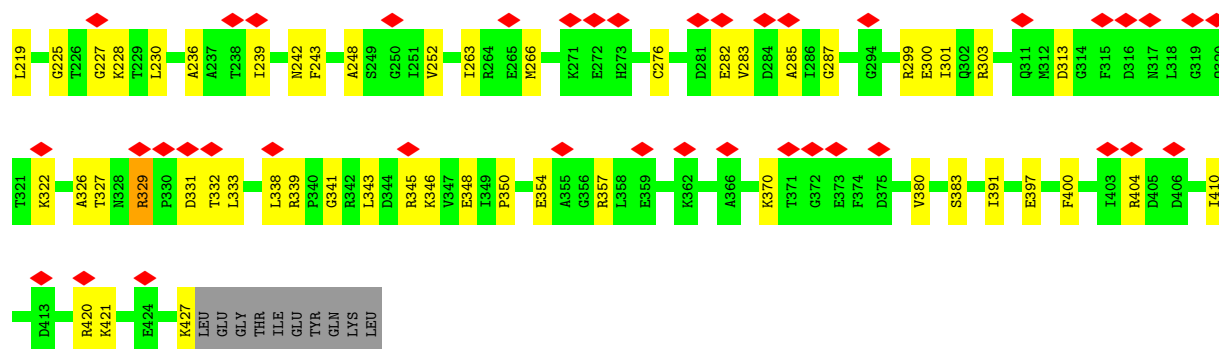


- Molecule 16: 26S protease regulatory subunit 8 homolog

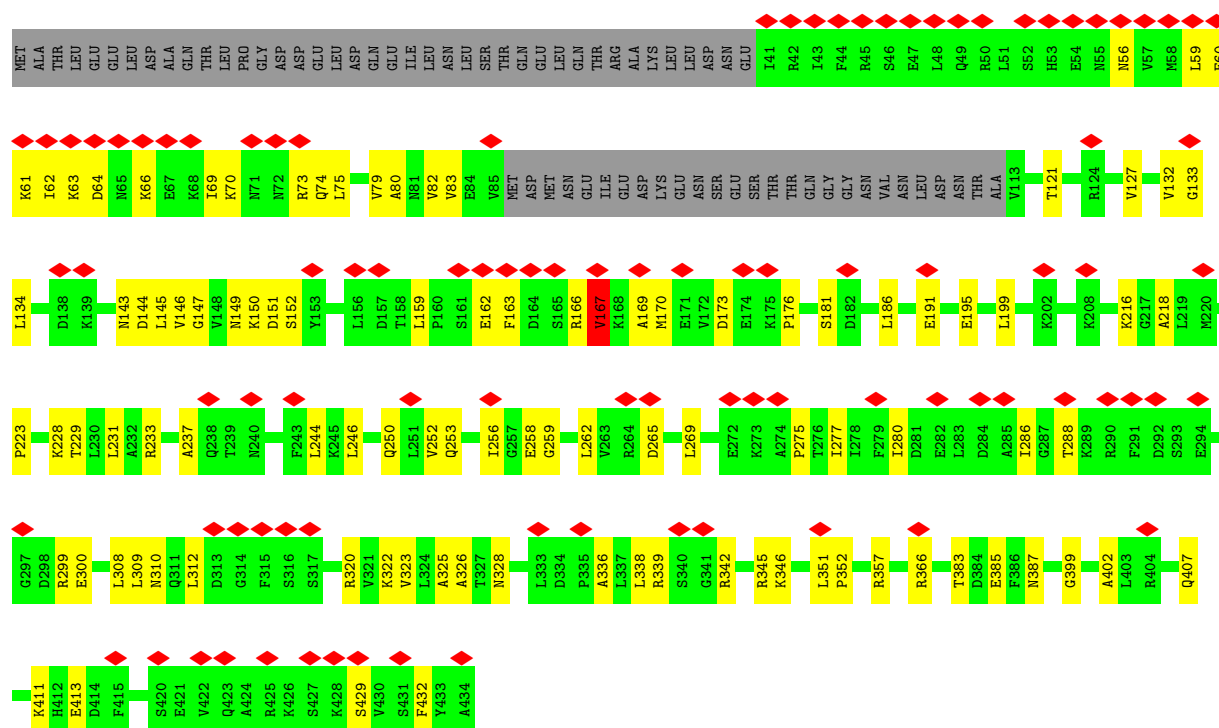


- Molecule 17: 26S protease subunit RPT4

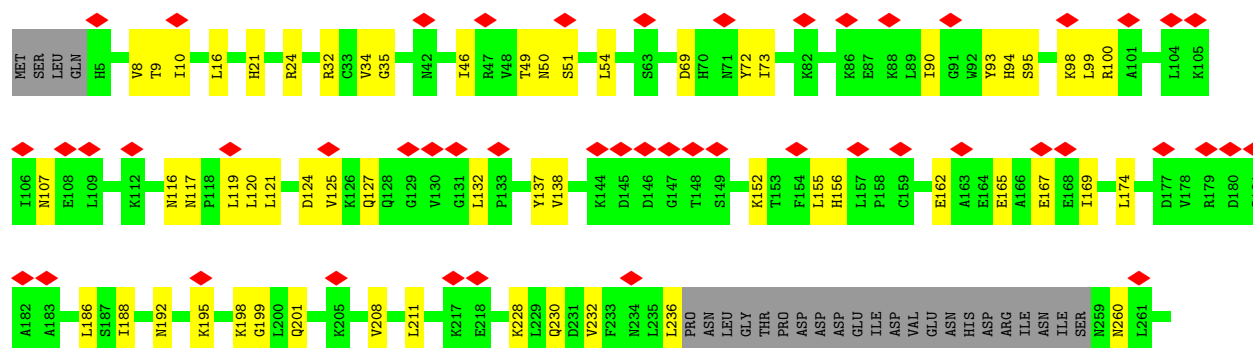


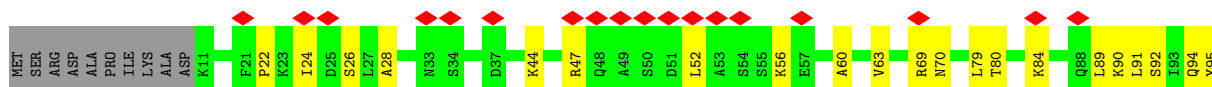


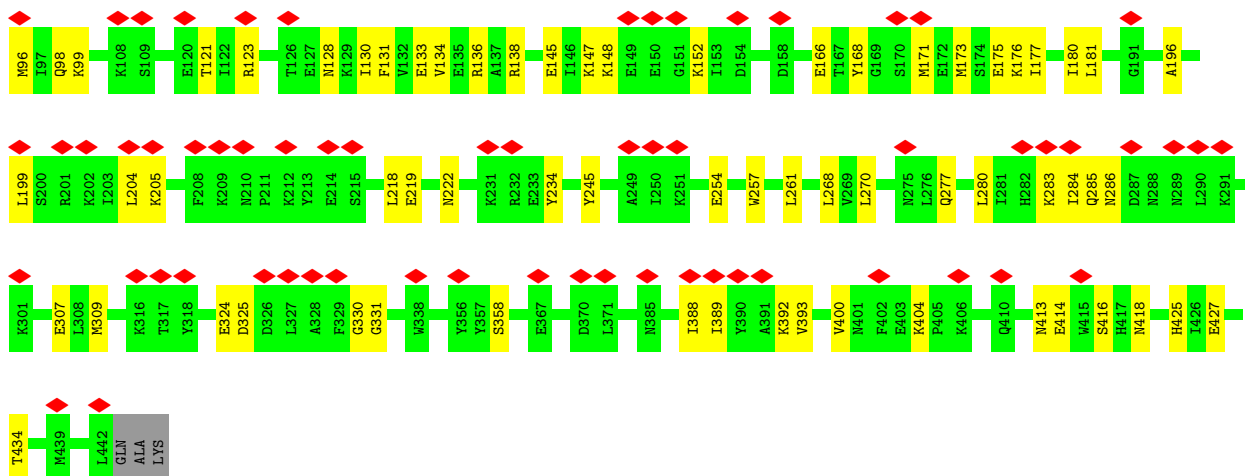
• Molecule 18: 26S protease regulatory subunit 6A



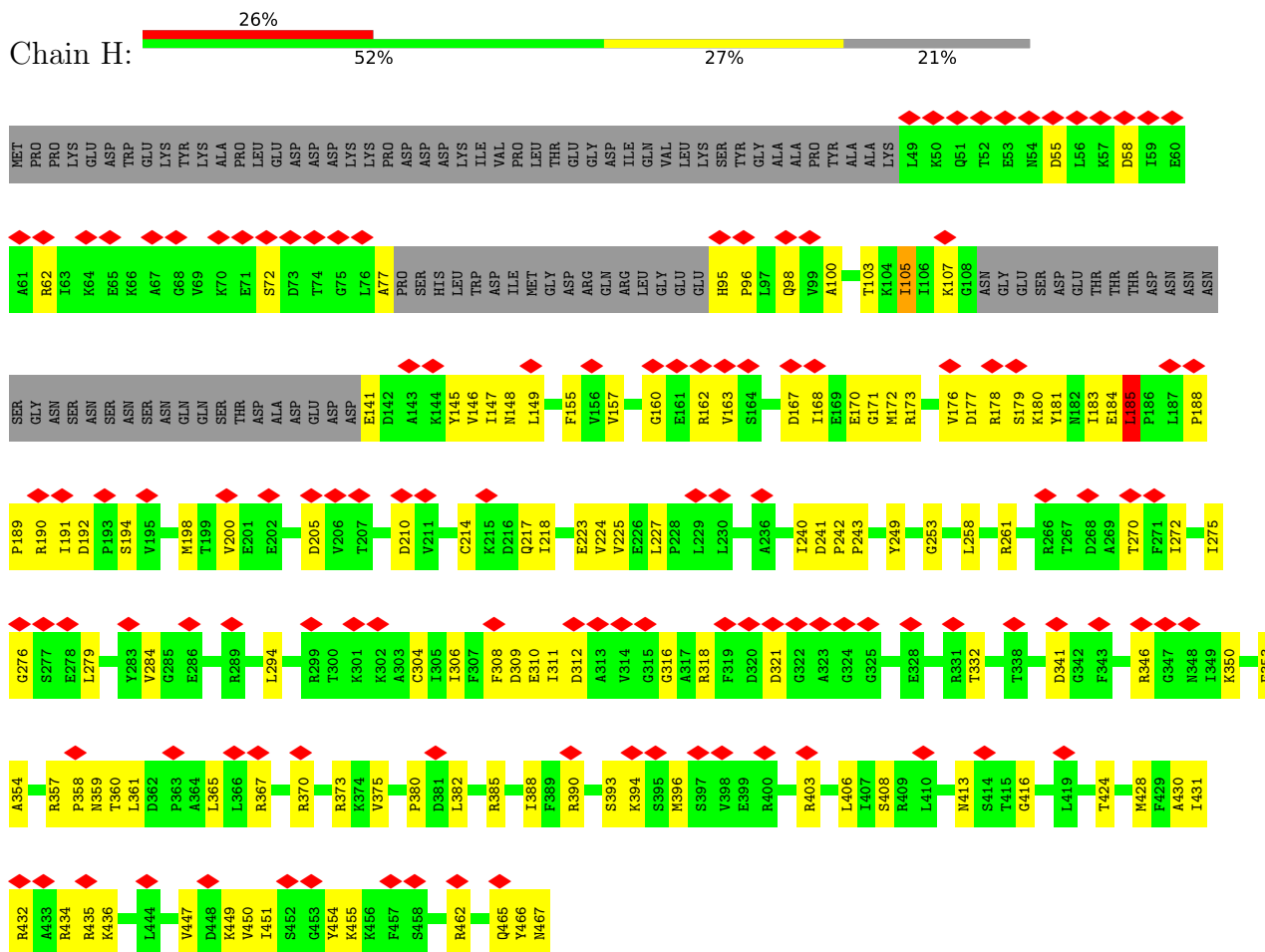
• Molecule 19: 26S proteasome regulatory subunit RPN8



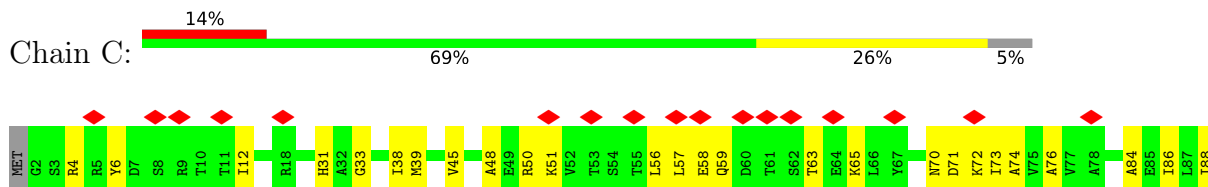


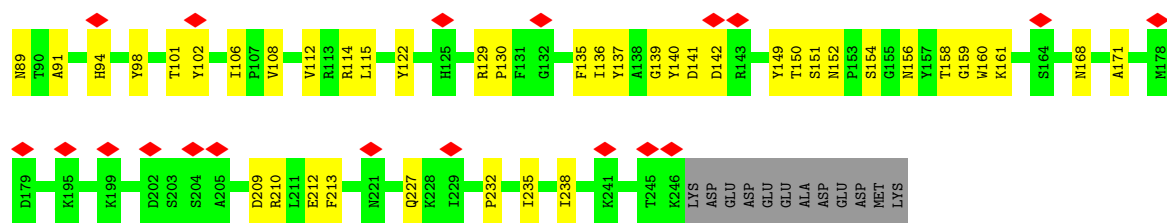


- Molecule 23: 26S protease regulatory subunit 7 homolog

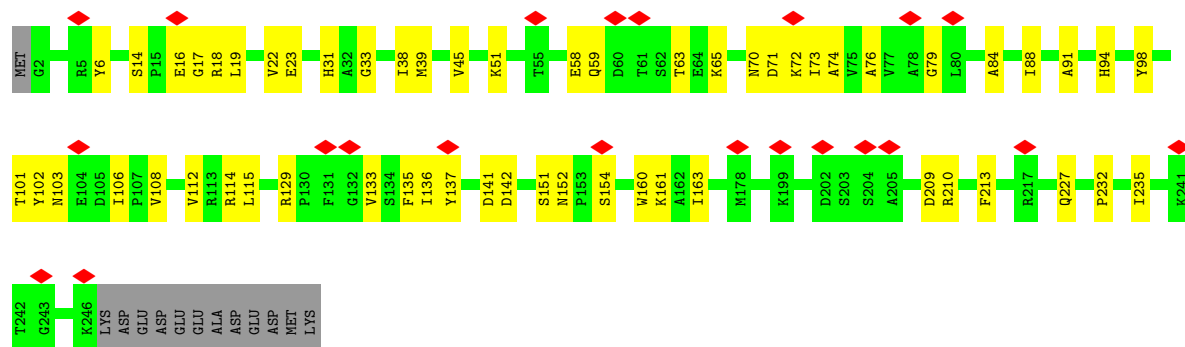
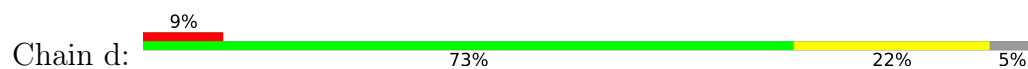


- Molecule 24: Proteasome subunit alpha type-3

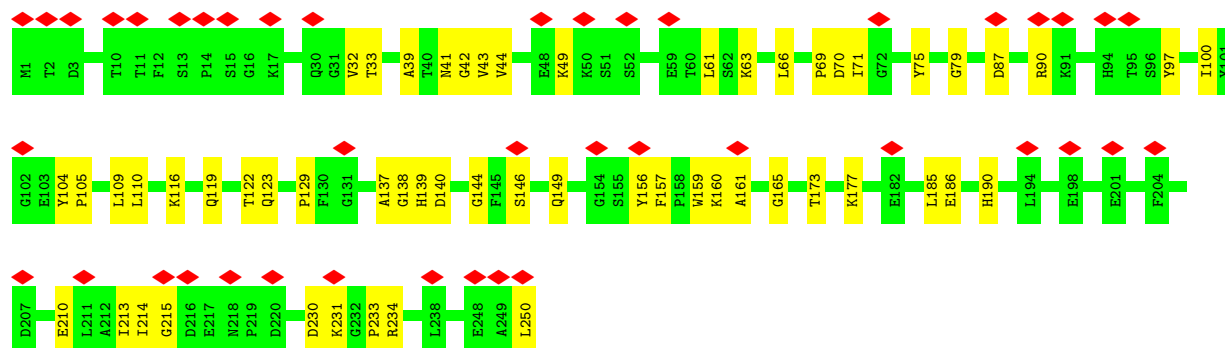
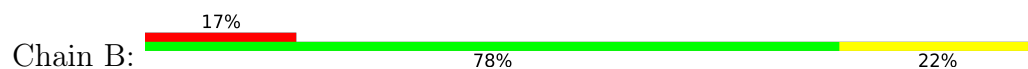




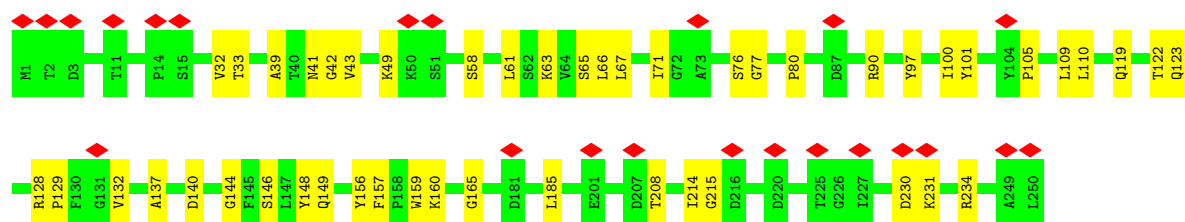
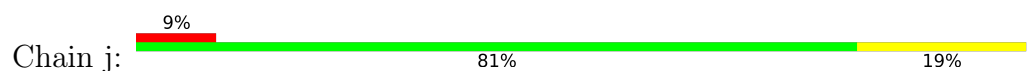
• Molecule 24: Proteasome subunit alpha type-3



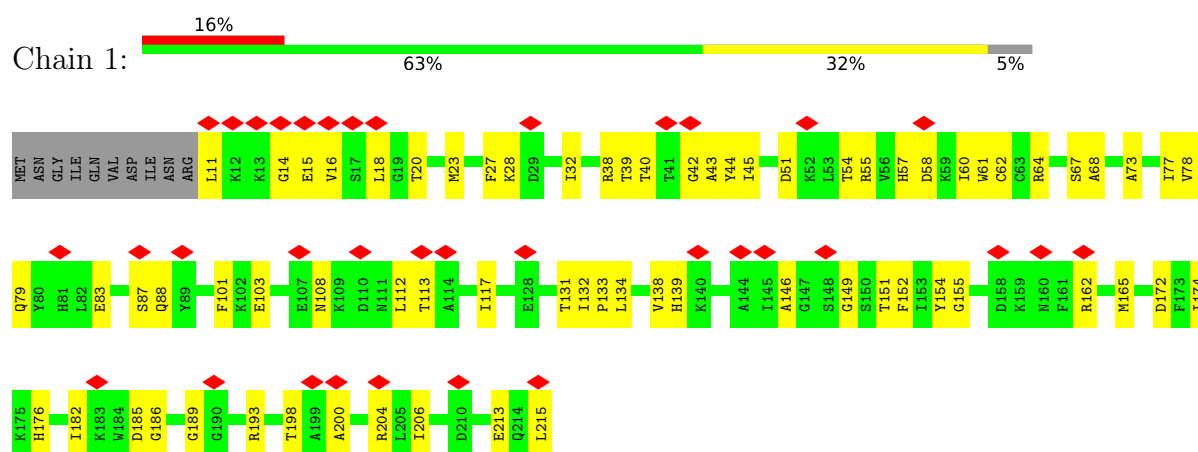
• Molecule 25: Proteasome subunit alpha type-2



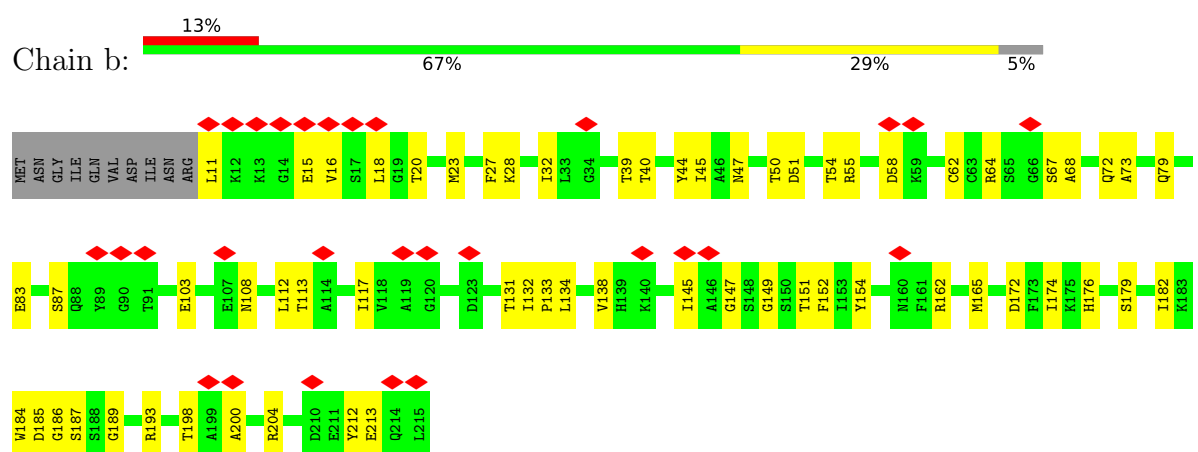
• Molecule 25: Proteasome subunit alpha type-2



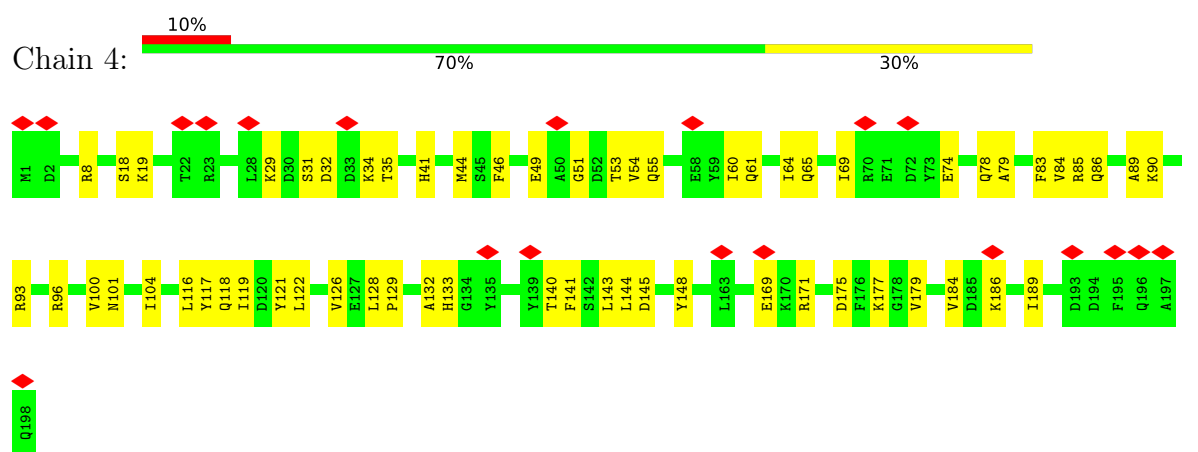
• Molecule 26: Proteasome subunit beta type-1



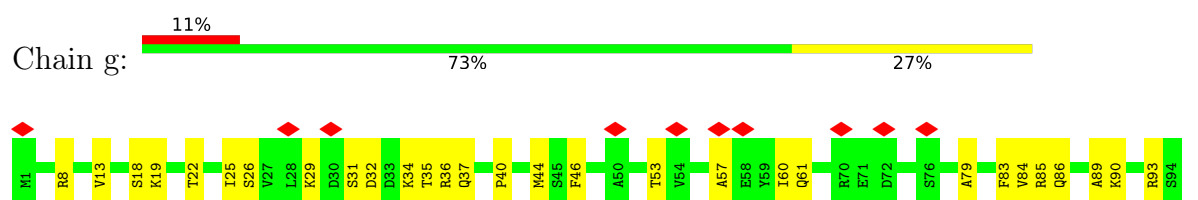
• Molecule 26: Proteasome subunit beta type-1



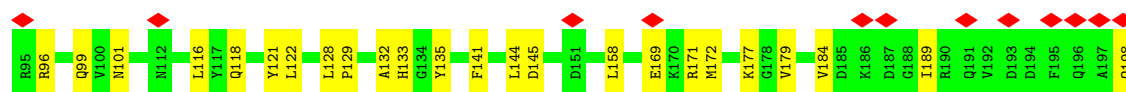
• Molecule 27: Proteasome subunit beta type-4



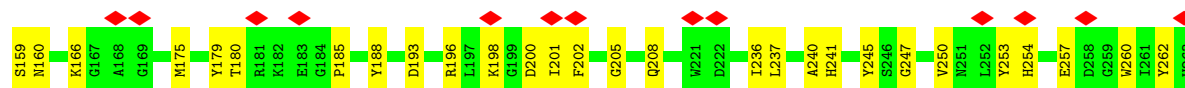
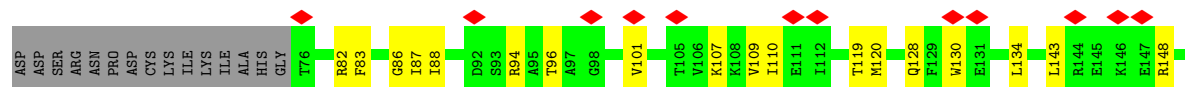
• Molecule 27: Proteasome subunit beta type-4



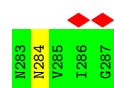
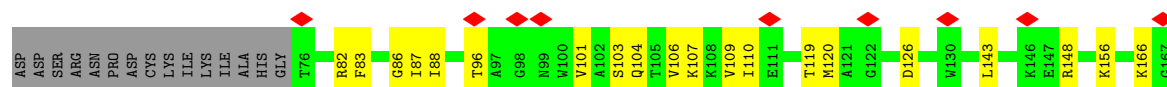
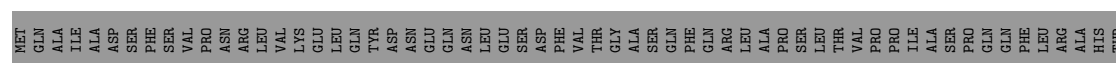




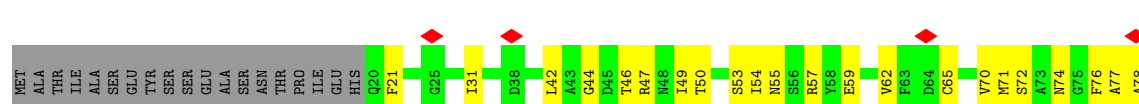
• Molecule 28: Proteasome subunit beta type-5

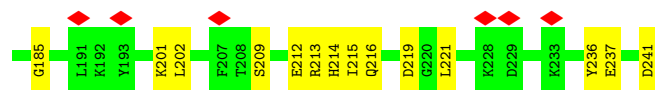


• Molecule 28: Proteasome subunit beta type-5

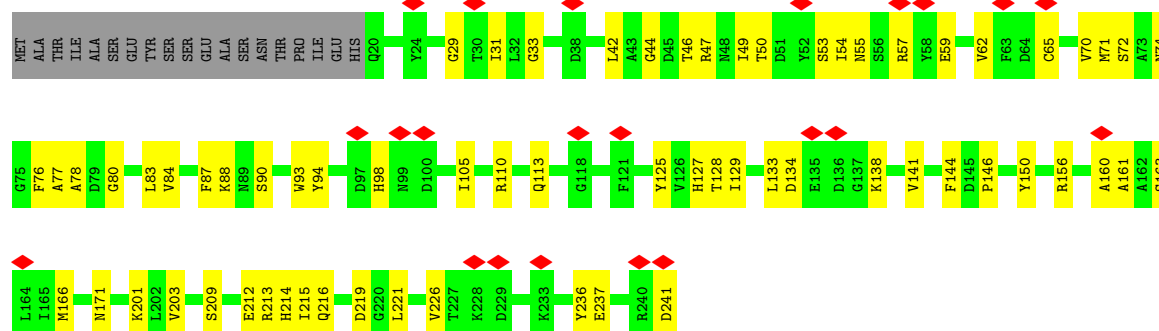


• Molecule 29: Proteasome subunit beta type-6

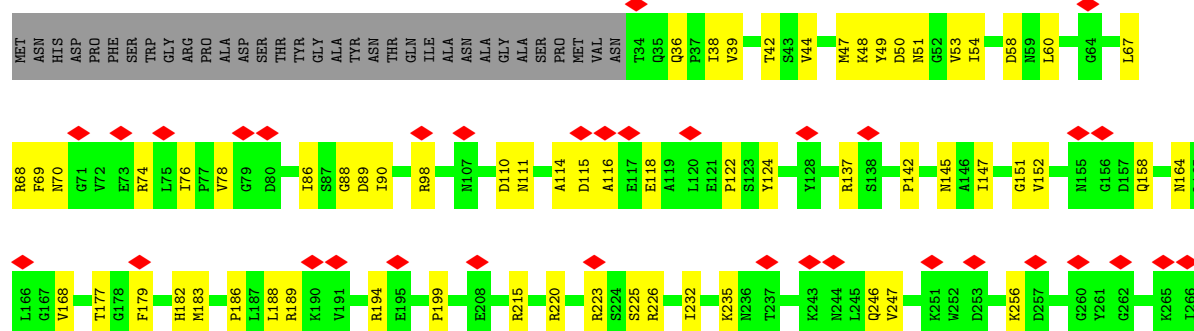




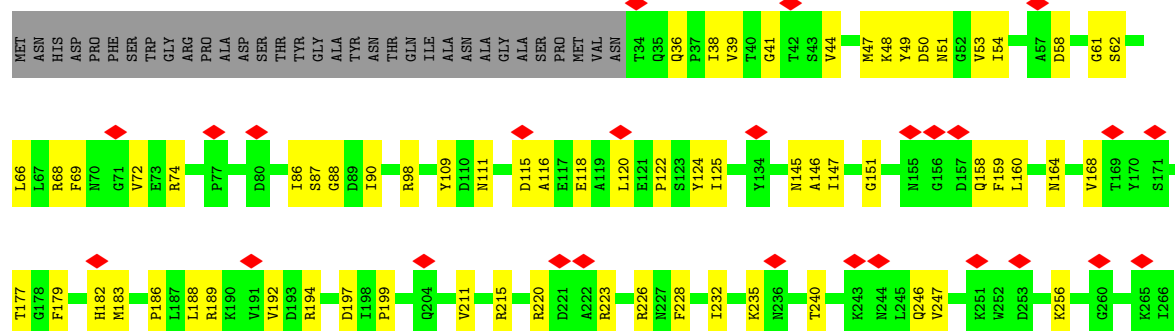
- Molecule 29: Proteasome subunit beta type-6



- Molecule 30: Proteasome subunit beta type-7

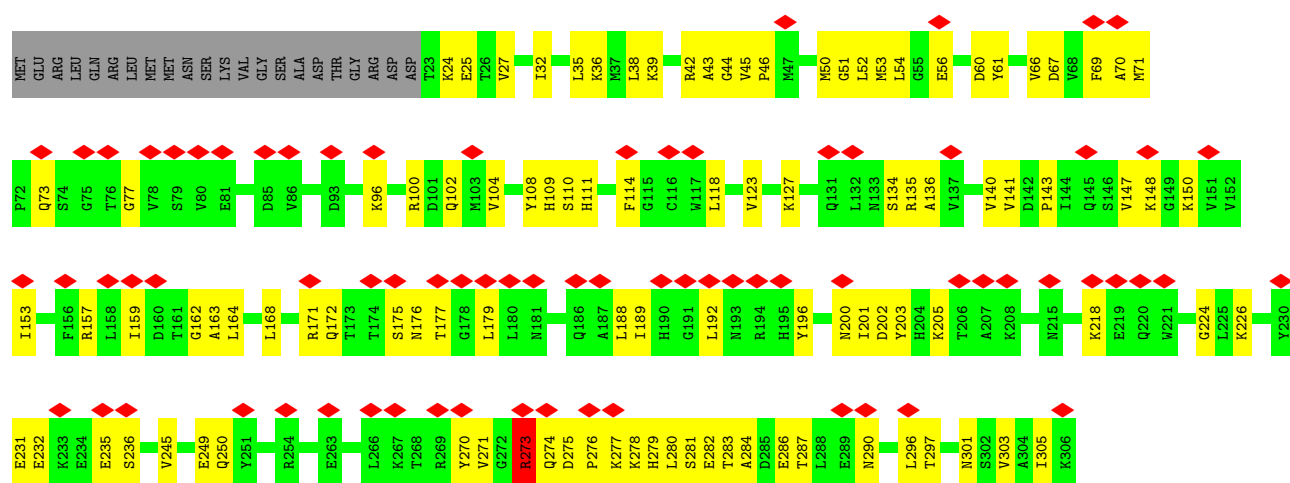
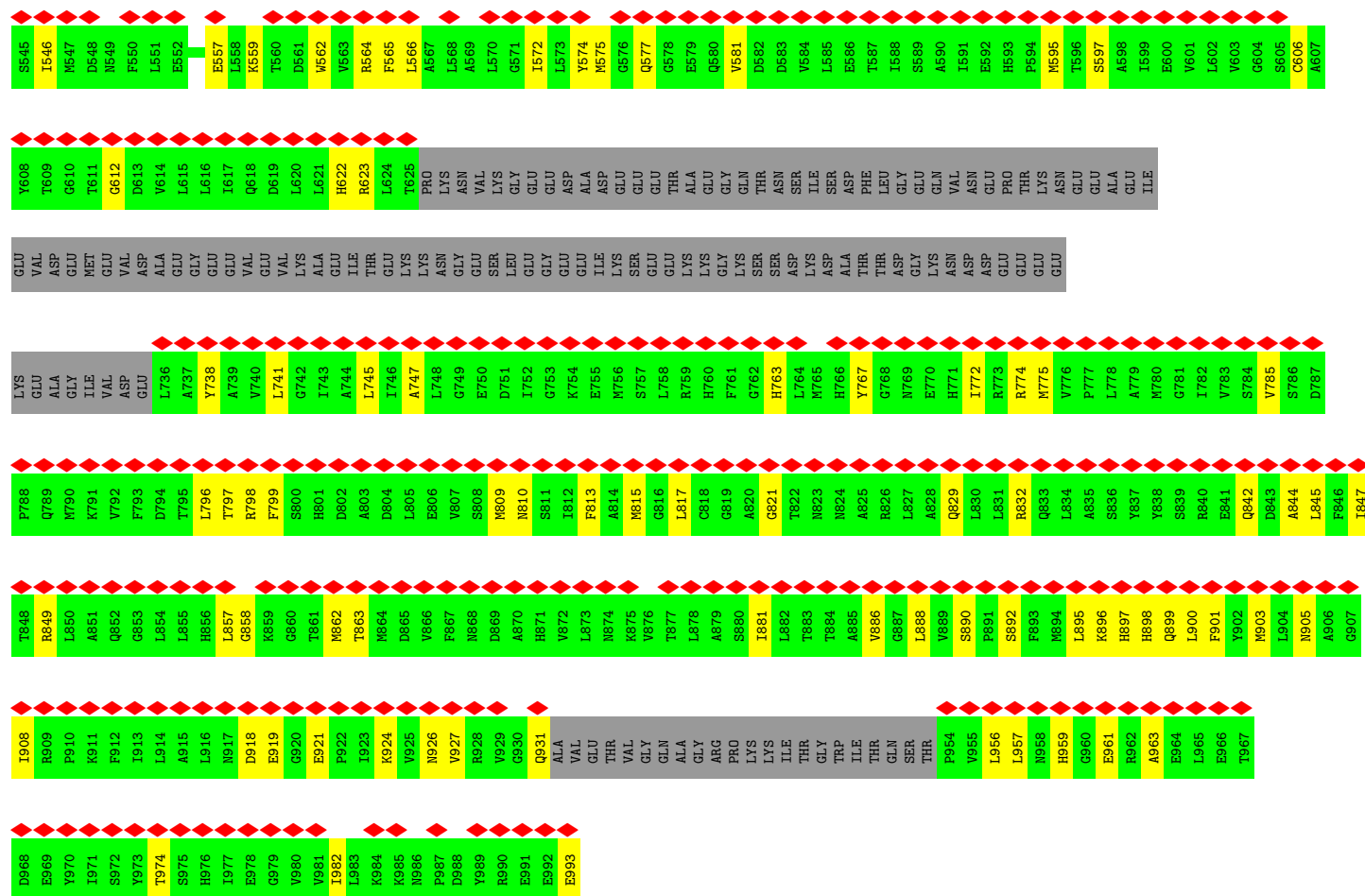


- Molecule 30: Proteasome subunit beta type-7



- Molecule 31: 26S proteasome regulatory subunit RPN13





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 26000                                   | 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 ( $e^-/\text{\AA}^2$ ) | 25                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON II (4k x 4k)                 | Depositor |
| Maximum map value                    | 2.237                                   | Depositor |
| Minimum map value                    | -1.142                                  | Depositor |
| Average map value                    | 0.012                                   | Depositor |
| Map value standard deviation         | 0.123                                   | Depositor |
| Recommended contour level            | 0.755                                   | 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 [i](#)

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

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

| Mol | Chain | Bond lengths |               | Bond angles |             |
|-----|-------|--------------|---------------|-------------|-------------|
|     |       | RMSZ         | # $ Z  > 5$   | RMSZ        | # $ Z  > 5$ |
| 1   | I     | 0.10         | 0/2860        | 0.34        | 0/3856      |
| 2   | K     | 0.11         | 0/3062        | 0.35        | 0/4132      |
| 3   | 2     | 0.07         | 0/1715        | 0.23        | 0/2326      |
| 3   | i     | 0.07         | 0/1715        | 0.22        | 0/2326      |
| 4   | A     | 0.07         | 0/1959        | 0.25        | 0/2652      |
| 4   | c     | 0.07         | 0/1959        | 0.23        | 0/2652      |
| 5   | 3     | 0.08         | 0/1611        | 0.25        | 0/2174      |
| 5   | h     | 0.09         | 0/1611        | 0.28        | 0/2174      |
| 6   | G     | 0.07         | 0/1940        | 0.23        | 0/2619      |
| 6   | k     | 0.07         | 0/1940        | 0.24        | 0/2619      |
| 7   | F     | 0.07         | 0/1823        | 0.25        | 0/2463      |
| 7   | l     | 0.07         | 0/1823        | 0.23        | 0/2463      |
| 8   | E     | 0.06         | 0/1892        | 0.22        | 0/2549      |
| 8   | m     | 0.06         | 0/1892        | 0.23        | 0/2549      |
| 9   | D     | 0.08         | 0/1928        | 0.26        | 0/2610      |
| 9   | n     | 0.07         | 0/1928        | 0.23        | 0/2610      |
| 10  | Y     | 0.07         | 0/239         | 0.21        | 0/322       |
| 11  | N     | 0.08         | 0/6670        | 0.25        | 0/9023      |
| 12  | S     | 0.08         | 0/2945        | 0.26        | 0/3976      |
| 13  | T     | 0.08         | 0/2279        | 0.27        | 0/3077      |
| 14  | R     | 0.08         | 0/3272        | 0.25        | 0/4412      |
| 15  | Q     | 0.07         | 0/3527        | 0.23        | 0/4748      |
| 16  | J     | 0.21         | 1/2964 (0.0%) | 0.28        | 0/3981      |
| 17  | L     | 0.15         | 1/2896 (0.0%) | 0.30        | 0/3895      |
| 18  | M     | 0.09         | 0/2903        | 0.30        | 0/3909      |
| 19  | U     | 0.07         | 0/2287        | 0.23        | 0/3087      |
| 20  | W     | 0.08         | 0/1557        | 0.26        | 0/2111      |
| 21  | O     | 0.08         | 0/3243        | 0.26        | 0/4374      |
| 22  | P     | 0.07         | 0/3599        | 0.24        | 0/4854      |
| 23  | H     | 0.23         | 1/2931 (0.0%) | 0.37        | 0/3941      |
| 24  | C     | 0.07         | 0/1943        | 0.23        | 0/2629      |
| 24  | d     | 0.07         | 0/1943        | 0.23        | 0/2629      |
| 25  | B     | 0.08         | 0/1952        | 0.25        | 0/2642      |
| 25  | j     | 0.08         | 0/1952        | 0.26        | 0/2642      |

| Mol | Chain | Bond lengths |                 | Bond angles |          |
|-----|-------|--------------|-----------------|-------------|----------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5  |
| 26  | 1     | 0.08         | 0/1605          | 0.31        | 0/2171   |
| 26  | b     | 0.07         | 0/1603          | 0.27        | 0/2168   |
| 27  | 4     | 0.07         | 0/1613          | 0.24        | 0/2173   |
| 27  | g     | 0.08         | 0/1613          | 0.29        | 0/2173   |
| 28  | 5     | 0.07         | 0/1681          | 0.23        | 0/2274   |
| 28  | f     | 0.06         | 0/1681          | 0.23        | 0/2274   |
| 29  | 6     | 0.07         | 0/1795          | 0.24        | 0/2420   |
| 29  | e     | 0.07         | 0/1795          | 0.24        | 0/2420   |
| 30  | 7     | 0.08         | 0/1855          | 0.25        | 0/2514   |
| 30  | a     | 0.08         | 0/1855          | 0.25        | 0/2514   |
| 31  | X     | 0.07         | 0/1058          | 0.25        | 0/1432   |
| 32  | Z     | 0.09         | 0/6403          | 0.29        | 0/8686   |
| 33  | V     | 0.13         | 0/2271          | 0.38        | 0/3064   |
| All | All   | 0.10         | 3/107588 (0.0%) | 0.27        | 0/145309 |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | I     | 0                   | 1                   |
| 5   | h     | 0                   | 1                   |
| 18  | M     | 0                   | 1                   |
| 26  | 1     | 0                   | 1                   |
| 33  | V     | 0                   | 2                   |
| All | All   | 0                   | 6                   |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 23  | H     | 185 | LEU  | C-N   | 10.56 | 1.58        | 1.33     |
| 16  | J     | 241 | ALA  | C-N   | 10.36 | 1.58        | 1.33     |
| 17  | L     | 329 | ARG  | C-N   | 6.95  | 1.50        | 1.33     |

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 26  | 1     | 42  | GLY  | Peptide |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | I     | 102 | ASN  | Peptide |
| 18  | M     | 167 | VAL  | Peptide |
| 33  | V     | 162 | GLY  | Peptide |
| 33  | V     | 273 | ARG  | Peptide |
| 5   | h     | 45  | HIS  | Peptide |

## 5.2 Too-close contacts [i](#)

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   | I     | 2822  | 0        | 2870     | 79      | 0            |
| 2   | K     | 3019  | 0        | 3084     | 100     | 0            |
| 3   | 2     | 1684  | 0        | 1685     | 37      | 0            |
| 3   | i     | 1684  | 0        | 1685     | 32      | 0            |
| 4   | A     | 1921  | 0        | 1910     | 49      | 0            |
| 4   | c     | 1921  | 0        | 1910     | 42      | 0            |
| 5   | 3     | 1581  | 0        | 1571     | 46      | 0            |
| 5   | h     | 1581  | 0        | 1571     | 62      | 0            |
| 6   | G     | 1900  | 0        | 1889     | 41      | 0            |
| 6   | k     | 1900  | 0        | 1889     | 41      | 0            |
| 7   | F     | 1795  | 0        | 1797     | 39      | 0            |
| 7   | l     | 1795  | 0        | 1797     | 41      | 0            |
| 8   | E     | 1867  | 0        | 1841     | 51      | 0            |
| 8   | m     | 1867  | 0        | 1841     | 48      | 0            |
| 9   | D     | 1899  | 0        | 1908     | 39      | 0            |
| 9   | n     | 1899  | 0        | 1908     | 43      | 0            |
| 10  | Y     | 236   | 0        | 203      | 2       | 0            |
| 11  | N     | 6562  | 0        | 6625     | 130     | 0            |
| 12  | S     | 2893  | 0        | 2937     | 55      | 0            |
| 13  | T     | 2235  | 0        | 2207     | 37      | 0            |
| 14  | R     | 3218  | 0        | 3216     | 58      | 0            |
| 15  | Q     | 3471  | 0        | 3495     | 48      | 0            |
| 16  | J     | 2928  | 0        | 3057     | 76      | 0            |
| 17  | L     | 2853  | 0        | 2926     | 78      | 0            |
| 18  | M     | 2866  | 0        | 2938     | 81      | 0            |
| 19  | U     | 2257  | 0        | 2312     | 52      | 0            |
| 20  | W     | 1534  | 0        | 1542     | 35      | 0            |
| 21  | O     | 3182  | 0        | 3207     | 59      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 22  | P     | 3545   | 0        | 3629     | 52      | 0            |
| 23  | H     | 2889   | 0        | 2964     | 108     | 0            |
| 24  | C     | 1913   | 0        | 1914     | 46      | 0            |
| 24  | d     | 1913   | 0        | 1914     | 38      | 0            |
| 25  | B     | 1915   | 0        | 1929     | 41      | 0            |
| 25  | j     | 1915   | 0        | 1929     | 37      | 0            |
| 26  | 1     | 1576   | 0        | 1552     | 48      | 0            |
| 26  | b     | 1574   | 0        | 1547     | 43      | 0            |
| 27  | 4     | 1585   | 0        | 1590     | 53      | 0            |
| 27  | g     | 1585   | 0        | 1590     | 39      | 0            |
| 28  | 5     | 1644   | 0        | 1592     | 39      | 0            |
| 28  | f     | 1644   | 0        | 1592     | 35      | 0            |
| 29  | 6     | 1757   | 0        | 1708     | 53      | 0            |
| 29  | e     | 1757   | 0        | 1708     | 53      | 0            |
| 30  | 7     | 1824   | 0        | 1829     | 48      | 0            |
| 30  | a     | 1824   | 0        | 1829     | 54      | 0            |
| 31  | X     | 1032   | 0        | 1015     | 19      | 0            |
| 32  | Z     | 6289   | 0        | 6236     | 129     | 0            |
| 33  | V     | 2236   | 0        | 2242     | 81      | 0            |
| All | All   | 105787 | 0        | 106130   | 2162    | 0            |

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

All (2162) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:N:25:LEU:HB3   | 11:N:29:ASN:HB2   | 1.63                     | 0.80              |
| 18:M:162:GLU:HG2  | 18:M:166:ARG:HG2  | 1.64                     | 0.80              |
| 5:h:133:ALA:H     | 5:h:137:ILE:HD11  | 1.47                     | 0.79              |
| 9:D:63:LYS:HE2    | 9:D:76:SER:HB2    | 1.64                     | 0.76              |
| 32:Z:233:LEU:HB3  | 32:Z:271:ILE:HD11 | 1.66                     | 0.75              |
| 4:A:61:ASP:HB3    | 4:A:64:LEU:HG     | 1.68                     | 0.75              |
| 32:Z:926:ASN:HB3  | 32:Z:956:LEU:HD22 | 1.68                     | 0.75              |
| 29:e:71:MET:HE3   | 29:e:84:VAL:HG22  | 1.69                     | 0.74              |
| 23:H:214:CYS:HA   | 23:H:217:GLN:HB3  | 1.70                     | 0.74              |
| 11:N:330:THR:HG23 | 11:N:366:THR:HG21 | 1.69                     | 0.74              |
| 18:M:170:MET:HB2  | 23:H:180:LYS:HZ3  | 1.52                     | 0.74              |
| 30:a:54:ILE:HG12  | 30:a:232:ILE:HG12 | 1.70                     | 0.74              |
| 5:h:107:PRO:HG2   | 5:h:124:PHE:H     | 1.53                     | 0.74              |
| 7:l:58:SER:HB2    | 8:m:166:ARG:HB3   | 1.69                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:h:56:LEU:HD11   | 27:g:122:LEU:HB3  | 1.70                     | 0.73              |
| 16:J:328:LEU:HB3  | 16:J:343:LEU:HD22 | 1.71                     | 0.73              |
| 1:I:218:GLY:H     | 1:I:344:ILE:HG12  | 1.53                     | 0.73              |
| 12:S:231:ALA:O    | 12:S:235:ASN:ND2  | 2.22                     | 0.73              |
| 16:J:195:LYS:NZ   | 16:J:294:THR:O    | 2.22                     | 0.73              |
| 26:b:55:ARG:O     | 26:b:79:GLN:NE2   | 2.21                     | 0.73              |
| 3:i:126:TYR:HB3   | 3:i:156:LEU:HD13  | 1.72                     | 0.71              |
| 6:k:30:ALA:HB2    | 7:l:17:GLY:HA3    | 1.72                     | 0.71              |
| 1:I:128:TYR:HB3   | 1:I:130:VAL:HG13  | 1.72                     | 0.71              |
| 11:N:341:ALA:HA   | 11:N:374:ILE:HA   | 1.72                     | 0.71              |
| 16:J:98:VAL:HA    | 16:J:122:LEU:HB3  | 1.72                     | 0.71              |
| 1:I:113:ILE:HG22  | 1:I:115:ASP:H     | 1.56                     | 0.71              |
| 2:K:211:LEU:HG    | 2:K:219:LYS:HE2   | 1.72                     | 0.71              |
| 18:M:170:MET:HB2  | 23:H:180:LYS:NZ   | 2.05                     | 0.71              |
| 5:3:56:LEU:HD11   | 27:4:122:LEU:HB3  | 1.72                     | 0.71              |
| 11:N:770:LYS:HA   | 11:N:870:ASN:HD22 | 1.56                     | 0.71              |
| 30:7:54:ILE:HG12  | 30:7:232:ILE:HG12 | 1.72                     | 0.71              |
| 5:3:29:LEU:HB3    | 5:3:37:SER:HB3    | 1.73                     | 0.71              |
| 19:U:186:LEU:HD21 | 33:V:296:LEU:HD12 | 1.72                     | 0.71              |
| 33:V:277:LYS:HG3  | 33:V:282:GLU:HB2  | 1.73                     | 0.70              |
| 11:N:884:PHE:HZ   | 11:N:897:LYS:HB2  | 1.56                     | 0.70              |
| 4:A:15:HIS:HB2    | 24:C:6:TYR:HE2    | 1.56                     | 0.70              |
| 8:E:223:THR:HG22  | 8:E:225:GLN:H     | 1.57                     | 0.70              |
| 27:4:118:GLN:NE2  | 27:4:132:ALA:O    | 2.25                     | 0.70              |
| 33:V:54:LEU:HB3   | 33:V:102:GLN:HB2  | 1.73                     | 0.70              |
| 3:i:70:ILE:HG12   | 3:i:131:GLY:HA3   | 1.73                     | 0.70              |
| 11:N:19:SER:HA    | 11:N:22:THR:HB    | 1.74                     | 0.70              |
| 13:T:200:LEU:HD12 | 13:T:201:PRO:HD2  | 1.74                     | 0.70              |
| 23:H:163:VAL:HG22 | 23:H:185:LEU:HD11 | 1.74                     | 0.70              |
| 3:2:70:ILE:HG12   | 3:2:131:GLY:HA3   | 1.74                     | 0.69              |
| 1:I:300:ARG:HB3   | 1:I:304:ARG:HE    | 1.57                     | 0.69              |
| 22:P:325:ASP:HB2  | 22:P:330:GLY:H    | 1.56                     | 0.69              |
| 1:I:358:LYS:HD3   | 1:I:384:LYS:HD3   | 1.74                     | 0.69              |
| 16:J:217:GLU:O    | 16:J:220:GLN:NE2  | 2.26                     | 0.69              |
| 25:j:97:TYR:HA    | 25:j:100:ILE:HB   | 1.75                     | 0.69              |
| 28:f:166:LYS:O    | 27:g:96:ARG:NH2   | 2.24                     | 0.69              |
| 4:A:114:CYS:SG    | 4:A:145:SER:OG    | 2.51                     | 0.69              |
| 2:K:276:SER:HB2   | 17:L:303:ARG:HG3  | 1.73                     | 0.69              |
| 8:E:52:LYS:HE3    | 8:E:218:GLN:HB2   | 1.73                     | 0.69              |
| 3:2:126:TYR:HB3   | 3:2:156:LEU:HD13  | 1.73                     | 0.69              |
| 5:3:55:GLY:HA3    | 5:3:105:VAL:HG12  | 1.75                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:j:42:GLY:HA3   | 25:j:185:LEU:HD13 | 1.74                     | 0.69              |
| 23:H:311:ILE:HD12 | 23:H:361:LEU:HD11 | 1.75                     | 0.68              |
| 26:1:11:LEU:N     | 26:1:113:THR:HG1  | 1.91                     | 0.68              |
| 2:K:180:GLN:NE2   | 2:K:339:GLU:O     | 2.20                     | 0.68              |
| 8:m:52:LYS:HE3    | 8:m:218:GLN:HB2   | 1.75                     | 0.68              |
| 22:P:90:LYS:HB3   | 22:P:130:ILE:HG12 | 1.76                     | 0.68              |
| 23:H:149:LEU:HD22 | 23:H:178:ARG:HD2  | 1.74                     | 0.68              |
| 6:G:136:THR:HB    | 6:G:151:LEU:HB3   | 1.74                     | 0.68              |
| 9:D:163:THR:HG23  | 9:D:168:SER:HB3   | 1.76                     | 0.68              |
| 11:N:6:ALA:HB1    | 11:N:45:ASP:HB2   | 1.76                     | 0.68              |
| 4:c:36:ASN:HD22   | 4:c:173:PRO:HD3   | 1.58                     | 0.68              |
| 28:5:148:ARG:NH1  | 28:5:179:TYR:O    | 2.27                     | 0.68              |
| 29:6:71:MET:HE3   | 29:6:84:VAL:HG22  | 1.75                     | 0.68              |
| 4:c:114:CYS:SG    | 4:c:145:SER:OG    | 2.52                     | 0.68              |
| 8:m:63:SER:HB2    | 9:n:158:SER:HB2   | 1.75                     | 0.68              |
| 8:m:223:THR:HG22  | 8:m:225:GLN:H     | 1.59                     | 0.68              |
| 2:K:248:GLY:O     | 2:K:252:ARG:NH1   | 2.27                     | 0.67              |
| 26:1:20:THR:HA    | 26:1:149:GLY:H    | 1.60                     | 0.67              |
| 1:I:225:PRO:O     | 16:J:306:ARG:NH1  | 2.28                     | 0.67              |
| 6:k:222:SER:O     | 6:k:225:ASN:ND2   | 2.27                     | 0.67              |
| 11:N:634:LEU:HG   | 11:N:636:SER:H    | 1.58                     | 0.67              |
| 32:Z:774:ARG:HH12 | 32:Z:886:VAL:HG13 | 1.59                     | 0.67              |
| 24:d:129:ARG:O    | 25:j:123:GLN:NE2  | 2.28                     | 0.67              |
| 19:U:198:LYS:HE2  | 21:O:378:GLU:HG3  | 1.76                     | 0.67              |
| 4:c:88:PRO:HD3    | 6:k:156:SER:HB3   | 1.77                     | 0.67              |
| 21:O:76:LEU:HB2   | 21:O:122:HIS:HB2  | 1.76                     | 0.67              |
| 6:G:222:SER:O     | 6:G:225:ASN:ND2   | 2.28                     | 0.67              |
| 2:K:187:ALA:O     | 2:K:313:LYS:NZ    | 2.27                     | 0.67              |
| 15:Q:411:SER:O    | 33:V:250:GLN:NE2  | 2.28                     | 0.67              |
| 21:O:1:MET:N      | 21:O:36:LYS:O     | 2.27                     | 0.67              |
| 16:J:320:SER:H    | 16:J:323:ALA:HB3  | 1.60                     | 0.66              |
| 5:h:29:LEU:HB3    | 5:h:37:SER:HB3    | 1.77                     | 0.66              |
| 27:4:29:LYS:HE2   | 27:4:31:SER:HB2   | 1.76                     | 0.66              |
| 1:I:196:GLU:HA    | 1:I:200:LEU:HD12  | 1.76                     | 0.66              |
| 9:n:163:THR:HG23  | 9:n:168:SER:HB3   | 1.77                     | 0.66              |
| 15:Q:75:ARG:HD2   | 15:Q:116:PHE:HB2  | 1.78                     | 0.66              |
| 5:h:49:VAL:HG11   | 5:h:109:VAL:HG13  | 1.78                     | 0.66              |
| 25:B:122:THR:HG22 | 25:B:129:PRO:HB3  | 1.76                     | 0.66              |
| 22:P:204:LEU:HG   | 22:P:205:LYS:H    | 1.60                     | 0.66              |
| 9:D:158:SER:HB2   | 8:E:63:SER:HB2    | 1.77                     | 0.66              |
| 2:K:217:THR:HG22  | 2:K:381:ALA:HB2   | 1.78                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:F:78:ALA:HB1    | 7:F:81:ALA:HB3    | 1.78                     | 0.66              |
| 33:V:114:PHE:HB2  | 33:V:118:LEU:HD23 | 1.76                     | 0.66              |
| 33:V:245:VAL:HG12 | 33:V:290:ASN:HB3  | 1.78                     | 0.66              |
| 2:K:119:VAL:H     | 16:J:70:SER:H     | 1.44                     | 0.66              |
| 2:K:132:LYS:HZ3   | 2:K:262:ARG:HD3   | 1.61                     | 0.65              |
| 6:k:40:ILE:HD11   | 6:k:196:ALA:HB2   | 1.78                     | 0.65              |
| 29:e:49:ILE:HG22  | 29:e:54:ILE:HG12  | 1.77                     | 0.65              |
| 28:5:148:ARG:NH2  | 28:5:257:GLU:O    | 2.30                     | 0.65              |
| 26:1:55:ARG:NH2   | 26:1:58:ASP:OD1   | 2.29                     | 0.65              |
| 30:a:182:HIS:HD1  | 29:e:53:SER:HG    | 1.42                     | 0.65              |
| 33:V:148:LYS:HE3  | 33:V:150:LYS:HB3  | 1.79                     | 0.65              |
| 11:N:885:ILE:HG22 | 11:N:887:ASP:H    | 1.60                     | 0.65              |
| 32:Z:453:LEU:HA   | 32:Z:492:GLY:HA2  | 1.76                     | 0.65              |
| 12:S:415:SER:OG   | 12:S:418:THR:OG1  | 2.14                     | 0.65              |
| 23:H:176:VAL:HB   | 23:H:191:ILE:H    | 1.61                     | 0.65              |
| 23:H:176:VAL:HG23 | 23:H:190:ARG:HB2  | 1.78                     | 0.65              |
| 25:B:43:VAL:HB    | 25:B:214:ILE:HB   | 1.79                     | 0.65              |
| 24:d:33:GLY:H     | 24:d:65:LYS:HE3   | 1.60                     | 0.65              |
| 33:V:54:LEU:HB2   | 33:V:67:ASP:HB3   | 1.79                     | 0.65              |
| 2:K:119:VAL:HB    | 16:J:70:SER:HB2   | 1.78                     | 0.65              |
| 26:1:51:ASP:OD2   | 26:1:204:ARG:NH2  | 2.29                     | 0.65              |
| 3:i:141:SER:HB2   | 3:i:154:LEU:HD13  | 1.78                     | 0.65              |
| 23:H:214:CYS:HB3  | 23:H:218:ILE:HG13 | 1.77                     | 0.65              |
| 23:H:276:GLY:H    | 23:H:310:GLU:HB2  | 1.61                     | 0.65              |
| 3:2:230:LYS:HB2   | 29:e:201:LYS:HD3  | 1.79                     | 0.65              |
| 32:Z:308:LYS:HB2  | 32:Z:982:ILE:HD11 | 1.79                     | 0.65              |
| 32:Z:518:LEU:HD13 | 32:Z:559:LYS:HB3  | 1.78                     | 0.65              |
| 11:N:766:GLN:O    | 11:N:921:ARG:NH2  | 2.30                     | 0.65              |
| 18:M:66:LYS:HA    | 18:M:69:ILE:HB    | 1.79                     | 0.65              |
| 33:V:273:ARG:HG3  | 33:V:274:GLN:H    | 1.62                     | 0.65              |
| 27:4:29:LYS:HG2   | 27:4:31:SER:H     | 1.61                     | 0.65              |
| 2:K:385:ALA:HB3   | 2:K:414:GLN:HE22  | 1.62                     | 0.64              |
| 16:J:67:GLU:OE2   | 16:J:116:ARG:NH2  | 2.30                     | 0.64              |
| 7:F:117:GLN:NE2   | 7:F:120:THR:OG1   | 2.30                     | 0.64              |
| 5:3:101:GLY:O     | 27:4:93:ARG:NH1   | 2.30                     | 0.64              |
| 30:7:111:ASN:HD21 | 30:7:118:GLU:HB3  | 1.61                     | 0.64              |
| 9:D:124:GLY:H     | 8:E:133:LEU:HB3   | 1.63                     | 0.64              |
| 14:R:313:ALA:HA   | 14:R:317:ILE:HD12 | 1.79                     | 0.64              |
| 27:4:169:GLU:O    | 27:g:177:LYS:NZ   | 2.30                     | 0.64              |
| 18:M:195:GLU:HA   | 18:M:199:LEU:HD12 | 1.79                     | 0.64              |
| 32:Z:253:VAL:HG13 | 32:Z:264:PHE:HD2  | 1.63                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:g:118:GLN:NE2  | 27:g:132:ALA:O    | 2.30                     | 0.64              |
| 11:N:870:ASN:OD1  | 11:N:871:MET:N    | 2.30                     | 0.64              |
| 32:Z:413:ASP:HB2  | 32:Z:898:HIS:HD2  | 1.62                     | 0.64              |
| 26:b:23:MET:HE2   | 26:b:174:ILE:HG12 | 1.80                     | 0.64              |
| 25:j:122:THR:HG22 | 25:j:129:PRO:HB3  | 1.79                     | 0.64              |
| 3:i:230:LYS:HB2   | 29:6:201:LYS:HD3  | 1.80                     | 0.64              |
| 23:H:272:ILE:HB   | 23:H:306:ILE:HG12 | 1.79                     | 0.64              |
| 26:b:182:ILE:HG23 | 26:b:189:GLY:HA2  | 1.79                     | 0.64              |
| 25:B:97:TYR:HA    | 25:B:100:ILE:HB   | 1.80                     | 0.64              |
| 27:4:184:VAL:HG22 | 27:4:189:ILE:HG12 | 1.79                     | 0.64              |
| 14:R:35:GLN:O     | 14:R:323:ASN:ND2  | 2.31                     | 0.64              |
| 24:C:76:ALA:HB3   | 24:C:136:ILE:HB   | 1.80                     | 0.64              |
| 32:Z:888:LEU:HB3  | 32:Z:901:PHE:HE1  | 1.63                     | 0.64              |
| 6:k:136:THR:HB    | 6:k:151:LEU:HB3   | 1.79                     | 0.64              |
| 21:O:239:MET:HE1  | 21:O:251:LEU:HB2  | 1.79                     | 0.64              |
| 5:3:172:LEU:HD22  | 5:3:202:MET:HB3   | 1.79                     | 0.64              |
| 30:7:38:ILE:HG22  | 30:7:39:VAL:HG23  | 1.80                     | 0.64              |
| 32:Z:317:GLN:HB3  | 32:Z:321:PHE:HB2  | 1.79                     | 0.64              |
| 11:N:339:MET:HE2  | 11:N:707:ASN:HD21 | 1.63                     | 0.63              |
| 14:R:71:LEU:HG    | 14:R:72:VAL:HG23  | 1.80                     | 0.63              |
| 19:U:120:LEU:HB3  | 19:U:137:TYR:HB2  | 1.79                     | 0.63              |
| 2:K:244:HIS:CE1   | 2:K:246:TYR:HB3   | 2.33                     | 0.63              |
| 7:l:82:ARG:O      | 7:l:86:ASN:ND2    | 2.31                     | 0.63              |
| 32:Z:537:THR:O    | 32:Z:577:GLN:NE2  | 2.30                     | 0.63              |
| 5:h:172:LEU:HD22  | 5:h:202:MET:HB3   | 1.81                     | 0.63              |
| 2:K:339:GLU:HG2   | 2:K:341:PRO:HD3   | 1.79                     | 0.63              |
| 6:G:40:ILE:HD11   | 6:G:196:ALA:HB2   | 1.81                     | 0.63              |
| 24:d:14:SER:OG    | 24:d:18:ARG:O     | 2.16                     | 0.63              |
| 5:h:109:VAL:O     | 5:h:122:ALA:N     | 2.28                     | 0.63              |
| 21:O:105:GLN:HG2  | 21:O:109:LEU:HD12 | 1.79                     | 0.63              |
| 27:4:100:VAL:H    | 27:4:121:TYR:HB3  | 1.63                     | 0.63              |
| 8:m:86:ARG:NH2    | 9:n:156:TYR:OH    | 2.32                     | 0.63              |
| 26:1:23:MET:HE2   | 26:1:174:ILE:HG12 | 1.80                     | 0.63              |
| 5:h:121:ILE:HD12  | 5:h:137:ILE:HG12  | 1.81                     | 0.63              |
| 11:N:595:LEU:HB3  | 11:N:602:VAL:HG22 | 1.81                     | 0.63              |
| 18:M:336:ALA:O    | 18:M:342:ARG:NH1  | 2.32                     | 0.63              |
| 4:c:144:VAL:HG12  | 4:c:154:ILE:HG12  | 1.80                     | 0.63              |
| 11:N:711:ARG:O    | 11:N:873:ARG:NH2  | 2.32                     | 0.63              |
| 18:M:411:LYS:HE3  | 18:M:413:GLU:HB3  | 1.79                     | 0.63              |
| 22:P:413:ASN:OD1  | 22:P:414:GLU:N    | 2.32                     | 0.63              |
| 7:F:40:SER:OG     | 7:F:43:HIS:O      | 2.15                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:4:54:VAL:HG11  | 28:5:196:ARG:H    | 1.63                     | 0.63              |
| 33:V:249:GLU:OE2  | 33:V:290:ASN:ND2  | 2.32                     | 0.63              |
| 22:P:98:GLN:OE1   | 22:P:136:ARG:NH1  | 2.32                     | 0.63              |
| 7:F:105:VAL:HB    | 7:F:145:LEU:HB2   | 1.81                     | 0.63              |
| 3:2:65:ARG:NH1    | 3:2:93:GLU:OE2    | 2.32                     | 0.63              |
| 9:D:187:THR:HB    | 9:D:190:GLU:HG2   | 1.80                     | 0.62              |
| 24:C:31:HIS:O     | 24:C:51:LYS:NZ    | 2.31                     | 0.62              |
| 30:7:226:ARG:HE   | 30:7:246:GLN:HB3  | 1.63                     | 0.62              |
| 8:m:83:ALA:O      | 9:n:118:GLN:NE2   | 2.32                     | 0.62              |
| 23:H:141:GLU:OE1  | 23:H:162:ARG:NH1  | 2.30                     | 0.62              |
| 32:Z:858:GLY:HA3  | 32:Z:862:MET:HB2  | 1.81                     | 0.62              |
| 30:a:226:ARG:HE   | 30:a:246:GLN:HB3  | 1.63                     | 0.62              |
| 26:b:20:THR:HA    | 26:b:149:GLY:H    | 1.65                     | 0.62              |
| 29:e:50:THR:OG1   | 29:e:55:ASN:ND2   | 2.31                     | 0.62              |
| 1:I:294:SER:O     | 1:I:303:GLN:NE2   | 2.31                     | 0.62              |
| 14:R:168:ILE:HD11 | 16:J:333:ARG:HH22 | 1.64                     | 0.62              |
| 17:L:183:ILE:HD13 | 17:L:230:LEU:HB2  | 1.81                     | 0.62              |
| 22:P:131:PHE:CZ   | 22:P:133:GLU:HB3  | 2.34                     | 0.62              |
| 22:P:147:LYS:HB3  | 22:P:152:LYS:HB2  | 1.80                     | 0.62              |
| 4:A:105:ARG:HG3   | 4:A:109:GLY:HA2   | 1.82                     | 0.62              |
| 7:F:82:ARG:O      | 7:F:86:ASN:ND2    | 2.32                     | 0.62              |
| 11:N:545:SER:OG   | 11:N:580:ASN:ND2  | 2.32                     | 0.62              |
| 11:N:614:ASN:OD1  | 11:N:615:ALA:N    | 2.33                     | 0.62              |
| 19:U:54:LEU:HG    | 19:U:73:ILE:HD13  | 1.82                     | 0.62              |
| 2:K:95:VAL:O      | 2:K:139:LEU:N     | 2.32                     | 0.62              |
| 4:c:15:HIS:HB2    | 24:d:6:TYR:HE2    | 1.63                     | 0.62              |
| 19:U:201:GLN:NE2  | 21:O:375:ASP:OD1  | 2.33                     | 0.62              |
| 23:H:224:VAL:HG22 | 23:H:243:PRO:HG2  | 1.81                     | 0.62              |
| 30:7:58:ASP:OD1   | 30:7:74:ARG:NH2   | 2.33                     | 0.62              |
| 30:a:111:ASN:HD21 | 30:a:118:GLU:HB3  | 1.64                     | 0.62              |
| 29:e:125:TYR:HD1  | 29:e:146:PRO:HB3  | 1.63                     | 0.62              |
| 23:H:436:LYS:NZ   | 32:Z:959:HIS:O    | 2.32                     | 0.62              |
| 24:C:70:ASN:OD1   | 24:C:71:ASP:N     | 2.32                     | 0.62              |
| 3:2:50:THR:HG22   | 3:2:55:VAL:HG22   | 1.82                     | 0.62              |
| 6:k:68:GLN:OE1    | 6:k:93:ARG:NH2    | 2.33                     | 0.61              |
| 11:N:325:PHE:HE1  | 33:V:24:LYS:HD3   | 1.65                     | 0.61              |
| 13:T:107:SER:HB3  | 13:T:142:LEU:HD23 | 1.82                     | 0.61              |
| 16:J:245:ILE:HB   | 16:J:290:ILE:HG12 | 1.82                     | 0.61              |
| 21:O:341:ILE:HG12 | 21:O:348:VAL:HG13 | 1.82                     | 0.61              |
| 2:K:174:VAL:O     | 2:K:181:LYS:NZ    | 2.34                     | 0.61              |
| 23:H:184:GLU:OE1  | 23:H:190:ARG:NE   | 2.32                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:N:230:VAL:HG11 | 11:N:724:THR:HG21 | 1.81                     | 0.61              |
| 12:S:284:LEU:HA   | 12:S:382:ARG:HH21 | 1.65                     | 0.61              |
| 14:R:24:TYR:HB2   | 14:R:242:GLU:HA   | 1.81                     | 0.61              |
| 4:A:86:PRO:HG2    | 4:A:89:ASP:HB2    | 1.82                     | 0.61              |
| 24:C:102:TYR:HB3  | 27:4:79:ALA:HB1   | 1.81                     | 0.61              |
| 24:d:76:ALA:HB3   | 24:d:136:ILE:HB   | 1.80                     | 0.61              |
| 33:V:277:LYS:HD2  | 33:V:281:SER:HB2  | 1.83                     | 0.61              |
| 2:K:300:LEU:HA    | 2:K:333:ARG:HE    | 1.64                     | 0.61              |
| 2:K:344:ARG:O     | 2:K:349:ARG:NH1   | 2.33                     | 0.61              |
| 30:a:88:GLY:HA3   | 30:a:145:ASN:HA   | 1.82                     | 0.61              |
| 7:l:52:ASN:ND2    | 7:l:54:ASP:O      | 2.33                     | 0.61              |
| 9:n:187:THR:HB    | 9:n:190:GLU:HG2   | 1.83                     | 0.61              |
| 17:L:357:ARG:HD2  | 17:L:391:ILE:HD11 | 1.81                     | 0.61              |
| 26:1:182:ILE:HG23 | 26:1:189:GLY:HA2  | 1.82                     | 0.61              |
| 23:H:403:ARG:NH2  | 8:E:206:GLN:OE1   | 2.34                     | 0.61              |
| 23:H:462:ARG:O    | 23:H:465:GLN:NE2  | 2.33                     | 0.61              |
| 32:Z:564:ARG:NH2  | 32:Z:595:MET:SD   | 2.73                     | 0.61              |
| 2:K:281:ARG:NH2   | 17:L:300:GLU:OE2  | 2.34                     | 0.61              |
| 22:P:181:LEU:HD13 | 22:P:219:GLU:HG2  | 1.83                     | 0.61              |
| 8:m:116:VAL:O     | 8:m:120:ALA:N     | 2.32                     | 0.61              |
| 16:J:78:ILE:HG22  | 16:J:84:VAL:HG23  | 1.82                     | 0.61              |
| 29:6:47:ARG:NH1   | 29:6:215:ILE:O    | 2.34                     | 0.61              |
| 1:I:340:ARG:HH11  | 1:I:343:ARG:HG2   | 1.66                     | 0.61              |
| 5:h:67:PHE:HE1    | 5:h:91:VAL:HG22   | 1.65                     | 0.61              |
| 5:h:91:VAL:HG11   | 5:h:107:PRO:HG3   | 1.82                     | 0.60              |
| 15:Q:263:LYS:HG2  | 15:Q:299:MET:HG3  | 1.83                     | 0.60              |
| 16:J:220:GLN:HG3  | 16:J:225:GLU:HB2  | 1.83                     | 0.60              |
| 31:X:37:PRO:HA    | 31:X:46:TRP:HA    | 1.83                     | 0.60              |
| 32:Z:436:LEU:HD21 | 32:Z:455:ILE:HA   | 1.83                     | 0.60              |
| 28:f:272:PHE:HZ   | 28:f:282:PHE:HB2  | 1.66                     | 0.60              |
| 1:I:315:GLY:O     | 23:H:261:ARG:NH1  | 2.35                     | 0.60              |
| 3:i:228:LYS:HE2   | 3:i:231:SER:HA    | 1.82                     | 0.60              |
| 11:N:608:LEU:HD23 | 11:N:611:LYS:HD2  | 1.83                     | 0.60              |
| 20:W:161:VAL:O    | 20:W:163:ASN:ND2  | 2.34                     | 0.60              |
| 25:B:97:TYR:HB2   | 25:B:105:PRO:HD3  | 1.83                     | 0.60              |
| 27:g:19:LYS:HB3   | 27:g:31:SER:HA    | 1.83                     | 0.60              |
| 2:K:268:ILE:HA    | 2:K:313:LYS:HB2   | 1.84                     | 0.60              |
| 17:L:354:GLU:HB2  | 17:L:380:VAL:HG11 | 1.81                     | 0.60              |
| 24:C:63:THR:O     | 25:B:156:TYR:OH   | 2.20                     | 0.60              |
| 5:3:58:THR:OG1    | 27:4:122:LEU:O    | 2.19                     | 0.60              |
| 24:d:74:ALA:HB2   | 24:d:227:GLN:HE22 | 1.65                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:k:116:LEU:HB3   | 6:k:151:LEU:HD22  | 1.84                     | 0.60              |
| 19:U:124:ASP:H    | 19:U:127:GLN:HE21 | 1.47                     | 0.60              |
| 20:W:150:ASN:OD1  | 20:W:151:THR:N    | 2.34                     | 0.60              |
| 25:B:100:ILE:HG23 | 5:3:90:LEU:HD13   | 1.82                     | 0.60              |
| 1:I:319:ARG:HH22  | 32:Z:829:GLN:HG2  | 1.66                     | 0.60              |
| 4:c:86:PRO:HG2    | 4:c:89:ASP:HB2    | 1.83                     | 0.60              |
| 5:h:50:PHE:HZ     | 5:h:195:VAL:HG21  | 1.66                     | 0.60              |
| 7:F:129:GLY:HA2   | 7:F:149:PRO:HB3   | 1.82                     | 0.60              |
| 11:N:778:LYS:HE2  | 11:N:780:ASP:HB2  | 1.84                     | 0.60              |
| 17:L:197:ILE:HA   | 17:L:322:LYS:HE3  | 1.83                     | 0.60              |
| 18:M:132:VAL:HG12 | 18:M:134:LEU:H    | 1.66                     | 0.60              |
| 18:M:402:ALA:HB1  | 18:M:407:GLN:HB2  | 1.83                     | 0.60              |
| 19:U:116:ASN:OD1  | 19:U:117:ASN:N    | 2.29                     | 0.60              |
| 32:Z:213:LYS:HE2  | 32:Z:240:ASN:HB2  | 1.83                     | 0.60              |
| 25:j:49:LYS:NZ    | 25:j:58:SER:O     | 2.34                     | 0.60              |
| 9:n:29:ARG:HE     | 24:d:17:GLY:HA3   | 1.66                     | 0.60              |
| 11:N:778:LYS:NZ   | 11:N:861:TYR:OH   | 2.35                     | 0.60              |
| 22:P:176:LYS:HE2  | 22:P:180:ILE:HD11 | 1.84                     | 0.60              |
| 4:A:86:PRO:HD2    | 4:A:139:VAL:HG22  | 1.83                     | 0.60              |
| 30:a:164:ASN:OD1  | 30:a:168:VAL:N    | 2.34                     | 0.60              |
| 4:c:141:LEU:HB2   | 4:c:157:THR:HB    | 1.84                     | 0.60              |
| 32:Z:844:ALA:HA   | 32:Z:847:ILE:HD12 | 1.83                     | 0.60              |
| 5:h:11:ILE:HG21   | 5:h:142:ALA:HB3   | 1.83                     | 0.60              |
| 11:N:456:GLY:H    | 11:N:490:LEU:HD12 | 1.67                     | 0.60              |
| 6:G:70:VAL:N      | 6:G:74:ILE:O      | 2.35                     | 0.60              |
| 11:N:668:THR:HG22 | 11:N:671:LEU:HD12 | 1.84                     | 0.60              |
| 24:d:19:LEU:HB2   | 24:d:22:VAL:HG23  | 1.82                     | 0.60              |
| 26:b:117:ILE:HG12 | 26:b:131:THR:HG23 | 1.84                     | 0.60              |
| 14:R:139:GLU:OE1  | 14:R:176:ARG:NH2  | 2.34                     | 0.59              |
| 20:W:97:THR:HA    | 20:W:100:HIS:HD2  | 1.66                     | 0.59              |
| 4:A:144:VAL:HG12  | 4:A:154:ILE:HG12  | 1.84                     | 0.59              |
| 25:B:119:GLN:NE2  | 25:B:122:THR:OG1  | 2.35                     | 0.59              |
| 32:Z:337:GLU:HB3  | 32:Z:340:LEU:HA   | 1.84                     | 0.59              |
| 25:j:43:VAL:HB    | 25:j:214:ILE:HB   | 1.84                     | 0.59              |
| 28:f:96:THR:HG22  | 28:f:101:VAL:HG22 | 1.83                     | 0.59              |
| 33:V:188:LEU:HB3  | 33:V:192:LEU:HD12 | 1.83                     | 0.59              |
| 7:l:21:GLN:NE2    | 8:m:13:SER:O      | 2.35                     | 0.59              |
| 18:M:288:THR:HG23 | 23:H:321:ASP:HB3  | 1.84                     | 0.59              |
| 32:Z:543:THR:HG1  | 32:Z:574:TYR:HH   | 1.46                     | 0.59              |
| 29:e:134:ASP:OD1  | 29:e:138:LYS:N    | 2.34                     | 0.59              |
| 11:N:324:LYS:HD2  | 11:N:360:GLN:HE21 | 1.67                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:Q:3:LEU:HD12   | 15:Q:4:PRO:HD2    | 1.84                     | 0.59              |
| 23:H:360:THR:HG22 | 23:H:467:ASN:HD22 | 1.68                     | 0.59              |
| 4:A:220:LYS:HB3   | 4:A:242:GLU:HB2   | 1.83                     | 0.59              |
| 5:3:50:PHE:HZ     | 5:3:195:VAL:HG11  | 1.67                     | 0.59              |
| 5:3:62:THR:OG1    | 27:4:85:ARG:NH1   | 2.35                     | 0.59              |
| 27:4:19:LYS:HB3   | 27:4:31:SER:HA    | 1.85                     | 0.59              |
| 32:Z:905:ASN:HA   | 32:Z:908:ILE:HD12 | 1.85                     | 0.59              |
| 30:a:194:ARG:NH1  | 29:e:237:GLU:OE2  | 2.35                     | 0.59              |
| 5:h:13:VAL:HA     | 5:h:138:VAL:HG12  | 1.84                     | 0.59              |
| 15:Q:170:ASP:O    | 15:Q:174:LEU:N    | 2.35                     | 0.59              |
| 16:J:75:VAL:HG22  | 16:J:86:VAL:HG22  | 1.84                     | 0.59              |
| 18:M:252:VAL:HG12 | 23:H:284:VAL:HG11 | 1.84                     | 0.59              |
| 8:E:10:ARG:HE     | 8:E:14:THR:HG21   | 1.67                     | 0.59              |
| 26:1:45:ILE:HB    | 30:a:220:ARG:HA   | 1.85                     | 0.59              |
| 26:1:117:ILE:HG12 | 26:1:131:THR:HG23 | 1.83                     | 0.59              |
| 32:Z:212:LEU:O    | 32:Z:244:ARG:NH2  | 2.35                     | 0.59              |
| 32:Z:546:ILE:HG23 | 32:Z:566:LEU:HD13 | 1.84                     | 0.59              |
| 29:e:47:ARG:NH2   | 29:e:241:ASP:OD1  | 2.36                     | 0.59              |
| 1:I:151:HIS:CD2   | 1:I:152:LYS:HG3   | 2.38                     | 0.59              |
| 11:N:685:VAL:HG13 | 11:N:691:GLN:HG3  | 1.84                     | 0.59              |
| 14:R:263:ARG:NH2  | 15:Q:383:ASP:OD1  | 2.33                     | 0.59              |
| 29:6:134:ASP:OD1  | 29:6:138:LYS:N    | 2.35                     | 0.59              |
| 32:Z:376:SER:H    | 32:Z:409:LYS:HZ2  | 1.48                     | 0.59              |
| 7:l:78:ALA:HB1    | 7:l:81:ALA:HB3    | 1.84                     | 0.59              |
| 14:R:235:LEU:O    | 16:J:376:HIS:NE2  | 2.34                     | 0.59              |
| 17:L:228:LYS:HE2  | 17:L:326:ALA:HB1  | 1.85                     | 0.59              |
| 1:I:168:VAL:O     | 16:J:231:ARG:NH2  | 2.35                     | 0.59              |
| 1:I:188:GLU:HA    | 1:I:191:ILE:HB    | 1.83                     | 0.59              |
| 3:i:50:THR:HG22   | 3:i:55:VAL:HG22   | 1.85                     | 0.59              |
| 11:N:454:ALA:HB1  | 11:N:488:CYS:HA   | 1.83                     | 0.59              |
| 7:F:52:ASN:ND2    | 7:F:54:ASP:O      | 2.36                     | 0.59              |
| 27:4:34:LYS:HB3   | 27:4:46:PHE:HB2   | 1.85                     | 0.59              |
| 25:j:32:VAL:HG11  | 25:j:63:LYS:HE3   | 1.85                     | 0.59              |
| 11:N:774:ASN:HA   | 11:N:867:LYS:HA   | 1.85                     | 0.59              |
| 12:S:449:LEU:HA   | 14:R:397:ASN:HD21 | 1.68                     | 0.59              |
| 22:P:80:THR:HG22  | 22:P:84:LYS:HE3   | 1.85                     | 0.59              |
| 24:d:18:ARG:NH2   | 24:d:23:GLU:OE2   | 2.36                     | 0.59              |
| 26:b:51:ASP:OD2   | 26:b:204:ARG:NH2  | 2.36                     | 0.59              |
| 24:d:63:THR:O     | 25:j:156:TYR:OH   | 2.21                     | 0.59              |
| 11:N:650:ASP:HB3  | 11:N:694:LEU:HD23 | 1.83                     | 0.59              |
| 23:H:311:ILE:HD13 | 23:H:353:PHE:HB3  | 1.85                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 27:4:18:SER:HA   | 27:4:179:VAL:HG12 | 1.84                     | 0.59              |
| 32:Z:772:ILE:HA  | 32:Z:775:MET:HE3  | 1.83                     | 0.59              |
| 1:I:148:LEU:HB2  | 1:I:158:GLY:H     | 1.68                     | 0.58              |
| 11:N:897:LYS:NZ  | 11:N:904:VAL:O    | 2.35                     | 0.58              |
| 12:S:302:HIS:HB2 | 12:S:305:LYS:HB2  | 1.84                     | 0.58              |
| 17:L:348:GLU:HG3 | 17:L:350:PRO:HD3  | 1.85                     | 0.58              |
| 17:L:420:ARG:NH2 | 6:G:177:GLU:OE2   | 2.36                     | 0.58              |
| 25:j:97:TYR:HD2  | 25:j:105:PRO:HB3  | 1.66                     | 0.58              |
| 26:b:55:ARG:NH2  | 26:b:58:ASP:OD1   | 2.33                     | 0.58              |
| 24:C:152:ASN:ND2 | 24:C:154:SER:OG   | 2.36                     | 0.58              |
| 1:I:129:TYR:CZ   | 23:H:77:ALA:HA    | 2.38                     | 0.58              |
| 11:N:297:ASP:HB3 | 11:N:921:ARG:HB2  | 1.85                     | 0.58              |
| 22:P:254:GLU:HA  | 22:P:257:TRP:HB3  | 1.84                     | 0.58              |
| 26:l:54:THR:HB   | 26:l:62:CYS:HB3   | 1.84                     | 0.58              |
| 5:h:58:THR:OG1   | 27:g:122:LEU:O    | 2.19                     | 0.58              |
| 5:h:102:PRO:O    | 27:g:93:ARG:NH2   | 2.31                     | 0.58              |
| 30:7:122:PRO:HG2 | 30:7:151:GLY:HA3  | 1.85                     | 0.58              |
| 29:e:46:THR:HB   | 29:e:59:GLU:H     | 1.66                     | 0.58              |
| 27:g:19:LYS:HB3  | 27:g:32:ASP:H     | 1.67                     | 0.58              |
| 5:h:48:HIS:CD2   | 5:h:49:VAL:HG23   | 2.39                     | 0.58              |
| 14:R:44:LYS:HD3  | 14:R:88:LEU:HD12  | 1.86                     | 0.58              |
| 6:G:41:LYS:HD3   | 6:G:161:LYS:HA    | 1.85                     | 0.58              |
| 24:C:38:ILE:O    | 24:C:45:VAL:N     | 2.36                     | 0.58              |
| 30:7:164:ASN:OD1 | 30:7:168:VAL:N    | 2.35                     | 0.58              |
| 33:V:297:THR:OG1 | 33:V:301:ASN:ND2  | 2.37                     | 0.58              |
| 18:M:149:ASN:OD1 | 18:M:150:LYS:N    | 2.36                     | 0.58              |
| 22:P:52:LEU:HD21 | 22:P:56:LYS:HD3   | 1.85                     | 0.58              |
| 22:P:89:LEU:HG   | 22:P:91:LEU:H     | 1.68                     | 0.58              |
| 2:K:281:ARG:NH2  | 2:K:288:SER:O     | 2.35                     | 0.58              |
| 6:k:58:LEU:HD23  | 7:l:176:LEU:HD22  | 1.86                     | 0.58              |
| 6:k:70:VAL:N     | 6:k:74:ILE:O      | 2.35                     | 0.58              |
| 7:l:95:SER:O     | 7:l:100:ASN:N     | 2.37                     | 0.58              |
| 8:m:93:ARG:HD3   | 28:f:143:LEU:HD22 | 1.86                     | 0.58              |
| 8:m:138:PHE:HB2  | 8:m:160:PRO:HA    | 1.85                     | 0.58              |
| 11:N:25:LEU:HA   | 11:N:28:ILE:HB    | 1.84                     | 0.58              |
| 14:R:37:LYS:HG3  | 14:R:38:VAL:HG23  | 1.86                     | 0.58              |
| 22:P:94:GLN:HG2  | 22:P:131:PHE:HD1  | 1.69                     | 0.58              |
| 25:B:90:ARG:HD3  | 3:2:94:LEU:HD22   | 1.84                     | 0.58              |
| 28:5:166:LYS:NZ  | 28:5:193:ASP:OD1  | 2.36                     | 0.58              |
| 29:6:77:ALA:HB3  | 30:7:168:VAL:HA   | 1.86                     | 0.58              |
| 30:a:58:ASP:OD1  | 30:a:74:ARG:NH2   | 2.36                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:L:84:LEU:HD22  | 18:M:59:LEU:HD13  | 1.84                     | 0.58              |
| 20:W:73:LEU:HD23  | 20:W:76:LEU:HD12  | 1.84                     | 0.58              |
| 3:2:143:HIS:HB2   | 3:2:147:SER:HB3   | 1.85                     | 0.58              |
| 3:2:196:LEU:HB3   | 29:e:215:ILE:HB   | 1.86                     | 0.58              |
| 32:Z:518:LEU:HD12 | 32:Z:557:GLU:HA   | 1.86                     | 0.58              |
| 5:h:151:GLU:HB3   | 29:6:209:SER:HB3  | 1.86                     | 0.58              |
| 11:N:261:LEU:HA   | 11:N:264:SER:HB2  | 1.86                     | 0.58              |
| 1:I:435:LEU:HB2   | 9:D:79:ASN:HD21   | 1.69                     | 0.58              |
| 13:T:253:GLU:OE2  | 21:O:376:GLN:NE2  | 2.37                     | 0.58              |
| 17:L:192:GLU:OE2  | 17:L:345:ARG:NH1  | 2.36                     | 0.58              |
| 24:C:58:GLU:HB2   | 25:B:160:LYS:HG3  | 1.86                     | 0.58              |
| 26:1:55:ARG:O     | 26:1:79:GLN:NE2   | 2.33                     | 0.58              |
| 24:d:102:TYR:HB3  | 27:g:79:ALA:HB1   | 1.86                     | 0.58              |
| 11:N:307:LYS:HG3  | 11:N:710:GLY:HA3  | 1.86                     | 0.57              |
| 17:L:132:ARG:HD3  | 17:L:156:MET:HA   | 1.84                     | 0.57              |
| 20:W:179:ARG:HE   | 20:W:183:GLU:HG2  | 1.69                     | 0.57              |
| 6:G:130:ARG:HB3   | 7:F:121:GLN:HA    | 1.85                     | 0.57              |
| 30:7:49:TYR:HE2   | 30:7:54:ILE:HG13  | 1.68                     | 0.57              |
| 32:Z:354:PRO:HA   | 32:Z:357:ILE:HG12 | 1.85                     | 0.57              |
| 3:i:193:TRP:HB3   | 29:6:57:ARG:HH22  | 1.67                     | 0.57              |
| 7:l:117:GLN:NE2   | 7:l:120:THR:OG1   | 2.37                     | 0.57              |
| 30:a:49:TYR:HE2   | 30:a:54:ILE:HG13  | 1.69                     | 0.57              |
| 33:V:280:LEU:O    | 33:V:283:THR:OG1  | 2.22                     | 0.57              |
| 2:K:113:THR:HB    | 2:K:252:ARG:NH2   | 2.19                     | 0.57              |
| 11:N:176:GLN:O    | 11:N:182:ASN:ND2  | 2.37                     | 0.57              |
| 13:T:230:ASN:OD1  | 13:T:231:SER:N    | 2.37                     | 0.57              |
| 14:R:134:TRP:HB2  | 14:R:157:SER:HB3  | 1.85                     | 0.57              |
| 17:L:133:ASN:H    | 33:V:45:VAL:HG11  | 1.69                     | 0.57              |
| 17:L:228:LYS:NZ   | 17:L:327:THR:O    | 2.37                     | 0.57              |
| 32:Z:575:MET:HA   | 32:Z:606:CYS:HB3  | 1.85                     | 0.57              |
| 30:a:62:SER:OG    | 30:a:66:LEU:O     | 2.22                     | 0.57              |
| 2:K:89:ILE:HD13   | 16:J:62:LEU:HD13  | 1.86                     | 0.57              |
| 2:K:245:LYS:NZ    | 17:L:300:GLU:OE1  | 2.33                     | 0.57              |
| 3:i:240:ALA:HB2   | 29:6:185:GLY:HA3  | 1.86                     | 0.57              |
| 12:S:469:ASN:ND2  | 13:T:269:SER:OG   | 2.37                     | 0.57              |
| 12:S:478:SER:HA   | 16:J:43:ARG:HH22  | 1.68                     | 0.57              |
| 22:P:138:ARG:NH2  | 22:P:175:GLU:OE1  | 2.37                     | 0.57              |
| 25:B:90:ARG:HB3   | 3:2:94:LEU:HD13   | 1.87                     | 0.57              |
| 32:Z:56:LEU:HD13  | 32:Z:99:LEU:HD21  | 1.86                     | 0.57              |
| 32:Z:427:GLN:HG2  | 32:Z:428:TRP:CD1  | 2.40                     | 0.57              |
| 24:d:70:ASN:HB3   | 24:d:73:ILE:HB    | 1.87                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:h:11:ILE:HD12   | 5:h:146:LEU:HD11  | 1.87                     | 0.57              |
| 8:E:68:VAL:HB     | 8:E:93:ARG:HH21   | 1.70                     | 0.57              |
| 9:n:29:ARG:NH2    | 24:d:16:GLU:O     | 2.38                     | 0.57              |
| 18:M:277:ILE:HA   | 18:M:322:LYS:HB2  | 1.86                     | 0.57              |
| 20:W:179:ARG:HG2  | 20:W:180:LEU:H    | 1.69                     | 0.57              |
| 23:H:465:GLN:HB3  | 8:E:10:ARG:HH22   | 1.69                     | 0.57              |
| 2:K:126:LEU:HD22  | 2:K:149:ILE:H     | 1.68                     | 0.57              |
| 12:S:464:ARG:HE   | 14:R:403:LEU:HD11 | 1.70                     | 0.57              |
| 20:W:30:ILE:HG23  | 20:W:76:LEU:HD13  | 1.85                     | 0.57              |
| 22:P:388:ILE:HG22 | 22:P:389:ILE:HG23 | 1.86                     | 0.57              |
| 4:A:57:LYS:NZ     | 4:A:66:PRO:O      | 2.36                     | 0.57              |
| 8:E:110:GLU:HA    | 8:E:156:PHE:HE2   | 1.70                     | 0.57              |
| 5:h:53:ILE:HG22   | 5:h:60:VAL:HG22   | 1.85                     | 0.57              |
| 11:N:476:THR:OG1  | 33:V:61:TYR:OH    | 2.23                     | 0.57              |
| 13:T:69:SER:HG    | 13:T:77:SER:HG    | 1.53                     | 0.57              |
| 8:E:116:VAL:O     | 8:E:120:ALA:N     | 2.38                     | 0.57              |
| 32:Z:524:ALA:O    | 32:Z:562:TRP:NE1  | 2.37                     | 0.57              |
| 1:I:127:ASP:OD1   | 23:H:173:ARG:NH2  | 2.37                     | 0.57              |
| 4:c:86:PRO:HD2    | 4:c:139:VAL:HG22  | 1.86                     | 0.57              |
| 12:S:149:SER:HB3  | 12:S:196:ARG:HH11 | 1.70                     | 0.57              |
| 12:S:273:PHE:HA   | 12:S:276:LEU:HB2  | 1.86                     | 0.57              |
| 14:R:270:VAL:HG12 | 14:R:276:LEU:HD22 | 1.87                     | 0.57              |
| 22:P:128:ASN:ND2  | 22:P:166:GLU:O    | 2.38                     | 0.57              |
| 4:A:51:THR:HB     | 4:A:228:ALA:HB3   | 1.86                     | 0.57              |
| 27:4:19:LYS:HB3   | 27:4:32:ASP:H     | 1.69                     | 0.57              |
| 29:6:46:THR:HB    | 29:6:59:GLU:H     | 1.68                     | 0.57              |
| 32:Z:490:ILE:HG21 | 32:Z:526:ALA:HA   | 1.87                     | 0.57              |
| 7:l:88:LEU:HD22   | 7:l:112:LEU:HD11  | 1.87                     | 0.56              |
| 11:N:352:ASN:HB2  | 11:N:355:TRP:HE1  | 1.69                     | 0.56              |
| 11:N:614:ASN:HB3  | 11:N:617:VAL:HB   | 1.87                     | 0.56              |
| 16:J:55:VAL:HA    | 16:J:58:ILE:HD12  | 1.87                     | 0.56              |
| 23:H:279:LEU:HD21 | 23:H:332:THR:HG21 | 1.85                     | 0.56              |
| 8:E:80:GLY:HA3    | 8:E:140:VAL:HA    | 1.87                     | 0.56              |
| 9:D:34:VAL:O      | 9:D:45:GLY:N      | 2.38                     | 0.56              |
| 24:C:91:ALA:HB2   | 24:C:115:LEU:HD21 | 1.87                     | 0.56              |
| 3:2:228:LYS:HE2   | 3:2:231:SER:HA    | 1.87                     | 0.56              |
| 25:j:149:GLN:HB3  | 25:j:157:PHE:HB2  | 1.86                     | 0.56              |
| 1:I:340:ARG:NE    | 23:H:253:GLY:O    | 2.37                     | 0.56              |
| 3:i:65:ARG:NH1    | 3:i:93:GLU:OE2    | 2.37                     | 0.56              |
| 7:l:18:ARG:HH12   | 7:l:23:GLU:HB2    | 1.69                     | 0.56              |
| 12:S:276:LEU:HD22 | 12:S:279:ILE:HD11 | 1.86                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:S:280:ASN:O    | 12:S:382:ARG:NH2  | 2.39                     | 0.56              |
| 14:R:138:GLY:HA3  | 14:R:154:LEU:HD13 | 1.87                     | 0.56              |
| 17:L:164:ASP:O    | 17:L:169:ASN:ND2  | 2.30                     | 0.56              |
| 21:O:147:ARG:HH21 | 22:P:284:ILE:HB   | 1.69                     | 0.56              |
| 23:H:95:HIS:N     | 23:H:192:ASP:OD2  | 2.38                     | 0.56              |
| 24:d:39:MET:HE2   | 24:d:161:LYS:HG2  | 1.86                     | 0.56              |
| 24:d:70:ASN:OD1   | 24:d:71:ASP:N     | 2.38                     | 0.56              |
| 26:b:11:LEU:N     | 26:b:113:THR:HG1  | 2.03                     | 0.56              |
| 29:e:90:SER:HA    | 29:e:93:TRP:HD1   | 1.69                     | 0.56              |
| 33:V:235:GLU:HG3  | 33:V:236:SER:H    | 1.69                     | 0.56              |
| 19:U:99:LEU:HB2   | 22:P:434:THR:HG21 | 1.86                     | 0.56              |
| 23:H:179:SER:O    | 23:H:181:TYR:N    | 2.38                     | 0.56              |
| 4:A:170:ALA:HB3   | 4:A:175:GLN:HG3   | 1.87                     | 0.56              |
| 2:K:131:LEU:HD11  | 33:V:273:ARG:HH21 | 1.70                     | 0.56              |
| 5:h:61:THR:OG1    | 27:g:85:ARG:NH1   | 2.39                     | 0.56              |
| 24:C:50:ARG:HH21  | 24:C:57:LEU:HD21  | 1.71                     | 0.56              |
| 29:6:49:ILE:HA    | 29:6:55:ASN:H     | 1.71                     | 0.56              |
| 29:6:80:GLY:O     | 29:6:84:VAL:N     | 2.37                     | 0.56              |
| 25:j:215:GLY:H    | 25:j:234:ARG:HB3  | 1.71                     | 0.56              |
| 18:M:186:LEU:HD13 | 18:M:231:LEU:HD22 | 1.87                     | 0.56              |
| 29:6:237:GLU:OE2  | 30:7:194:ARG:NH1  | 2.39                     | 0.56              |
| 26:b:162:ARG:H    | 26:b:165:MET:HE3  | 1.71                     | 0.56              |
| 28:f:83:PHE:HE2   | 28:f:88:ILE:HG12  | 1.70                     | 0.56              |
| 11:N:258:ALA:HB1  | 11:N:290:LEU:HD21 | 1.88                     | 0.56              |
| 24:C:129:ARG:O    | 25:B:123:GLN:NE2  | 2.39                     | 0.56              |
| 26:1:18:LEU:HD13  | 26:1:64:ARG:HG2   | 1.88                     | 0.56              |
| 27:4:8:ARG:HH11   | 27:4:116:LEU:HB3  | 1.69                     | 0.56              |
| 29:e:42:LEU:HD23  | 29:e:70:VAL:HG12  | 1.86                     | 0.56              |
| 17:L:198:GLU:HA   | 17:L:201:LEU:HD12 | 1.87                     | 0.56              |
| 21:O:31:LYS:HA    | 21:O:39:PHE:HE2   | 1.71                     | 0.56              |
| 9:D:41:CYS:HA     | 9:D:138:PHE:HZ    | 1.71                     | 0.56              |
| 24:d:31:HIS:O     | 24:d:51:LYS:NZ    | 2.34                     | 0.56              |
| 1:I:408:ARG:HG2   | 1:I:410:GLN:H     | 1.70                     | 0.56              |
| 16:J:140:GLU:OE1  | 16:J:200:ARG:NH2  | 2.38                     | 0.56              |
| 18:M:170:MET:HE2  | 18:M:244:LEU:HD22 | 1.88                     | 0.56              |
| 9:D:4:TYR:HD2     | 9:D:125:GLY:HA2   | 1.70                     | 0.56              |
| 30:7:60:LEU:HA    | 30:7:70:ASN:HA    | 1.88                     | 0.56              |
| 32:Z:233:LEU:HB2  | 32:Z:234:PRO:HD3  | 1.87                     | 0.56              |
| 11:N:34:GLN:NE2   | 12:S:215:MET:O    | 2.39                     | 0.56              |
| 17:L:427:LYS:NZ   | 6:G:18:ASP:OD2    | 2.33                     | 0.56              |
| 18:M:75:LEU:HB3   | 23:H:146:VAL:HB   | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:W:172:LEU:HG   | 20:W:189:PRO:HD2  | 1.88                     | 0.56              |
| 25:B:149:GLN:HB3  | 25:B:157:PHE:HB2  | 1.88                     | 0.56              |
| 32:Z:166:ASN:ND2  | 32:Z:226:GLU:O    | 2.38                     | 0.56              |
| 6:k:69:VAL:HA     | 6:k:75:GLY:HA2    | 1.88                     | 0.55              |
| 7:l:40:SER:HB2    | 7:l:180:ILE:HA    | 1.86                     | 0.55              |
| 20:W:109:ARG:HE   | 20:W:140:ASP:HB2  | 1.70                     | 0.55              |
| 23:H:105:ILE:HA   | 23:H:170:GLU:HG3  | 1.88                     | 0.55              |
| 23:H:382:LEU:HD11 | 23:H:408:SER:HB2  | 1.88                     | 0.55              |
| 29:6:65:CYS:HA    | 29:6:88:LYS:HG2   | 1.88                     | 0.55              |
| 29:6:172:GLN:HE21 | 29:6:202:LEU:HD21 | 1.71                     | 0.55              |
| 29:e:65:CYS:HA    | 29:e:88:LYS:HG2   | 1.88                     | 0.55              |
| 2:K:170:THR:HA    | 2:K:228:ASN:HD22  | 1.70                     | 0.55              |
| 11:N:728:LYS:HD3  | 11:N:751:LEU:HD22 | 1.88                     | 0.55              |
| 20:W:133:LYS:HD3  | 20:W:163:ASN:HD21 | 1.70                     | 0.55              |
| 9:D:122:GLN:NE2   | 8:E:84:ASP:OD1    | 2.31                     | 0.55              |
| 24:C:135:PHE:HB2  | 24:C:151:SER:HB3  | 1.88                     | 0.55              |
| 3:2:164:MET:SD    | 30:a:220:ARG:NH2  | 2.79                     | 0.55              |
| 32:Z:797:THR:HG22 | 32:Z:798:ARG:HG2  | 1.89                     | 0.55              |
| 14:R:240:SER:OG   | 14:R:243:LEU:HB2  | 2.07                     | 0.55              |
| 23:H:200:VAL:HG22 | 23:H:272:ILE:HG12 | 1.88                     | 0.55              |
| 25:B:109:LEU:HD13 | 5:3:77:LYS:HB3    | 1.89                     | 0.55              |
| 5:3:44:PHE:O      | 5:3:51:LEU:N      | 2.35                     | 0.55              |
| 30:a:50:ASP:O     | 30:a:158:GLN:NE2  | 2.36                     | 0.55              |
| 33:V:52:LEU:HD11  | 33:V:104:VAL:HG13 | 1.86                     | 0.55              |
| 1:I:221:LEU:HG    | 1:I:348:ILE:HB    | 1.87                     | 0.55              |
| 5:h:10:GLY:N      | 5:h:180:LEU:O     | 2.37                     | 0.55              |
| 6:k:130:ARG:O     | 7:l:121:GLN:NE2   | 2.39                     | 0.55              |
| 9:n:32:CYS:HA     | 9:n:165:GLY:HA3   | 1.87                     | 0.55              |
| 9:n:111:ARG:O     | 9:n:115:GLY:N     | 2.40                     | 0.55              |
| 19:U:49:THR:HB    | 33:V:39:LYS:HE3   | 1.88                     | 0.55              |
| 29:6:53:SER:OG    | 30:7:182:HIS:ND1  | 2.38                     | 0.55              |
| 31:X:78:ILE:HG12  | 31:X:80:SER:H     | 1.71                     | 0.55              |
| 24:d:94:HIS:HB3   | 24:d:114:ARG:HH11 | 1.70                     | 0.55              |
| 30:a:72:VAL:HG11  | 30:a:90:ILE:HD13  | 1.88                     | 0.55              |
| 2:K:88:ARG:O      | 2:K:91:SER:OG     | 2.24                     | 0.55              |
| 7:l:52:ASN:ND2    | 7:l:57:SER:O      | 2.26                     | 0.55              |
| 11:N:416:GLY:O    | 11:N:420:THR:OG1  | 2.23                     | 0.55              |
| 24:C:72:LYS:HB2   | 24:C:140:TYR:HB3  | 1.87                     | 0.55              |
| 25:B:215:GLY:H    | 25:B:234:ARG:HB3  | 1.71                     | 0.55              |
| 29:6:54:ILE:HB    | 30:7:189:ARG:HH12 | 1.71                     | 0.55              |
| 25:j:67:LEU:HD23  | 25:j:90:ARG:HE    | 1.72                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:f:260:TRP:HZ3  | 28:f:262:TYR:HB2  | 1.71                     | 0.55              |
| 33:V:270:TYR:CD2  | 33:V:271:VAL:HG22 | 2.41                     | 0.55              |
| 7:l:34:VAL:HG22   | 7:l:163:ALA:H     | 1.72                     | 0.55              |
| 29:e:47:ARG:HB2   | 29:e:219:ASP:HB2  | 1.87                     | 0.55              |
| 16:J:324:ARG:NE   | 16:J:347:ALA:O    | 2.35                     | 0.55              |
| 23:H:406:LEU:HD22 | 8:E:209:GLU:HA    | 1.89                     | 0.55              |
| 9:D:65:SER:OG     | 9:D:73:LEU:O      | 2.22                     | 0.55              |
| 3:2:201:ASN:ND2   | 3:2:218:ASN:OD1   | 2.30                     | 0.55              |
| 32:Z:262:VAL:HG21 | 32:Z:288:LEU:HD21 | 1.88                     | 0.55              |
| 8:m:86:ARG:HD3    | 9:n:111:ARG:HE    | 1.72                     | 0.55              |
| 21:O:47:LYS:HE3   | 21:O:80:LYS:HD2   | 1.87                     | 0.55              |
| 27:4:44:MET:HE1   | 27:4:84:VAL:HG11  | 1.89                     | 0.55              |
| 19:U:107:ASN:HD22 | 19:U:152:LYS:HD3  | 1.71                     | 0.55              |
| 28:5:96:THR:HG22  | 28:5:101:VAL:HG22 | 1.89                     | 0.55              |
| 29:6:42:LEU:HD23  | 29:6:70:VAL:HG12  | 1.87                     | 0.55              |
| 24:d:91:ALA:HB2   | 24:d:115:LEU:HD21 | 1.87                     | 0.55              |
| 11:N:376:LYS:HA   | 11:N:411:ILE:HA   | 1.87                     | 0.55              |
| 11:N:625:LEU:HB3  | 11:N:663:ILE:HD11 | 1.88                     | 0.55              |
| 14:R:219:LEU:HA   | 14:R:224:PHE:HE1  | 1.71                     | 0.55              |
| 6:G:8:TYR:HB3     | 6:G:22:PHE:H      | 1.71                     | 0.55              |
| 6:G:69:VAL:HA     | 6:G:75:GLY:HA2    | 1.88                     | 0.55              |
| 4:A:82:VAL:HB     | 4:A:142:THR:HB    | 1.89                     | 0.55              |
| 9:D:27:VAL:HG22   | 9:D:77:GLY:HA2    | 1.89                     | 0.55              |
| 27:g:8:ARG:HH11   | 27:g:116:LEU:HB3  | 1.72                     | 0.55              |
| 2:K:104:ASP:HB3   | 2:K:107:THR:HB    | 1.87                     | 0.54              |
| 7:l:140:SER:OG    | 7:l:143:HIS:NE2   | 2.35                     | 0.54              |
| 8:m:18:GLU:OE1    | 8:m:20:ARG:NH2    | 2.40                     | 0.54              |
| 12:S:348:LEU:O    | 12:S:352:VAL:N    | 2.38                     | 0.54              |
| 18:M:262:LEU:HA   | 18:M:265:ASP:HB2  | 1.89                     | 0.54              |
| 7:F:58:SER:HB2    | 8:E:166:ARG:HB3   | 1.90                     | 0.54              |
| 24:C:158:THR:OG1  | 24:C:160:TRP:NE1  | 2.40                     | 0.54              |
| 24:d:152:ASN:ND2  | 24:d:154:SER:OG   | 2.40                     | 0.54              |
| 9:n:34:VAL:O      | 9:n:45:GLY:N      | 2.35                     | 0.54              |
| 13:T:111:LEU:HB3  | 13:T:181:LEU:HD21 | 1.88                     | 0.54              |
| 14:R:279:LEU:HD21 | 14:R:286:LEU:HD22 | 1.89                     | 0.54              |
| 16:J:139:VAL:HG22 | 16:J:211:ILE:HG12 | 1.87                     | 0.54              |
| 18:M:216:LYS:HB3  | 18:M:323:VAL:H    | 1.71                     | 0.54              |
| 21:O:120:LYS:HB2  | 21:O:166:ARG:HH12 | 1.73                     | 0.54              |
| 23:H:167:ASP:OD1  | 23:H:168:ILE:N    | 2.40                     | 0.54              |
| 28:5:83:PHE:HE2   | 28:5:88:ILE:HG12  | 1.71                     | 0.54              |
| 29:6:90:SER:HA    | 29:6:93:TRP:HD1   | 1.72                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:Z:796:LEU:HD13 | 32:Z:815:MET:HE2  | 1.89                     | 0.54              |
| 27:g:36:ARG:HH21  | 27:g:57:ALA:H     | 1.54                     | 0.54              |
| 1:I:225:PRO:HG2   | 16:J:306:ARG:HH22 | 1.71                     | 0.54              |
| 5:h:77:LYS:HB3    | 25:j:109:LEU:HD13 | 1.89                     | 0.54              |
| 14:R:410:LEU:HD13 | 15:Q:419:LEU:HD13 | 1.89                     | 0.54              |
| 21:O:114:GLN:HE22 | 21:O:126:ILE:HD12 | 1.72                     | 0.54              |
| 23:H:223:GLU:HA   | 23:H:227:LEU:HB2  | 1.90                     | 0.54              |
| 32:Z:763:HIS:ND1  | 32:Z:767:TYR:OH   | 2.32                     | 0.54              |
| 33:V:171:ARG:HD2  | 33:V:179:LEU:HD11 | 1.90                     | 0.54              |
| 1:I:130:VAL:HB    | 1:I:155:SER:HA    | 1.89                     | 0.54              |
| 3:i:201:ASN:ND2   | 3:i:218:ASN:OD1   | 2.32                     | 0.54              |
| 11:N:661:SER:HB3  | 11:N:702:ALA:HB1  | 1.90                     | 0.54              |
| 17:L:131:VAL:HG12 | 17:L:155:ILE:HD12 | 1.90                     | 0.54              |
| 18:M:169:ALA:H    | 18:M:246:LEU:HD13 | 1.72                     | 0.54              |
| 19:U:54:LEU:HG    | 19:U:73:ILE:HG21  | 1.89                     | 0.54              |
| 22:P:44:LYS:HG2   | 22:P:47:ARG:HH21  | 1.73                     | 0.54              |
| 27:4:86:GLN:HE21  | 27:4:90:LYS:HE3   | 1.71                     | 0.54              |
| 33:V:231:GLU:HG3  | 33:V:301:ASN:HD21 | 1.71                     | 0.54              |
| 12:S:282:ILE:HG23 | 13:T:123:HIS:HB2  | 1.90                     | 0.54              |
| 14:R:78:ASP:HB2   | 14:R:92:ILE:HG12  | 1.89                     | 0.54              |
| 18:M:275:PRO:HA   | 18:M:320:ARG:HA   | 1.89                     | 0.54              |
| 19:U:10:ILE:O     | 19:U:162:GLU:N    | 2.37                     | 0.54              |
| 27:g:86:GLN:HE21  | 27:g:90:LYS:HE3   | 1.72                     | 0.54              |
| 4:c:170:ALA:HB3   | 4:c:175:GLN:HG3   | 1.90                     | 0.54              |
| 8:m:89:ILE:HG23   | 8:m:93:ARG:HD2    | 1.90                     | 0.54              |
| 18:M:229:THR:OG1  | 23:H:341:ASP:OD1  | 2.24                     | 0.54              |
| 24:d:58:GLU:HB2   | 25:j:160:LYS:HG3  | 1.89                     | 0.54              |
| 1:I:251:GLU:O     | 1:I:254:GLN:HG2   | 2.07                     | 0.54              |
| 9:D:32:CYS:HA     | 9:D:165:GLY:HA3   | 1.90                     | 0.54              |
| 33:V:53:MET:HG3   | 33:V:108:TYR:HD2  | 1.71                     | 0.54              |
| 1:I:220:ILE:H     | 1:I:346:ARG:HB3   | 1.72                     | 0.54              |
| 6:k:130:ARG:HB2   | 7:l:11:VAL:HG12   | 1.90                     | 0.54              |
| 11:N:529:GLN:HE22 | 11:N:558:ALA:HB3  | 1.72                     | 0.54              |
| 19:U:50:ASN:OD1   | 19:U:51:SER:N     | 2.40                     | 0.54              |
| 26:1:16:VAL:HG11  | 26:1:39:THR:HG23  | 1.89                     | 0.54              |
| 30:7:51:ASN:HA    | 30:7:235:LYS:HE2  | 1.90                     | 0.54              |
| 4:c:82:VAL:HB     | 4:c:142:THR:HB    | 1.90                     | 0.54              |
| 4:c:147:ASP:HB3   | 4:c:151:GLY:H     | 1.73                     | 0.54              |
| 5:h:169:GLN:OE1   | 5:h:173:ASN:ND2   | 2.39                     | 0.54              |
| 19:U:165:GLU:HB2  | 33:V:43:ALA:HB2   | 1.89                     | 0.54              |
| 23:H:241:ASP:HB3  | 23:H:346:ARG:HD2  | 1.90                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:103:GLU:OE1   | 4:A:120:ARG:NH2   | 2.41                     | 0.54              |
| 28:5:87:ILE:HD11  | 28:5:185:PRO:HB3  | 1.89                     | 0.54              |
| 28:f:208:GLN:HE21 | 27:g:25:ILE:HD11  | 1.72                     | 0.54              |
| 10:Y:66:ASP:OD1   | 14:R:222:ARG:NH1  | 2.41                     | 0.54              |
| 11:N:422:TYR:HD2  | 11:N:423:LEU:HD12 | 1.73                     | 0.54              |
| 11:N:521:LEU:HB3  | 11:N:535:LEU:HD21 | 1.89                     | 0.54              |
| 12:S:406:ASP:OD1  | 14:R:383:ARG:NH1  | 2.41                     | 0.54              |
| 14:R:333:MET:HA   | 14:R:336:LYS:HD3  | 1.90                     | 0.54              |
| 22:P:284:ILE:HG13 | 22:P:285:GLN:HG2  | 1.89                     | 0.54              |
| 23:H:318:ARG:HD2  | 23:H:321:ASP:HA   | 1.89                     | 0.54              |
| 29:6:62:VAL:HA    | 29:6:72:SER:HB2   | 1.89                     | 0.54              |
| 32:Z:564:ARG:HD2  | 32:Z:738:TYR:HE2  | 1.72                     | 0.54              |
| 29:e:80:GLY:O     | 29:e:84:VAL:N     | 2.36                     | 0.54              |
| 5:h:20:CYS:HA     | 5:h:112:ILE:HD11  | 1.89                     | 0.53              |
| 5:h:155:GLU:HB3   | 5:h:158:LEU:HD21  | 1.90                     | 0.53              |
| 16:J:88:VAL:HG12  | 16:J:90:PRO:HD2   | 1.90                     | 0.53              |
| 26:1:162:ARG:H    | 26:1:165:MET:HE3  | 1.72                     | 0.53              |
| 33:V:282:GLU:O    | 33:V:286:GLU:N    | 2.35                     | 0.53              |
| 1:I:366:THR:HA    | 1:I:369:MET:HB2   | 1.90                     | 0.53              |
| 4:c:138:GLY:HA2   | 4:c:159:PRO:HB3   | 1.91                     | 0.53              |
| 9:n:66:LYS:H      | 9:n:90:ARG:HH21   | 1.57                     | 0.53              |
| 16:J:272:MET:HG3  | 16:J:292:MET:HE2  | 1.90                     | 0.53              |
| 17:L:339:ARG:HG2  | 17:L:341:GLY:H    | 1.72                     | 0.53              |
| 29:6:50:THR:OG1   | 29:6:55:ASN:ND2   | 2.31                     | 0.53              |
| 32:Z:927:VAL:H    | 32:Z:956:LEU:HA   | 1.74                     | 0.53              |
| 29:e:74:ASN:N     | 29:e:127:HIS:O    | 2.40                     | 0.53              |
| 1:I:299:GLU:HG3   | 1:I:301:GLU:H     | 1.73                     | 0.53              |
| 9:n:37:LYS:HD3    | 9:n:160:SER:HA    | 1.90                     | 0.53              |
| 17:L:225:GLY:HA3  | 18:M:342:ARG:HH22 | 1.71                     | 0.53              |
| 18:M:223:PRO:HB3  | 23:H:367:ARG:HD3  | 1.90                     | 0.53              |
| 18:M:429:SER:OG   | 8:E:20:ARG:NH2    | 2.35                     | 0.53              |
| 6:G:156:SER:HB3   | 4:A:88:PRO:HD3    | 1.88                     | 0.53              |
| 27:4:44:MET:HE2   | 27:4:46:PHE:HE1   | 1.74                     | 0.53              |
| 29:6:94:TYR:O     | 29:6:98:HIS:ND1   | 2.40                     | 0.53              |
| 1:I:102:ASN:HD22  | 16:J:97:ASP:HB3   | 1.72                     | 0.53              |
| 4:c:14:ARG:HB3    | 6:k:7:GLY:HA3     | 1.91                     | 0.53              |
| 11:N:668:THR:HB   | 11:N:785:PRO:HB3  | 1.91                     | 0.53              |
| 24:C:33:GLY:H     | 24:C:65:LYS:HE3   | 1.74                     | 0.53              |
| 24:C:39:MET:HE2   | 24:C:161:LYS:HG2  | 1.90                     | 0.53              |
| 24:C:168:ASN:HB3  | 24:C:171:ALA:HB3  | 1.91                     | 0.53              |
| 4:c:40:ILE:HG12   | 4:c:71:TYR:HE2    | 1.73                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:k:130:ARG:HB3   | 7:l:121:GLN:HA    | 1.90                     | 0.53              |
| 11:N:726:ASP:HB3  | 11:N:729:SER:HB3  | 1.90                     | 0.53              |
| 12:S:402:ILE:HB   | 12:S:443:ILE:HB   | 1.91                     | 0.53              |
| 16:J:324:ARG:HH21 | 16:J:348:GLU:HA   | 1.73                     | 0.53              |
| 23:H:393:SER:HA   | 23:H:396:MET:HB3  | 1.89                     | 0.53              |
| 4:A:16:ILE:HG13   | 4:A:17:THR:H      | 1.72                     | 0.53              |
| 8:E:142:LEU:HB2   | 8:E:158:ALA:HB3   | 1.90                     | 0.53              |
| 32:Z:378:GLN:NE2  | 32:Z:842:GLN:O    | 2.39                     | 0.53              |
| 30:a:87:SER:HB3   | 30:a:146:ALA:HB3  | 1.90                     | 0.53              |
| 29:e:113:GLN:HB2  | 29:e:150:TYR:HE2  | 1.72                     | 0.53              |
| 1:I:108:THR:HB    | 1:I:121:THR:HB    | 1.91                     | 0.53              |
| 3:i:143:HIS:HB2   | 3:i:147:SER:HB3   | 1.89                     | 0.53              |
| 15:Q:40:ALA:HA    | 15:Q:46:VAL:HA    | 1.91                     | 0.53              |
| 23:H:380:PRO:HG2  | 23:H:385:ARG:HH11 | 1.74                     | 0.53              |
| 32:Z:212:LEU:HD22 | 32:Z:245:VAL:HG22 | 1.90                     | 0.53              |
| 32:Z:821:GLY:H    | 32:Z:863:THR:HG21 | 1.73                     | 0.53              |
| 30:a:86:ILE:HG12  | 30:a:147:ILE:HG12 | 1.89                     | 0.53              |
| 27:g:29:LYS:HG2   | 27:g:31:SER:H     | 1.73                     | 0.53              |
| 21:O:55:THR:HG22  | 21:O:57:LEU:HG    | 1.90                     | 0.53              |
| 31:X:91:PHE:HB3   | 31:X:94:ASN:HD22  | 1.73                     | 0.53              |
| 11:N:59:GLU:HB2   | 11:N:88:ARG:HE    | 1.74                     | 0.53              |
| 11:N:607:GLN:HG2  | 11:N:611:LYS:HE3  | 1.90                     | 0.53              |
| 19:U:192:ASN:HB3  | 33:V:226:LYS:HG3  | 1.91                     | 0.53              |
| 20:W:51:LEU:HB3   | 20:W:63:SER:HB3   | 1.90                     | 0.53              |
| 9:D:157:SER:OG    | 9:D:159:TRP:NE1   | 2.42                     | 0.53              |
| 24:C:152:ASN:OD1  | 24:C:156:ASN:N    | 2.41                     | 0.53              |
| 5:3:30:GLY:HA3    | 5:3:35:GLY:HA2    | 1.91                     | 0.53              |
| 25:j:119:GLN:NE2  | 25:j:122:THR:OG1  | 2.41                     | 0.53              |
| 2:K:345:ASP:OD2   | 2:K:347:ARG:NH1   | 2.42                     | 0.53              |
| 4:c:51:THR:HB     | 4:c:228:ALA:HB3   | 1.90                     | 0.53              |
| 5:h:30:GLY:HA3    | 5:h:35:GLY:HA2    | 1.91                     | 0.53              |
| 15:Q:50:ARG:O     | 15:Q:54:GLN:N     | 2.37                     | 0.53              |
| 17:L:252:VAL:HB   | 18:M:256:ILE:HG22 | 1.90                     | 0.53              |
| 17:L:421:LYS:NZ   | 18:M:345:ARG:HH12 | 2.07                     | 0.53              |
| 18:M:69:ILE:O     | 18:M:73:ARG:N     | 2.40                     | 0.53              |
| 18:M:79:VAL:HA    | 18:M:147:GLY:HA2  | 1.91                     | 0.53              |
| 18:M:259:GLY:N    | 18:M:300:GLU:OE2  | 2.36                     | 0.53              |
| 5:3:57:ALA:HA     | 5:3:60:VAL:HB     | 1.91                     | 0.53              |
| 32:Z:272:TYR:CG   | 32:Z:277:GLU:HB2  | 2.44                     | 0.53              |
| 30:a:38:ILE:HG22  | 30:a:39:VAL:HG23  | 1.90                     | 0.53              |
| 28:f:87:ILE:HD11  | 28:f:185:PRO:HB3  | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:g:60:ILE:HG21  | 27:g:84:VAL:HG22  | 1.90                     | 0.53              |
| 8:m:111:SER:HB2   | 29:e:98:HIS:HA    | 1.90                     | 0.53              |
| 14:R:149:ASN:O    | 14:R:153:THR:OG1  | 2.26                     | 0.53              |
| 15:Q:281:ILE:O    | 15:Q:287:THR:OG1  | 2.25                     | 0.53              |
| 20:W:6:THR:HB     | 20:W:49:VAL:HG22  | 1.90                     | 0.53              |
| 5:3:5:SER:HA      | 5:3:56:LEU:HB2    | 1.91                     | 0.53              |
| 27:g:101:ASN:HB3  | 27:g:133:HIS:CG   | 2.44                     | 0.53              |
| 3:i:113:LYS:HZ1   | 26:b:72:GLN:HB3   | 1.74                     | 0.52              |
| 6:G:60:VAL:HG21   | 7:F:39:ARG:HH21   | 1.74                     | 0.52              |
| 27:4:101:ASN:HB3  | 27:4:133:HIS:CG   | 2.43                     | 0.52              |
| 2:K:190:LEU:HD11  | 2:K:197:LEU:HD12  | 1.90                     | 0.52              |
| 5:h:125:ASP:OD1   | 5:h:129:CYS:N     | 2.42                     | 0.52              |
| 6:k:68:GLN:N      | 6:k:76:CYS:O      | 2.37                     | 0.52              |
| 9:n:138:PHE:HE1   | 9:n:145:PRO:HB3   | 1.75                     | 0.52              |
| 14:R:411:LEU:HD23 | 14:R:414:LEU:HD12 | 1.90                     | 0.52              |
| 16:J:183:LYS:HG2  | 16:J:286:LYS:NZ   | 2.24                     | 0.52              |
| 19:U:32:ARG:HG3   | 19:U:95:SER:H     | 1.75                     | 0.52              |
| 20:W:186:ALA:HA   | 20:W:191:ILE:HG21 | 1.90                     | 0.52              |
| 26:1:151:THR:HA   | 26:1:154:TYR:CE2  | 2.43                     | 0.52              |
| 3:i:49:SER:HB3    | 3:i:57:ASP:HB3    | 1.92                     | 0.52              |
| 11:N:694:LEU:HA   | 11:N:697:PHE:HB3  | 1.91                     | 0.52              |
| 17:L:331:ASP:C    | 17:L:333:LEU:H    | 2.18                     | 0.52              |
| 23:H:147:ILE:HD11 | 23:H:157:VAL:HB   | 1.91                     | 0.52              |
| 26:1:57:HIS:HB3   | 26:1:60:ILE:HB    | 1.90                     | 0.52              |
| 30:7:220:ARG:HA   | 26:b:45:ILE:HB    | 1.92                     | 0.52              |
| 12:S:295:ALA:HA   | 12:S:298:ARG:HE   | 1.75                     | 0.52              |
| 18:M:80:ALA:HA    | 18:M:121:THR:HA   | 1.90                     | 0.52              |
| 20:W:12:ASN:ND2   | 20:W:53:SER:OG    | 2.42                     | 0.52              |
| 23:H:242:PRO:O    | 23:H:346:ARG:NH1  | 2.38                     | 0.52              |
| 4:A:105:ARG:HA    | 4:A:109:GLY:H     | 1.74                     | 0.52              |
| 24:C:129:ARG:HB3  | 25:B:123:GLN:HE22 | 1.75                     | 0.52              |
| 27:4:49:GLU:HG3   | 27:4:51:GLY:H     | 1.73                     | 0.52              |
| 29:6:31:ILE:HG22  | 29:6:44:GLY:HA3   | 1.90                     | 0.52              |
| 33:V:277:LYS:O    | 33:V:282:GLU:N    | 2.33                     | 0.52              |
| 11:N:306:ASN:HD21 | 11:N:871:MET:HB3  | 1.74                     | 0.52              |
| 11:N:610:SER:HB2  | 11:N:621:THR:HG21 | 1.92                     | 0.52              |
| 12:S:437:ASN:HB3  | 12:S:442:PHE:H    | 1.74                     | 0.52              |
| 13:T:241:GLU:HG2  | 13:T:242:LYS:HG3  | 1.91                     | 0.52              |
| 22:P:324:GLU:HA   | 22:P:331:GLY:HA3  | 1.92                     | 0.52              |
| 4:A:114:CYS:SG    | 4:A:153:SER:OG    | 2.68                     | 0.52              |
| 7:F:62:LYS:HD2    | 7:F:74:LEU:HD11   | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:Z:102:ILE:HD12 | 32:Z:105:LYS:HD2  | 1.91                     | 0.52              |
| 32:Z:810:ASN:HA   | 32:Z:813:PHE:HB2  | 1.91                     | 0.52              |
| 33:V:164:LEU:HD12 | 33:V:168:LEU:HD23 | 1.92                     | 0.52              |
| 2:K:218:GLY:HA2   | 2:K:221:MET:HB2   | 1.92                     | 0.52              |
| 4:c:240:ASN:HB3   | 4:c:244:ARG:HH12  | 1.74                     | 0.52              |
| 15:Q:426:LEU:HB3  | 19:U:292:ILE:HG21 | 1.91                     | 0.52              |
| 16:J:186:ILE:HG12 | 16:J:292:MET:HB2  | 1.92                     | 0.52              |
| 23:H:359:ASN:HB2  | 23:H:466:TYR:O    | 2.09                     | 0.52              |
| 6:G:116:LEU:HB3   | 6:G:151:LEU:HD22  | 1.92                     | 0.52              |
| 9:D:13:PRO:HA     | 8:E:26:TYR:HB3    | 1.91                     | 0.52              |
| 27:g:184:VAL:HG22 | 27:g:189:ILE:HG12 | 1.91                     | 0.52              |
| 1:I:193:GLU:HG2   | 23:H:432:ARG:HH22 | 1.75                     | 0.52              |
| 11:N:36:TRP:HB2   | 11:N:68:VAL:HG13  | 1.91                     | 0.52              |
| 22:P:24:ILE:O     | 22:P:69:ARG:NH2   | 2.43                     | 0.52              |
| 5:3:13:VAL:HA     | 5:3:138:VAL:HG12  | 1.92                     | 0.52              |
| 27:4:78:GLN:HA    | 27:4:117:TYR:HE2  | 1.75                     | 0.52              |
| 26:b:18:LEU:HD13  | 26:b:64:ARG:HG2   | 1.91                     | 0.52              |
| 28:f:119:THR:HG1  | 28:f:175:MET:H    | 1.53                     | 0.52              |
| 27:g:44:MET:HE1   | 27:g:84:VAL:HG11  | 1.92                     | 0.52              |
| 8:m:71:ASP:OD1    | 8:m:72:ARG:N      | 2.41                     | 0.52              |
| 11:N:728:LYS:HB3  | 11:N:751:LEU:HB3  | 1.92                     | 0.52              |
| 17:L:166:LEU:HD21 | 18:M:83:VAL:HG12  | 1.92                     | 0.52              |
| 19:U:138:VAL:HB   | 19:U:155:LEU:HB3  | 1.92                     | 0.52              |
| 20:W:1:MET:HG2    | 20:W:2:VAL:HG13   | 1.92                     | 0.52              |
| 32:Z:204:CYS:HA   | 32:Z:207:ILE:HD12 | 1.90                     | 0.52              |
| 6:k:164:ALA:HB3   | 6:k:169:ARG:HG3   | 1.92                     | 0.52              |
| 12:S:141:LEU:HD22 | 12:S:155:LEU:HD11 | 1.92                     | 0.52              |
| 16:J:141:LYS:HB2  | 16:J:209:LYS:HG2  | 1.91                     | 0.52              |
| 16:J:195:LYS:HG2  | 16:J:316:PHE:HE2  | 1.74                     | 0.52              |
| 16:J:351:ASN:OD1  | 16:J:352:GLY:N    | 2.43                     | 0.52              |
| 23:H:105:ILE:HB   | 23:H:146:VAL:HG13 | 1.92                     | 0.52              |
| 23:H:430:ALA:HA   | 23:H:435:ARG:H    | 1.75                     | 0.52              |
| 4:A:106:TYR:OH    | 3:2:114:GLN:NE2   | 2.42                     | 0.52              |
| 32:Z:89:LEU:HD22  | 32:Z:125:THR:HG21 | 1.92                     | 0.52              |
| 32:Z:169:VAL:HG13 | 32:Z:179:SER:HB2  | 1.91                     | 0.52              |
| 32:Z:488:ALA:HB1  | 32:Z:899:GLN:HE22 | 1.75                     | 0.52              |
| 33:V:276:PRO:O    | 33:V:280:LEU:N    | 2.43                     | 0.52              |
| 1:I:221:LEU:HD23  | 1:I:229:LYS:HG2   | 1.91                     | 0.52              |
| 11:N:384:LYS:HA   | 11:N:390:LEU:HD11 | 1.91                     | 0.52              |
| 12:S:424:SER:HB3  | 13:T:192:ASN:HB3  | 1.91                     | 0.52              |
| 13:T:248:GLU:OE2  | 13:T:258:ASN:ND2  | 2.43                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:Q:97:LEU:HD23  | 15:Q:133:LEU:HD11 | 1.92                     | 0.52              |
| 16:J:86:VAL:HG11  | 16:J:115:LEU:HD11 | 1.92                     | 0.52              |
| 8:E:89:ILE:HG23   | 8:E:93:ARG:HD2    | 1.91                     | 0.52              |
| 28:5:110:ILE:HD11 | 28:5:120:MET:HE3  | 1.92                     | 0.52              |
| 2:K:261:ALA:HB1   | 2:K:312:VAL:HG22  | 1.92                     | 0.51              |
| 3:i:196:LEU:HB3   | 29:6:215:ILE:HB   | 1.91                     | 0.51              |
| 6:k:45:GLY:HA3    | 6:k:220:SER:HA    | 1.93                     | 0.51              |
| 7:l:54:ASP:OD1    | 7:l:55:GLU:N      | 2.43                     | 0.51              |
| 17:L:219:LEU:HD23 | 17:L:346:LYS:HG2  | 1.92                     | 0.51              |
| 5:3:53:ILE:HG22   | 5:3:60:VAL:HG22   | 1.92                     | 0.51              |
| 29:6:49:ILE:HG22  | 29:6:54:ILE:HG12  | 1.90                     | 0.51              |
| 1:I:80:GLU:OE2    | 32:Z:622:HIS:ND1  | 2.43                     | 0.51              |
| 14:R:177:LEU:HD23 | 14:R:180:PHE:HD2  | 1.75                     | 0.51              |
| 18:M:280:ILE:HB   | 18:M:325:ALA:HA   | 1.91                     | 0.51              |
| 4:A:61:ASP:OD1    | 4:A:62:LYS:N      | 2.43                     | 0.51              |
| 24:C:45:VAL:HG13  | 24:C:213:PHE:HE1  | 1.74                     | 0.51              |
| 27:4:96:ARG:NH2   | 28:5:166:LYS:O    | 2.43                     | 0.51              |
| 28:5:240:ALA:HB1  | 28:5:247:GLY:HA2  | 1.91                     | 0.51              |
| 28:f:236:ILE:HG21 | 28:f:250:VAL:HG11 | 1.91                     | 0.51              |
| 33:V:51:GLY:HA2   | 33:V:71:MET:HG2   | 1.92                     | 0.51              |
| 33:V:56:GLU:HA    | 33:V:135:ARG:HH22 | 1.75                     | 0.51              |
| 4:c:220:LYS:HB3   | 4:c:242:GLU:HB2   | 1.92                     | 0.51              |
| 11:N:4:THR:OG1    | 13:T:76:ASP:O     | 2.19                     | 0.51              |
| 11:N:165:ILE:HA   | 11:N:168:SER:HB3  | 1.92                     | 0.51              |
| 15:Q:35:SER:HB3   | 15:Q:46:VAL:HG22  | 1.92                     | 0.51              |
| 23:H:217:GLN:HE21 | 23:H:375:VAL:HG13 | 1.74                     | 0.51              |
| 30:7:256:LYS:HA   | 26:b:193:ARG:HH12 | 1.75                     | 0.51              |
| 30:a:47:MET:HE3   | 30:a:188:LEU:HD22 | 1.92                     | 0.51              |
| 30:a:48:LYS:HA    | 30:a:53:VAL:HG12  | 1.92                     | 0.51              |
| 29:e:47:ARG:NH1   | 29:e:215:ILE:O    | 2.43                     | 0.51              |
| 29:e:62:VAL:HA    | 29:e:72:SER:HB2   | 1.91                     | 0.51              |
| 29:e:83:LEU:O     | 29:e:87:PHE:N     | 2.38                     | 0.51              |
| 8:m:74:ILE:HG22   | 8:m:146:GLY:HA3   | 1.91                     | 0.51              |
| 21:O:342:ASP:OD1  | 22:P:358:SER:OG   | 2.26                     | 0.51              |
| 6:G:45:GLY:HA3    | 6:G:220:SER:HA    | 1.92                     | 0.51              |
| 24:C:56:LEU:HD13  | 25:B:161:ALA:HB3  | 1.93                     | 0.51              |
| 25:j:105:PRO:HG2  | 25:j:110:LEU:HB2  | 1.93                     | 0.51              |
| 2:K:123:LEU:HB3   | 2:K:126:LEU:HG    | 1.92                     | 0.51              |
| 6:k:152:GLU:OE1   | 6:k:156:SER:OG    | 2.28                     | 0.51              |
| 11:N:208:ARG:NH2  | 11:N:234:ASP:OD2  | 2.42                     | 0.51              |
| 30:a:62:SER:HB3   | 30:a:223:ARG:HE   | 1.75                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:b:40:THR:HG21  | 26:b:187:SER:HA   | 1.92                     | 0.51              |
| 3:i:43:ILE:HD12   | 3:i:63:LEU:HD22   | 1.93                     | 0.51              |
| 8:m:213:ASP:OD1   | 8:m:214:GLU:N     | 2.43                     | 0.51              |
| 16:J:183:LYS:HZ2  | 16:J:309:ARG:NH1  | 2.09                     | 0.51              |
| 17:L:285:ALA:HB1  | 18:M:299:ARG:HB2  | 1.93                     | 0.51              |
| 19:U:236:LEU:H    | 22:P:418:ASN:HD22 | 1.59                     | 0.51              |
| 23:H:308:PHE:HD2  | 23:H:353:PHE:HE1  | 1.56                     | 0.51              |
| 24:C:73:ILE:HA    | 24:C:139:GLY:HA2  | 1.93                     | 0.51              |
| 29:6:54:ILE:O     | 30:7:189:ARG:NH2  | 2.44                     | 0.51              |
| 29:6:113:GLN:HB2  | 29:6:150:TYR:HE2  | 1.76                     | 0.51              |
| 30:a:182:HIS:ND1  | 29:e:53:SER:OG    | 2.33                     | 0.51              |
| 30:a:215:ARG:HG2  | 30:a:247:VAL:HG13 | 1.93                     | 0.51              |
| 2:K:110:VAL:HG11  | 2:K:139:LEU:HD11  | 1.92                     | 0.51              |
| 2:K:190:LEU:HD21  | 16:J:370:LEU:HD22 | 1.93                     | 0.51              |
| 4:c:57:LYS:NZ     | 4:c:66:PRO:O      | 2.44                     | 0.51              |
| 5:h:68:ARG:NH1    | 24:d:103:ASN:OD1  | 2.43                     | 0.51              |
| 8:m:142:LEU:HB2   | 8:m:158:ALA:HB3   | 1.93                     | 0.51              |
| 11:N:366:THR:O    | 11:N:370:SER:N    | 2.44                     | 0.51              |
| 15:Q:47:ASP:OD1   | 15:Q:50:ARG:NH2   | 2.43                     | 0.51              |
| 15:Q:266:LEU:HD22 | 15:Q:278:VAL:HG13 | 1.93                     | 0.51              |
| 15:Q:357:VAL:H    | 15:Q:397:LEU:HB3  | 1.76                     | 0.51              |
| 19:U:32:ARG:HD3   | 19:U:94:HIS:HB3   | 1.93                     | 0.51              |
| 7:F:54:ASP:OD1    | 7:F:55:GLU:N      | 2.43                     | 0.51              |
| 32:Z:311:ALA:HB2  | 32:Z:345:GLU:HG3  | 1.93                     | 0.51              |
| 30:a:189:ARG:HH12 | 29:e:54:ILE:HB    | 1.75                     | 0.51              |
| 33:V:109:HIS:HB2  | 33:V:140:VAL:HG12 | 1.92                     | 0.51              |
| 1:I:117:HIS:CD2   | 23:H:172:MET:HE1  | 2.46                     | 0.51              |
| 2:K:156:SER:OG    | 17:L:126:ARG:NH2  | 2.44                     | 0.51              |
| 2:K:177:LEU:HB2   | 2:K:181:LYS:HE2   | 1.93                     | 0.51              |
| 5:h:57:ALA:HA     | 5:h:60:VAL:HB     | 1.93                     | 0.51              |
| 11:N:371:LEU:HD12 | 11:N:386:MET:HE2  | 1.91                     | 0.51              |
| 4:A:220:LYS:HD2   | 4:A:238:ALA:HB1   | 1.93                     | 0.51              |
| 26:1:213:GLU:OE1  | 30:a:226:ARG:NH1  | 2.37                     | 0.51              |
| 30:7:226:ARG:NH1  | 26:b:213:GLU:OE1  | 2.42                     | 0.51              |
| 30:a:50:ASP:HB2   | 30:a:199:PRO:HA   | 1.91                     | 0.51              |
| 33:V:44:GLY:O     | 33:V:45:VAL:HG22  | 2.10                     | 0.51              |
| 7:l:129:GLY:HA2   | 7:l:149:PRO:HB3   | 1.92                     | 0.51              |
| 12:S:224:LYS:HB3  | 16:J:25:GLN:HG3   | 1.93                     | 0.51              |
| 13:T:39:LEU:HD22  | 13:T:46:ILE:HG22  | 1.93                     | 0.51              |
| 18:M:308:LEU:HD11 | 18:M:323:VAL:HG11 | 1.92                     | 0.51              |
| 19:U:34:VAL:HG13  | 19:U:94:HIS:CD2   | 2.46                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:H:223:GLU:OE1  | 23:H:373:ARG:NH1  | 2.29                     | 0.51              |
| 9:D:172:ARG:NH1   | 8:E:56:SER:OG     | 2.42                     | 0.51              |
| 8:E:213:ASP:OD1   | 8:E:214:GLU:N     | 2.44                     | 0.51              |
| 24:C:209:ASP:OD1  | 24:C:210:ARG:N    | 2.44                     | 0.51              |
| 30:7:50:ASP:HB2   | 30:7:199:PRO:HA   | 1.93                     | 0.51              |
| 32:Z:253:VAL:HB   | 32:Z:254:PRO:HD3  | 1.92                     | 0.51              |
| 32:Z:377:ALA:HA   | 32:Z:380:ASN:HB3  | 1.93                     | 0.51              |
| 26:b:198:THR:HG23 | 26:b:200:ALA:H    | 1.75                     | 0.51              |
| 1:I:213:ILE:HG21  | 23:H:424:THR:HA   | 1.93                     | 0.51              |
| 8:m:93:ARG:HH11   | 28:f:143:LEU:HB3  | 1.76                     | 0.51              |
| 8:E:111:SER:HB2   | 29:6:98:HIS:HA    | 1.92                     | 0.51              |
| 25:B:32:VAL:HG11  | 25:B:63:LYS:HE3   | 1.93                     | 0.51              |
| 27:4:55:GLN:OE1   | 28:5:159:SER:OG   | 2.22                     | 0.51              |
| 2:K:208:GLY:HA3   | 2:K:334:LEU:HA    | 1.93                     | 0.50              |
| 12:S:238:LEU:HG   | 12:S:276:LEU:HD21 | 1.93                     | 0.50              |
| 20:W:185:ILE:HG22 | 20:W:191:ILE:HB   | 1.92                     | 0.50              |
| 23:H:147:ILE:HA   | 23:H:155:PHE:HB2  | 1.91                     | 0.50              |
| 6:G:183:HIS:CD2   | 6:G:187:LEU:HD12  | 2.47                     | 0.50              |
| 8:E:71:ASP:OD1    | 8:E:72:ARG:N      | 2.41                     | 0.50              |
| 24:C:84:ALA:O     | 24:C:88:ILE:HG12  | 2.11                     | 0.50              |
| 9:n:4:TYR:HD2     | 9:n:125:GLY:HA2   | 1.76                     | 0.50              |
| 11:N:580:ASN:OD1  | 11:N:581:ASP:N    | 2.45                     | 0.50              |
| 14:R:73:ASN:HB3   | 14:R:76:GLN:HE21  | 1.77                     | 0.50              |
| 19:U:260:ASN:HD21 | 21:O:304:ASN:HB3  | 1.76                     | 0.50              |
| 21:O:134:ALA:HB1  | 21:O:174:THR:HG21 | 1.91                     | 0.50              |
| 21:O:289:GLN:HG3  | 21:O:317:THR:HG21 | 1.94                     | 0.50              |
| 23:H:100:ALA:N    | 23:H:177:ASP:OD2  | 2.30                     | 0.50              |
| 27:4:8:ARG:N      | 27:4:129:PRO:O    | 2.43                     | 0.50              |
| 5:h:51:LEU:HA     | 5:h:108:VAL:O     | 2.11                     | 0.50              |
| 15:Q:104:PHE:HE2  | 15:Q:114:GLN:HB2  | 1.76                     | 0.50              |
| 8:E:101:LEU:O     | 29:6:114:HIS:NE2  | 2.43                     | 0.50              |
| 5:3:61:THR:OG1    | 27:4:85:ARG:NH1   | 2.45                     | 0.50              |
| 32:Z:900:LEU:HA   | 32:Z:903:MET:HE2  | 1.94                     | 0.50              |
| 24:d:45:VAL:HG13  | 24:d:213:PHE:HE1  | 1.76                     | 0.50              |
| 2:K:155:ASP:OD1   | 2:K:259:ARG:NH2   | 2.44                     | 0.50              |
| 5:h:90:LEU:HB2    | 25:j:101:TYR:HE1  | 1.76                     | 0.50              |
| 7:l:206:LEU:HD11  | 7:l:211:LEU:HD22  | 1.94                     | 0.50              |
| 9:n:82:SER:HB3    | 9:n:131:VAL:HG11  | 1.94                     | 0.50              |
| 11:N:769:PRO:HG2  | 11:N:771:PHE:HE2  | 1.76                     | 0.50              |
| 16:J:208:CYS:HA   | 16:J:242:PRO:HB2  | 1.92                     | 0.50              |
| 22:P:218:LEU:O    | 22:P:222:ASN:ND2  | 2.45                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:E:16:SER:N      | 8:E:20:ARG:O      | 2.43                     | 0.50              |
| 29:e:105:ILE:HG12 | 29:e:133:LEU:H    | 1.76                     | 0.50              |
| 3:i:248:ASN:O     | 5:h:45:HIS:NE2    | 2.43                     | 0.50              |
| 11:N:163:LEU:HD13 | 11:N:206:ILE:HG12 | 1.94                     | 0.50              |
| 19:U:132:LEU:HB2  | 33:V:224:GLY:HA3  | 1.93                     | 0.50              |
| 7:F:34:VAL:HG22   | 7:F:163:ALA:H     | 1.77                     | 0.50              |
| 9:D:17:ILE:O      | 9:D:21:GLU:HG3    | 2.11                     | 0.50              |
| 5:3:173:ASN:ND2   | 29:e:171:ASN:OD1  | 2.45                     | 0.50              |
| 27:4:177:LYS:NZ   | 27:g:169:GLU:O    | 2.44                     | 0.50              |
| 8:m:10:ARG:HH21   | 8:m:14:THR:HG21   | 1.75                     | 0.50              |
| 8:m:159:GLU:OE2   | 8:m:167:TYR:OH    | 2.30                     | 0.50              |
| 11:N:721:ASP:OD1  | 11:N:899:ASN:ND2  | 2.45                     | 0.50              |
| 12:S:282:ILE:HD11 | 13:T:127:GLN:HG3  | 1.94                     | 0.50              |
| 6:G:68:GLN:N      | 6:G:76:CYS:O      | 2.41                     | 0.50              |
| 6:G:130:ARG:HB2   | 7:F:11:VAL:HG12   | 1.94                     | 0.50              |
| 7:F:95:SER:HB3    | 7:F:101:ARG:HB2   | 1.94                     | 0.50              |
| 5:3:48:HIS:CE1    | 5:3:81:ALA:HB1    | 2.46                     | 0.50              |
| 27:g:8:ARG:NH1    | 27:g:128:LEU:O    | 2.43                     | 0.50              |
| 14:R:40:ILE:HG23  | 14:R:87:SER:HA    | 1.94                     | 0.50              |
| 14:R:70:TYR:HE2   | 14:R:81:HIS:HB2   | 1.76                     | 0.50              |
| 16:J:85:LEU:HD11  | 16:J:93:LYS:HB3   | 1.92                     | 0.50              |
| 18:M:218:ALA:HB1  | 18:M:345:ARG:HB2  | 1.94                     | 0.50              |
| 25:j:65:SER:OG    | 25:j:90:ARG:NH2   | 2.44                     | 0.50              |
| 33:V:24:LYS:HD2   | 33:V:172:GLN:HG3  | 1.93                     | 0.50              |
| 1:I:150:HIS:N     | 1:I:155:SER:O     | 2.43                     | 0.50              |
| 11:N:117:TYR:O    | 11:N:201:LYS:NZ   | 2.42                     | 0.50              |
| 14:R:118:GLN:NE2  | 14:R:122:GLU:OE2  | 2.42                     | 0.50              |
| 17:L:149:ASP:OD2  | 17:L:152:THR:N    | 2.45                     | 0.50              |
| 18:M:170:MET:HE3  | 23:H:180:LYS:NZ   | 2.27                     | 0.50              |
| 23:H:258:LEU:HD23 | 23:H:261:ARG:HH21 | 1.77                     | 0.50              |
| 9:D:56:ASP:OD1    | 9:D:57:THR:N      | 2.45                     | 0.50              |
| 25:B:173:THR:HG22 | 25:B:177:LYS:HE3  | 1.93                     | 0.50              |
| 3:2:43:ILE:HD12   | 3:2:63:LEU:HD22   | 1.93                     | 0.50              |
| 3:2:121:GLY:O     | 3:2:145:HIS:NE2   | 2.44                     | 0.50              |
| 30:a:61:GLY:N     | 30:a:69:PHE:O     | 2.44                     | 0.50              |
| 28:f:240:ALA:HB1  | 28:f:247:GLY:HA2  | 1.92                     | 0.50              |
| 33:V:51:GLY:HA3   | 33:V:70:ALA:HA    | 1.93                     | 0.50              |
| 33:V:171:ARG:NH2  | 33:V:177:THR:O    | 2.43                     | 0.50              |
| 14:R:209:ARG:HA   | 14:R:243:LEU:HD21 | 1.93                     | 0.50              |
| 4:A:54:ILE:HG23   | 4:A:225:VAL:HG22  | 1.94                     | 0.50              |
| 33:V:110:SER:HB3  | 33:V:143:PRO:HD3  | 1.94                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:K:295:ILE:O     | 2:K:299:LEU:N     | 2.40                     | 0.49              |
| 9:n:70:HIS:HB3    | 9:n:138:PHE:HB2   | 1.94                     | 0.49              |
| 11:N:158:LEU:HD13 | 11:N:196:THR:HG21 | 1.94                     | 0.49              |
| 11:N:250:ASP:HB3  | 11:N:253:LEU:HB3  | 1.94                     | 0.49              |
| 7:F:88:LEU:HD22   | 7:F:112:LEU:HD11  | 1.94                     | 0.49              |
| 30:7:60:LEU:HD21  | 30:7:67:LEU:HD13  | 1.93                     | 0.49              |
| 33:V:35:LEU:HD23  | 33:V:38:LEU:HD12  | 1.93                     | 0.49              |
| 1:I:147:VAL:HA    | 1:I:159:VAL:HA    | 1.94                     | 0.49              |
| 4:c:73:PHE:HB2    | 4:c:81:MET:HE2    | 1.92                     | 0.49              |
| 17:L:139:LYS:HB2  | 17:L:158:ILE:HD13 | 1.95                     | 0.49              |
| 21:O:4:ASN:HD22   | 21:O:39:PHE:HD2   | 1.60                     | 0.49              |
| 21:O:134:ALA:HA   | 21:O:149:LEU:HD23 | 1.95                     | 0.49              |
| 22:P:392:LYS:HE3  | 22:P:404:LYS:HG2  | 1.93                     | 0.49              |
| 7:F:95:SER:O      | 7:F:100:ASN:N     | 2.45                     | 0.49              |
| 8:E:122:ARG:HD2   | 8:E:130:GLU:HB2   | 1.93                     | 0.49              |
| 2:K:86:VAL:HA     | 2:K:89:ILE:HD12   | 1.93                     | 0.49              |
| 12:S:242:LEU:HD21 | 12:S:275:TYR:HB3  | 1.93                     | 0.49              |
| 21:O:56:PRO:HG3   | 21:O:85:SER:HB3   | 1.94                     | 0.49              |
| 4:A:106:TYR:HE1   | 26:1:77:ILE:HG12  | 1.76                     | 0.49              |
| 32:Z:243:GLN:NE2  | 32:Z:974:THR:O    | 2.45                     | 0.49              |
| 24:d:72:LYS:HG3   | 24:d:73:ILE:HG13  | 1.93                     | 0.49              |
| 26:b:15:GLU:OE1   | 26:b:67:SER:OG    | 2.29                     | 0.49              |
| 27:g:34:LYS:HD3   | 27:g:53:THR:HG21  | 1.94                     | 0.49              |
| 1:I:340:ARG:NH1   | 1:I:343:ARG:HG2   | 2.28                     | 0.49              |
| 1:I:347:LYS:NZ    | 23:H:454:TYR:O    | 2.31                     | 0.49              |
| 3:i:41:VAL:HG13   | 3:i:207:MET:HE3   | 1.93                     | 0.49              |
| 7:l:105:VAL:HB    | 7:l:145:LEU:HB2   | 1.93                     | 0.49              |
| 7:l:172:LEU:HD11  | 7:l:196:ALA:HB2   | 1.95                     | 0.49              |
| 8:m:41:ALA:HB2    | 8:m:155:LEU:HB2   | 1.95                     | 0.49              |
| 11:N:622:ALA:HB1  | 11:N:659:ALA:HB2  | 1.95                     | 0.49              |
| 16:J:306:ARG:HD2  | 16:J:309:ARG:HG2  | 1.93                     | 0.49              |
| 17:L:74:LEU:HD23  | 17:L:77:ARG:HD2   | 1.94                     | 0.49              |
| 19:U:156:HIS:NE2  | 22:P:427:GLU:OE2  | 2.37                     | 0.49              |
| 19:U:208:VAL:HG22 | 21:O:367:LYS:HZ3  | 1.76                     | 0.49              |
| 20:W:103:ASN:OD1  | 33:V:96:LYS:NZ    | 2.43                     | 0.49              |
| 21:O:80:LYS:HA    | 21:O:119:SER:HA   | 1.95                     | 0.49              |
| 24:C:72:LYS:HG3   | 24:C:73:ILE:HG13  | 1.94                     | 0.49              |
| 29:6:164:LEU:HD21 | 29:6:213:ARG:HB2  | 1.93                     | 0.49              |
| 30:7:47:MET:HE3   | 30:7:188:LEU:HD22 | 1.93                     | 0.49              |
| 30:7:48:LYS:HA    | 30:7:53:VAL:HG12  | 1.94                     | 0.49              |
| 1:I:226:GLY:H     | 1:I:230:THR:HB    | 1.77                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:m:208:MET:HG2   | 8:m:210:GLU:H     | 1.77                     | 0.49              |
| 14:R:280:ILE:HG12 | 14:R:289:ILE:HD12 | 1.94                     | 0.49              |
| 18:M:352:PRO:O    | 18:M:357:ARG:NH1  | 2.45                     | 0.49              |
| 23:H:205:ASP:OD2  | 32:Z:832:ARG:NH2  | 2.42                     | 0.49              |
| 8:E:51:GLU:HG2    | 8:E:53:ARG:HG3    | 1.94                     | 0.49              |
| 24:C:101:THR:HG23 | 27:4:83:PHE:CD1   | 2.47                     | 0.49              |
| 30:a:168:VAL:HA   | 29:e:77:ALA:HB3   | 1.95                     | 0.49              |
| 1:I:109:LEU:O     | 1:I:144:GLY:N     | 2.43                     | 0.49              |
| 19:U:46:ILE:HD13  | 19:U:119:LEU:HD22 | 1.94                     | 0.49              |
| 5:3:138:VAL:HG23  | 5:3:143:SER:HB2   | 1.94                     | 0.49              |
| 11:N:535:LEU:HG   | 11:N:539:MET:HE2  | 1.95                     | 0.49              |
| 14:R:263:ARG:HH21 | 15:Q:382:LEU:HB2  | 1.77                     | 0.49              |
| 17:L:339:ARG:NH1  | 17:L:341:GLY:HA3  | 2.27                     | 0.49              |
| 20:W:81:ILE:HG21  | 21:O:115:ARG:HG3  | 1.94                     | 0.49              |
| 26:l:113:THR:HB   | 26:l:134:LEU:HD11 | 1.93                     | 0.49              |
| 26:b:39:THR:HG1   | 26:b:50:THR:HG1   | 1.61                     | 0.49              |
| 1:I:243:THR:HB    | 1:I:276:PRO:HG2   | 1.95                     | 0.49              |
| 2:K:99:PHE:HZ     | 2:K:102:PRO:HD3   | 1.77                     | 0.49              |
| 5:h:50:PHE:CZ     | 5:h:195:VAL:HG21  | 2.47                     | 0.49              |
| 16:J:211:ILE:HB   | 16:J:245:ILE:HA   | 1.93                     | 0.49              |
| 17:L:88:TYR:HB3   | 18:M:62:ILE:HG12  | 1.95                     | 0.49              |
| 18:M:181:SER:O    | 18:M:366:ARG:NH2  | 2.46                     | 0.49              |
| 21:O:70:TYR:HB3   | 21:O:75:GLN:HB2   | 1.95                     | 0.49              |
| 23:H:449:LYS:O    | 23:H:454:TYR:N    | 2.46                     | 0.49              |
| 8:E:18:GLU:OE1    | 8:E:20:ARG:NH2    | 2.45                     | 0.49              |
| 27:4:85:ARG:HB2   | 27:4:119:ILE:HD13 | 1.94                     | 0.49              |
| 31:X:120:GLU:HG2  | 31:X:124:LYS:HE3  | 1.95                     | 0.49              |
| 26:b:151:THR:HA   | 26:b:154:TYR:CE2  | 2.48                     | 0.49              |
| 28:f:110:ILE:HD11 | 28:f:120:MET:HE3  | 1.95                     | 0.49              |
| 28:f:126:ASP:HB3  | 28:f:172:MET:HB3  | 1.94                     | 0.49              |
| 33:V:202:ASP:OD1  | 33:V:203:TYR:N    | 2.45                     | 0.49              |
| 6:k:108:PRO:HB2   | 6:k:110:PRO:HD2   | 1.95                     | 0.49              |
| 11:N:9:LEU:HD21   | 13:T:80:ASN:HD22  | 1.78                     | 0.49              |
| 16:J:188:TYR:HA   | 16:J:195:LYS:HZ2  | 1.78                     | 0.49              |
| 18:M:145:LEU:HD11 | 18:M:163:PHE:HA   | 1.93                     | 0.49              |
| 20:W:148:GLU:HB3  | 21:O:14:LEU:HD22  | 1.94                     | 0.49              |
| 21:O:44:SER:HA    | 21:O:73:ILE:HD12  | 1.93                     | 0.49              |
| 22:P:168:TYR:HB3  | 22:P:171:MET:HB2  | 1.94                     | 0.49              |
| 27:4:55:GLN:NE2   | 28:5:160:ASN:OD1  | 2.46                     | 0.49              |
| 30:a:98:ARG:NH1   | 26:b:103:GLU:OE2  | 2.34                     | 0.49              |
| 26:b:108:ASN:O    | 26:b:112:LEU:N    | 2.46                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:I:282:ASP:OD1   | 1:I:283:GLU:HG2   | 2.12                     | 0.49              |
| 2:K:104:ASP:OD1   | 2:K:105:GLN:N     | 2.42                     | 0.49              |
| 6:k:183:HIS:CD2   | 6:k:187:LEU:HD12  | 2.48                     | 0.49              |
| 9:n:98:LEU:O      | 28:f:156:LYS:NZ   | 2.39                     | 0.49              |
| 11:N:588:VAL:HG11 | 11:N:623:PHE:HD2  | 1.78                     | 0.49              |
| 11:N:762:ARG:HB3  | 11:N:767:ALA:H    | 1.77                     | 0.49              |
| 11:N:762:ARG:HH21 | 11:N:913:PRO:HB3  | 1.77                     | 0.49              |
| 15:Q:326:MET:HG2  | 15:Q:335:PHE:HD2  | 1.78                     | 0.49              |
| 16:J:279:LEU:HD13 | 16:J:286:LYS:HG3  | 1.93                     | 0.49              |
| 20:W:5:ALA:N      | 20:W:107:HIS:O    | 2.42                     | 0.49              |
| 23:H:72:SER:HB3   | 23:H:107:LYS:HE3  | 1.95                     | 0.49              |
| 23:H:450:VAL:HA   | 23:H:454:TYR:HB3  | 1.94                     | 0.49              |
| 26:1:185:ASP:OD1  | 26:1:186:GLY:N    | 2.46                     | 0.49              |
| 27:4:8:ARG:NH1    | 27:4:128:LEU:O    | 2.45                     | 0.49              |
| 27:4:145:ASP:HB3  | 28:f:282:PHE:HA   | 1.94                     | 0.49              |
| 27:4:171:ARG:HH22 | 28:f:201:ILE:HD12 | 1.78                     | 0.49              |
| 29:6:47:ARG:HB2   | 29:6:219:ASP:HB2  | 1.95                     | 0.49              |
| 32:Z:419:VAL:O    | 32:Z:423:GLY:N    | 2.44                     | 0.49              |
| 2:K:208:GLY:HA3   | 2:K:335:ASP:H     | 1.78                     | 0.48              |
| 15:Q:223:GLY:HA2  | 15:Q:226:HIS:HD2  | 1.76                     | 0.48              |
| 6:G:165:THR:HA    | 6:G:169:ARG:HE    | 1.78                     | 0.48              |
| 9:D:39:LYS:HD2    | 9:D:186:ALA:HA    | 1.94                     | 0.48              |
| 25:B:42:GLY:HA3   | 25:B:185:LEU:HD13 | 1.95                     | 0.48              |
| 26:1:15:GLU:OE1   | 26:1:67:SER:OG    | 2.30                     | 0.48              |
| 3:2:141:SER:HB2   | 3:2:154:LEU:HD13  | 1.94                     | 0.48              |
| 28:5:260:TRP:HZ3  | 28:5:262:TYR:HB2  | 1.77                     | 0.48              |
| 25:j:97:TYR:CD2   | 25:j:105:PRO:HB3  | 2.47                     | 0.48              |
| 1:I:77:SER:HB3    | 1:I:81:ILE:HB     | 1.96                     | 0.48              |
| 11:N:150:LEU:HD21 | 11:N:189:LEU:HB2  | 1.95                     | 0.48              |
| 23:H:270:THR:HB   | 23:H:304:CYS:HA   | 1.94                     | 0.48              |
| 24:C:38:ILE:HB    | 24:C:45:VAL:HB    | 1.94                     | 0.48              |
| 31:X:117:LYS:HD3  | 31:X:120:GLU:HB2  | 1.94                     | 0.48              |
| 27:g:8:ARG:N      | 27:g:129:PRO:O    | 2.37                     | 0.48              |
| 8:m:36:THR:HG21   | 8:m:207:VAL:HG11  | 1.95                     | 0.48              |
| 12:S:406:ASP:HB2  | 14:R:384:VAL:HB   | 1.95                     | 0.48              |
| 14:R:214:TYR:OH   | 14:R:226:GLU:OE1  | 2.25                     | 0.48              |
| 15:Q:65:TYR:HA    | 15:Q:70:ALA:HB3   | 1.94                     | 0.48              |
| 21:O:99:LEU:HD22  | 21:O:129:ILE:HA   | 1.95                     | 0.48              |
| 23:H:145:TYR:CZ   | 23:H:160:GLY:HA2  | 2.47                     | 0.48              |
| 4:A:73:PHE:HB2    | 4:A:81:MET:HE2    | 1.95                     | 0.48              |
| 26:1:38:ARG:HG2   | 26:1:40:THR:HG23  | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:b:83:GLU:O     | 26:b:87:SER:OG    | 2.27                     | 0.48              |
| 33:V:27:VAL:HB    | 33:V:201:ILE:HA   | 1.95                     | 0.48              |
| 4:c:15:HIS:CE1    | 6:k:7:GLY:HA2     | 2.48                     | 0.48              |
| 4:c:54:ILE:HG23   | 4:c:225:VAL:HG22  | 1.94                     | 0.48              |
| 13:T:78:PHE:O     | 13:T:82:PHE:N     | 2.42                     | 0.48              |
| 18:M:339:ARG:HE   | 18:M:342:ARG:HG3  | 1.77                     | 0.48              |
| 19:U:124:ASP:OD1  | 19:U:125:VAL:N    | 2.46                     | 0.48              |
| 7:F:45:VAL:HG11   | 7:F:190:ILE:HA    | 1.94                     | 0.48              |
| 9:D:106:VAL:HB    | 9:D:146:LYS:HD2   | 1.95                     | 0.48              |
| 5:3:18:LYS:HB2    | 5:3:157:ASN:HA    | 1.94                     | 0.48              |
| 28:5:236:ILE:HG21 | 28:5:250:VAL:HG11 | 1.95                     | 0.48              |
| 32:Z:376:SER:O    | 32:Z:380:ASN:N    | 2.46                     | 0.48              |
| 26:b:185:ASP:OD1  | 26:b:186:GLY:N    | 2.46                     | 0.48              |
| 29:e:46:THR:OG1   | 29:e:219:ASP:O    | 2.31                     | 0.48              |
| 33:V:73:GLN:HE22  | 33:V:77:GLY:HA2   | 1.79                     | 0.48              |
| 13:T:94:HIS:NE2   | 13:T:96:LEU:HB2   | 2.29                     | 0.48              |
| 16:J:183:LYS:HD2  | 16:J:309:ARG:HA   | 1.95                     | 0.48              |
| 17:L:113:SER:OG   | 17:L:116:LYS:O    | 2.29                     | 0.48              |
| 19:U:8:VAL:HG11   | 19:U:121:LEU:HD21 | 1.94                     | 0.48              |
| 19:U:232:VAL:HG21 | 21:O:370:LEU:HD11 | 1.96                     | 0.48              |
| 23:H:58:ASP:O     | 23:H:62:ARG:N     | 2.47                     | 0.48              |
| 8:E:74:ILE:HG22   | 8:E:146:GLY:HA3   | 1.96                     | 0.48              |
| 3:2:66:ILE:HG23   | 3:2:89:GLY:HA2    | 1.95                     | 0.48              |
| 2:K:191:PRO:HB3   | 2:K:198:TYR:HE2   | 1.79                     | 0.48              |
| 2:K:259:ARG:NH1   | 2:K:263:GLU:OE2   | 2.47                     | 0.48              |
| 8:m:110:GLU:HA    | 8:m:156:PHE:HE2   | 1.78                     | 0.48              |
| 11:N:13:LEU:HD13  | 11:N:55:PHE:HB2   | 1.95                     | 0.48              |
| 11:N:762:ARG:NH1  | 11:N:764:SER:HB2  | 2.29                     | 0.48              |
| 12:S:452:TYR:HA   | 12:S:457:PRO:HD3  | 1.95                     | 0.48              |
| 6:G:68:GLN:HG3    | 6:G:89:VAL:HG21   | 1.95                     | 0.48              |
| 9:D:19:GLN:HE22   | 24:C:12:ILE:HB    | 1.79                     | 0.48              |
| 25:B:70:ASP:HB3   | 25:B:139:HIS:HB3  | 1.95                     | 0.48              |
| 30:7:215:ARG:HG2  | 30:7:247:VAL:HG13 | 1.96                     | 0.48              |
| 20:W:19:GLY:HA3   | 21:O:71:ASP:HA    | 1.96                     | 0.48              |
| 6:G:40:ILE:HB     | 6:G:47:VAL:HB     | 1.95                     | 0.48              |
| 8:E:93:ARG:HD3    | 28:5:143:LEU:HD22 | 1.95                     | 0.48              |
| 5:3:10:GLY:N      | 5:3:180:LEU:O     | 2.47                     | 0.48              |
| 26:b:16:VAL:HG11  | 26:b:39:THR:HG23  | 1.94                     | 0.48              |
| 3:i:48:ARG:NH2    | 29:6:212:GLU:OE1  | 2.47                     | 0.48              |
| 5:h:90:LEU:HB2    | 25:j:101:TYR:CE1  | 2.48                     | 0.48              |
| 6:k:220:SER:O     | 6:k:224:THR:OG1   | 2.32                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:N:352:ASN:HB2  | 11:N:355:TRP:NE1  | 2.28                     | 0.48              |
| 11:N:694:LEU:HB2  | 33:V:175:SER:HB3  | 1.96                     | 0.48              |
| 14:R:368:LEU:HD11 | 14:R:381:ILE:HG13 | 1.96                     | 0.48              |
| 15:Q:130:ARG:NH2  | 25:B:186:GLU:OE1  | 2.46                     | 0.48              |
| 7:F:38:LEU:HA     | 7:F:158:GLY:HA2   | 1.96                     | 0.48              |
| 25:B:69:PRO:HB2   | 25:B:233:PRO:HA   | 1.95                     | 0.48              |
| 5:h:58:THR:O      | 5:h:62:THR:HB     | 2.13                     | 0.48              |
| 6:k:56:SER:OG     | 7:l:173:GLU:OE2   | 2.29                     | 0.48              |
| 11:N:498:ILE:HG23 | 11:N:521:LEU:HD22 | 1.95                     | 0.48              |
| 22:P:94:GLN:HG2   | 22:P:131:PHE:CD1  | 2.48                     | 0.48              |
| 8:E:159:GLU:OE1   | 8:E:163:THR:OG1   | 2.32                     | 0.48              |
| 5:3:74:TYR:CE2    | 5:3:82:ILE:HB     | 2.49                     | 0.48              |
| 29:6:46:THR:OG1   | 29:6:219:ASP:O    | 2.29                     | 0.48              |
| 32:Z:224:LEU:HD23 | 32:Z:227:ILE:HD11 | 1.96                     | 0.48              |
| 32:Z:597:SER:HB2  | 32:Z:623:ARG:HH21 | 1.79                     | 0.48              |
| 6:k:47:VAL:HG13   | 6:k:218:TRP:HB3   | 1.96                     | 0.48              |
| 16:J:85:LEU:HA    | 16:J:95:ILE:HA    | 1.96                     | 0.48              |
| 17:L:282:GLU:HG3  | 18:M:310:ASN:HD21 | 1.78                     | 0.48              |
| 18:M:56:ASN:HA    | 18:M:60:GLU:HB2   | 1.96                     | 0.48              |
| 18:M:223:PRO:HG3  | 18:M:387:ASN:HD22 | 1.79                     | 0.48              |
| 19:U:24:ARG:HH21  | 33:V:66:VAL:HG11  | 1.79                     | 0.48              |
| 22:P:416:SER:HB3  | 33:V:232:GLU:HG2  | 1.95                     | 0.48              |
| 23:H:183:ILE:O    | 23:H:188:PRO:HB3  | 2.14                     | 0.48              |
| 25:B:44:VAL:HG22  | 25:B:213:ILE:HG22 | 1.95                     | 0.48              |
| 26:1:108:ASN:O    | 26:1:112:LEU:N    | 2.46                     | 0.48              |
| 26:1:172:ASP:O    | 26:1:176:HIS:ND1  | 2.32                     | 0.48              |
| 29:6:47:ARG:NH2   | 29:6:241:ASP:OD1  | 2.46                     | 0.48              |
| 29:6:156:ARG:HA   | 29:6:166:MET:SD   | 2.54                     | 0.48              |
| 30:7:36:GLN:HE21  | 30:7:38:ILE:HD11  | 1.78                     | 0.48              |
| 30:7:42:THR:HG22  | 30:7:223:ARG:HB3  | 1.95                     | 0.48              |
| 30:a:120:LEU:HD11 | 30:a:125:ILE:HD12 | 1.96                     | 0.48              |
| 1:I:287:ILE:HA    | 1:I:302:ILE:HG23  | 1.96                     | 0.47              |
| 4:c:174:LYS:HD3   | 4:c:213:ALA:HB1   | 1.95                     | 0.47              |
| 5:h:93:SER:O      | 5:h:97:GLU:HG3    | 2.15                     | 0.47              |
| 7:l:100:ASN:HB3   | 30:a:124:TYR:HA   | 1.95                     | 0.47              |
| 14:R:335:ARG:O    | 14:R:339:ALA:N    | 2.42                     | 0.47              |
| 17:L:357:ARG:NH2  | 17:L:383:SER:OG   | 2.47                     | 0.47              |
| 17:L:370:LYS:HB2  | 17:L:410:ILE:H    | 1.79                     | 0.47              |
| 20:W:68:GLU:HG2   | 20:W:70:GLY:H     | 1.79                     | 0.47              |
| 22:P:22:PRO:O     | 22:P:26:SER:OG    | 2.30                     | 0.47              |
| 4:A:147:ASP:OD1   | 4:A:148:GLU:N     | 2.47                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:A:164:VAL:HG22  | 4:A:165:GLY:H     | 1.78                     | 0.47              |
| 5:3:145:GLN:HG2   | 29:e:163:SER:HB2  | 1.96                     | 0.47              |
| 32:Z:286:VAL:C    | 32:Z:288:LEU:H    | 2.22                     | 0.47              |
| 24:d:141:ASP:OD1  | 24:d:142:ASP:N    | 2.46                     | 0.47              |
| 30:a:211:VAL:HG13 | 30:a:228:PHE:HZ   | 1.78                     | 0.47              |
| 2:K:388:GLN:HE22  | 17:L:212:ILE:HB   | 1.79                     | 0.47              |
| 5:h:7:ILE:HG23    | 5:h:32:GLN:HG3    | 1.95                     | 0.47              |
| 8:m:133:LEU:HB3   | 9:n:124:GLY:H     | 1.78                     | 0.47              |
| 9:n:71:VAL:HG22   | 9:n:137:GLY:HA3   | 1.96                     | 0.47              |
| 9:n:94:GLN:O      | 9:n:98:LEU:N      | 2.39                     | 0.47              |
| 11:N:122:GLN:NE2  | 11:N:164:ASP:OD2  | 2.47                     | 0.47              |
| 11:N:596:LEU:HD21 | 11:N:627:ILE:HG22 | 1.95                     | 0.47              |
| 12:S:224:LYS:HE3  | 12:S:225:HIS:HE1  | 1.78                     | 0.47              |
| 14:R:410:LEU:HD21 | 19:U:285:ILE:HD11 | 1.95                     | 0.47              |
| 21:O:162:SER:HB2  | 21:O:167:ILE:HD13 | 1.96                     | 0.47              |
| 23:H:148:ASN:H    | 23:H:155:PHE:HB2  | 1.80                     | 0.47              |
| 23:H:177:ASP:O    | 23:H:178:ARG:HG2  | 2.13                     | 0.47              |
| 23:H:450:VAL:O    | 23:H:455:LYS:N    | 2.38                     | 0.47              |
| 4:A:46:ARG:HH21   | 4:A:167:LYS:HA    | 1.79                     | 0.47              |
| 9:D:37:LYS:HA     | 9:D:42:VAL:HG23   | 1.95                     | 0.47              |
| 28:5:82:ARG:HD2   | 28:5:185:PRO:HB2  | 1.96                     | 0.47              |
| 29:6:57:ARG:HH21  | 30:7:189:ARG:HD3  | 1.80                     | 0.47              |
| 1:I:150:HIS:HB3   | 1:I:155:SER:H     | 1.79                     | 0.47              |
| 9:n:56:ASP:HB3    | 9:n:59:ILE:HG12   | 1.95                     | 0.47              |
| 15:Q:168:LEU:HD23 | 25:B:177:LYS:HB3  | 1.95                     | 0.47              |
| 15:Q:199:THR:OG1  | 16:J:380:GLU:OE2  | 2.30                     | 0.47              |
| 17:L:133:ASN:N    | 33:V:45:VAL:HG11  | 2.30                     | 0.47              |
| 18:M:145:LEU:HD21 | 18:M:163:PHE:HD1  | 1.78                     | 0.47              |
| 21:O:271:LYS:H    | 21:O:274:ILE:HG22 | 1.79                     | 0.47              |
| 23:H:176:VAL:HG21 | 23:H:191:ILE:HG13 | 1.96                     | 0.47              |
| 23:H:225:VAL:HG22 | 23:H:350:LYS:HG3  | 1.97                     | 0.47              |
| 6:G:220:SER:O     | 6:G:224:THR:OG1   | 2.33                     | 0.47              |
| 30:7:86:ILE:HG12  | 30:7:147:ILE:HG12 | 1.96                     | 0.47              |
| 24:d:84:ALA:O     | 24:d:88:ILE:HG12  | 2.14                     | 0.47              |
| 29:e:203:VAL:HG12 | 29:e:221:LEU:HD21 | 1.96                     | 0.47              |
| 1:I:295:ASN:ND2   | 23:H:312:ASP:O    | 2.46                     | 0.47              |
| 2:K:94:LEU:HB2    | 17:L:128:ILE:HB   | 1.96                     | 0.47              |
| 3:i:84:VAL:HG13   | 3:i:88:ILE:HD12   | 1.97                     | 0.47              |
| 5:h:26:ASP:OD1    | 5:h:42:LYS:NZ     | 2.32                     | 0.47              |
| 7:l:19:LEU:HG     | 7:l:21:GLN:H      | 1.78                     | 0.47              |
| 13:T:94:HIS:HD2   | 13:T:97:SER:HB2   | 1.78                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:M:173:ASP:OD2  | 18:M:233:ARG:NH2  | 2.47                     | 0.47              |
| 7:F:18:ARG:HH12   | 7:F:23:GLU:HB2    | 1.80                     | 0.47              |
| 26:b:39:THR:HB    | 26:b:47:ASN:H     | 1.79                     | 0.47              |
| 2:K:121:ARG:H     | 16:J:65:LEU:HD21  | 1.79                     | 0.47              |
| 3:i:58:LYS:HD3    | 29:6:212:GLU:HB3  | 1.96                     | 0.47              |
| 5:h:173:ASN:ND2   | 29:6:171:ASN:OD1  | 2.47                     | 0.47              |
| 5:h:179:ALA:HB2   | 28:5:101:VAL:HG23 | 1.97                     | 0.47              |
| 9:n:106:VAL:HB    | 9:n:146:LYS:HD2   | 1.95                     | 0.47              |
| 6:G:152:GLU:OE1   | 6:G:156:SER:OG    | 2.32                     | 0.47              |
| 32:Z:322:GLU:HA   | 32:Z:327:GLN:HB2  | 1.97                     | 0.47              |
| 32:Z:471:LEU:HD22 | 32:Z:504:GLU:HB3  | 1.97                     | 0.47              |
| 33:V:123:VAL:HG12 | 33:V:127:LYS:HE3  | 1.96                     | 0.47              |
| 7:l:226:ASP:OD1   | 7:l:227:GLY:N     | 2.48                     | 0.47              |
| 11:N:307:LYS:NZ   | 11:N:339:MET:O    | 2.47                     | 0.47              |
| 17:L:236:ALA:HA   | 17:L:239:ILE:HD12 | 1.96                     | 0.47              |
| 18:M:167:VAL:O    | 18:M:169:ALA:N    | 2.48                     | 0.47              |
| 18:M:250:GLN:O    | 18:M:253:GLN:NE2  | 2.45                     | 0.47              |
| 32:Z:392:LEU:HB3  | 32:Z:858:GLY:HA2  | 1.97                     | 0.47              |
| 24:d:129:ARG:HB3  | 25:j:123:GLN:HE22 | 1.79                     | 0.47              |
| 27:g:35:THR:O     | 27:g:36:ARG:NH1   | 2.39                     | 0.47              |
| 1:I:228:GLY:HA2   | 1:I:231:LEU:HB2   | 1.97                     | 0.47              |
| 2:K:118:TYR:HB3   | 16:J:69:GLY:HA3   | 1.96                     | 0.47              |
| 2:K:224:LYS:NZ    | 17:L:313:ASP:O    | 2.36                     | 0.47              |
| 2:K:366:ALA:HA    | 2:K:404:GLN:HB2   | 1.96                     | 0.47              |
| 3:i:55:VAL:HB     | 29:6:213:ARG:HA   | 1.96                     | 0.47              |
| 8:m:117:CYS:HA    | 8:m:120:ALA:HB3   | 1.97                     | 0.47              |
| 9:n:17:ILE:HG22   | 9:n:19:GLN:H      | 1.79                     | 0.47              |
| 9:n:139:ASP:HB2   | 9:n:142:ASP:HB3   | 1.97                     | 0.47              |
| 11:N:34:GLN:HE22  | 12:S:216:LYS:HA   | 1.78                     | 0.47              |
| 13:T:152:LEU:HD21 | 13:T:185:ILE:HG12 | 1.96                     | 0.47              |
| 13:T:213:ASN:OD1  | 13:T:214:GLU:N    | 2.47                     | 0.47              |
| 15:Q:387:TYR:HB2  | 15:Q:401:GLU:HB2  | 1.97                     | 0.47              |
| 16:J:375:ILE:HG13 | 16:J:376:HIS:ND1  | 2.28                     | 0.47              |
| 17:L:95:ILE:HD11  | 18:M:69:ILE:HD11  | 1.96                     | 0.47              |
| 19:U:46:ILE:HG23  | 19:U:90:ILE:HD12  | 1.97                     | 0.47              |
| 21:O:75:GLN:HG2   | 21:O:107:GLN:NE2  | 2.30                     | 0.47              |
| 22:P:89:LEU:O     | 22:P:92:SER:OG    | 2.30                     | 0.47              |
| 23:H:55:ASP:HA    | 23:H:58:ASP:HB2   | 1.96                     | 0.47              |
| 7:F:31:GLN:HG3    | 8:E:18:GLU:HB3    | 1.97                     | 0.47              |
| 26:1:193:ARG:HH12 | 30:a:256:LYS:HA   | 1.80                     | 0.47              |
| 5:3:58:THR:O      | 5:3:62:THR:HB     | 2.14                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:7:152:VAL:HA   | 30:7:158:GLN:HA   | 1.97                     | 0.47              |
| 24:d:38:ILE:HB    | 24:d:45:VAL:HB    | 1.95                     | 0.47              |
| 30:a:41:GLY:C     | 30:a:223:ARG:HH12 | 2.23                     | 0.47              |
| 26:b:172:ASP:O    | 26:b:176:HIS:ND1  | 2.33                     | 0.47              |
| 29:e:94:TYR:O     | 29:e:98:HIS:ND1   | 2.47                     | 0.47              |
| 33:V:153:ILE:HG22 | 33:V:201:ILE:HB   | 1.96                     | 0.47              |
| 33:V:163:ALA:HB3  | 33:V:168:LEU:HD22 | 1.97                     | 0.47              |
| 8:m:121:LEU:HD12  | 8:m:162:GLY:HA3   | 1.97                     | 0.47              |
| 9:n:56:ASP:OD1    | 9:n:57:THR:N      | 2.47                     | 0.47              |
| 11:N:299:TYR:HA   | 11:N:302:PHE:HB3  | 1.95                     | 0.47              |
| 12:S:208:ILE:HG12 | 13:T:91:SER:HB2   | 1.97                     | 0.47              |
| 12:S:395:ILE:HG12 | 12:S:410:LYS:HD2  | 1.96                     | 0.47              |
| 17:L:287:GLY:HA3  | 17:L:333:LEU:HD23 | 1.96                     | 0.47              |
| 18:M:216:LYS:HD2  | 18:M:312:LEU:HD22 | 1.96                     | 0.47              |
| 7:F:190:ILE:HD11  | 7:F:215:ILE:HD12  | 1.96                     | 0.47              |
| 2:K:88:ARG:HH12   | 19:U:169:ILE:HG13 | 1.80                     | 0.47              |
| 3:i:132:VAL:HG11  | 3:i:209:ILE:HA    | 1.96                     | 0.47              |
| 4:A:29:GLU:HB3    | 4:A:33:LYS:HE2    | 1.95                     | 0.47              |
| 8:E:134:MET:HE3   | 8:E:137:PRO:HA    | 1.96                     | 0.47              |
| 3:2:41:VAL:HG13   | 3:2:207:MET:HE3   | 1.96                     | 0.47              |
| 28:5:107:LYS:HE2  | 28:5:109:VAL:HB   | 1.97                     | 0.47              |
| 32:Z:531:ALA:HB1  | 32:Z:572:ILE:HB   | 1.96                     | 0.47              |
| 32:Z:890:SER:HB3  | 32:Z:895:LEU:HD12 | 1.97                     | 0.47              |
| 13:T:165:GLN:O    | 13:T:170:ASN:ND2  | 2.45                     | 0.47              |
| 19:U:9:THR:HG22   | 19:U:162:GLU:HB2  | 1.96                     | 0.47              |
| 19:U:98:LYS:HB2   | 19:U:100:ARG:HH12 | 1.80                     | 0.47              |
| 19:U:230:GLN:HG3  | 21:O:352:TRP:HH2  | 1.80                     | 0.47              |
| 23:H:103:THR:C    | 23:H:105:ILE:H    | 2.23                     | 0.47              |
| 3:2:55:VAL:HB     | 29:e:213:ARG:HA   | 1.98                     | 0.47              |
| 29:6:160:ALA:HB3  | 29:6:214:HIS:CE1  | 2.50                     | 0.47              |
| 23:H:434:ARG:HH22 | 32:Z:956:LEU:HD12 | 1.80                     | 0.46              |
| 4:A:174:LYS:HD3   | 4:A:213:ALA:HB1   | 1.96                     | 0.46              |
| 26:1:18:LEU:HD11  | 26:1:68:ALA:HA    | 1.96                     | 0.46              |
| 3:2:58:LYS:HD3    | 29:e:212:GLU:HB3  | 1.96                     | 0.46              |
| 5:3:78:GLU:HB3    | 5:3:80:ARG:HG2    | 1.97                     | 0.46              |
| 27:4:60:ILE:HG13  | 27:4:84:VAL:HG22  | 1.96                     | 0.46              |
| 30:a:232:ILE:HB   | 30:a:240:THR:HB   | 1.97                     | 0.46              |
| 1:I:435:LEU:HB2   | 9:D:79:ASN:ND2    | 2.30                     | 0.46              |
| 5:h:185:ALA:HB3   | 5:h:200:LEU:HD12  | 1.97                     | 0.46              |
| 11:N:666:GLN:HG2  | 11:N:873:ARG:NH2  | 2.31                     | 0.46              |
| 12:S:264:VAL:HA   | 12:S:268:LEU:HD12 | 1.96                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:S:462:ASP:OD1  | 13:T:262:LYS:NZ   | 2.48                     | 0.46              |
| 14:R:137:LEU:O    | 14:R:141:TYR:N    | 2.39                     | 0.46              |
| 15:Q:101:ILE:HG21 | 15:Q:140:LYS:HD3  | 1.97                     | 0.46              |
| 16:J:325:ALA:HA   | 16:J:328:LEU:HD12 | 1.98                     | 0.46              |
| 18:M:176:PRO:HD2  | 18:M:237:ALA:HB2  | 1.97                     | 0.46              |
| 23:H:357:ARG:CZ   | 23:H:467:ASN:HB2  | 2.46                     | 0.46              |
| 24:C:98:TYR:CD2   | 24:C:106:ILE:HB   | 2.50                     | 0.46              |
| 25:B:33:THR:HA    | 25:B:165:GLY:HA3  | 1.97                     | 0.46              |
| 26:1:198:THR:HG23 | 26:1:200:ALA:H    | 1.80                     | 0.46              |
| 29:6:74:ASN:HB3   | 29:6:127:HIS:HB3  | 1.97                     | 0.46              |
| 28:f:180:THR:OG1  | 28:f:184:GLY:O    | 2.25                     | 0.46              |
| 1:I:248:VAL:HG22  | 16:J:274:GLU:HG3  | 1.96                     | 0.46              |
| 2:K:354:GLY:O     | 2:K:358:SER:OG    | 2.29                     | 0.46              |
| 5:h:175:ALA:HB3   | 5:h:202:MET:HE1   | 1.97                     | 0.46              |
| 8:m:80:GLY:HA3    | 8:m:140:VAL:HA    | 1.98                     | 0.46              |
| 11:N:501:MET:HE1  | 11:N:520:GLY:HA3  | 1.98                     | 0.46              |
| 17:L:331:ASP:O    | 17:L:333:LEU:N    | 2.48                     | 0.46              |
| 17:L:404:ARG:HH22 | 18:M:191:GLU:HG3  | 1.80                     | 0.46              |
| 20:W:179:ARG:NH2  | 20:W:183:GLU:O    | 2.48                     | 0.46              |
| 26:b:39:THR:O     | 26:b:45:ILE:HA    | 2.15                     | 0.46              |
| 1:I:191:ILE:HG12  | 1:I:232:LEU:HD13  | 1.96                     | 0.46              |
| 4:c:92:ASN:HA     | 6:k:121:GLN:HE22  | 1.80                     | 0.46              |
| 5:h:18:LYS:HB2    | 5:h:157:ASN:HA    | 1.96                     | 0.46              |
| 7:l:67:ASP:OD1    | 7:l:68:GLU:N      | 2.43                     | 0.46              |
| 14:R:27:SER:HB2   | 14:R:179:PHE:HB2  | 1.97                     | 0.46              |
| 18:M:61:LYS:HA    | 18:M:64:ASP:HB2   | 1.96                     | 0.46              |
| 8:E:10:ARG:O      | 24:C:4:ARG:NH2    | 2.48                     | 0.46              |
| 5:3:17:GLY:HA3    | 5:3:163:LEU:HD22  | 1.97                     | 0.46              |
| 31:X:91:PHE:H     | 31:X:96:ARG:HE    | 1.63                     | 0.46              |
| 32:Z:525:MET:SD   | 32:Z:897:HIS:NE2  | 2.82                     | 0.46              |
| 24:d:38:ILE:O     | 24:d:45:VAL:N     | 2.37                     | 0.46              |
| 30:a:189:ARG:NH2  | 29:e:54:ILE:O     | 2.49                     | 0.46              |
| 33:V:67:ASP:HA    | 33:V:100:ARG:HH21 | 1.79                     | 0.46              |
| 11:N:726:ASP:OD1  | 11:N:727:THR:N    | 2.49                     | 0.46              |
| 15:Q:388:GLY:HA2  | 15:Q:400:TYR:HB3  | 1.98                     | 0.46              |
| 21:O:298:GLU:HB2  | 21:O:356:ARG:HH22 | 1.80                     | 0.46              |
| 26:1:83:GLU:O     | 26:1:87:SER:OG    | 2.20                     | 0.46              |
| 5:3:113:ASN:HB3   | 5:3:118:LYS:H     | 1.79                     | 0.46              |
| 30:7:50:ASP:O     | 30:7:158:GLN:NE2  | 2.41                     | 0.46              |
| 30:a:151:GLY:N    | 30:a:159:PHE:O    | 2.44                     | 0.46              |
| 1:I:201:PRO:HB3   | 32:Z:931:GLN:HG3  | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:K:300:LEU:HD23  | 2:K:333:ARG:HE    | 1.80                     | 0.46              |
| 11:N:331:ALA:HB2  | 11:N:697:PHE:CD1  | 2.50                     | 0.46              |
| 11:N:713:VAL:HA   | 11:N:755:PRO:HA   | 1.98                     | 0.46              |
| 16:J:186:ILE:HB   | 16:J:313:LYS:HG2  | 1.98                     | 0.46              |
| 17:L:132:ARG:HG2  | 33:V:46:PRO:HD2   | 1.98                     | 0.46              |
| 18:M:252:VAL:HG23 | 18:M:286:ILE:HG22 | 1.98                     | 0.46              |
| 32:Z:918:ASP:OD1  | 32:Z:919:GLU:N    | 2.49                     | 0.46              |
| 25:j:49:LYS:N     | 25:j:208:THR:O    | 2.42                     | 0.46              |
| 1:I:242:ALA:HB1   | 1:I:276:PRO:HG3   | 1.98                     | 0.46              |
| 2:K:281:ARG:NH1   | 17:L:299:ARG:HB3  | 2.31                     | 0.46              |
| 2:K:392:LEU:HD21  | 17:L:215:PRO:HG3  | 1.97                     | 0.46              |
| 18:M:357:ARG:NE   | 18:M:383:THR:OG1  | 2.48                     | 0.46              |
| 23:H:390:ARG:O    | 23:H:394:LYS:HG3  | 2.15                     | 0.46              |
| 9:D:73:LEU:HD11   | 9:D:135:ILE:HG12  | 1.97                     | 0.46              |
| 30:7:114:ALA:HA   | 30:7:118:GLU:HB2  | 1.98                     | 0.46              |
| 31:X:85:ARG:HD2   | 31:X:101:LEU:HD23 | 1.97                     | 0.46              |
| 32:Z:474:LEU:HD23 | 32:Z:508:LEU:HD23 | 1.98                     | 0.46              |
| 24:d:135:PHE:HB2  | 24:d:151:SER:HB3  | 1.97                     | 0.46              |
| 28:f:148:ARG:HH11 | 28:f:180:THR:HA   | 1.81                     | 0.46              |
| 33:V:136:ALA:O    | 33:V:157:ARG:NH1  | 2.48                     | 0.46              |
| 2:K:272:ASP:OD1   | 2:K:273:GLU:N     | 2.48                     | 0.46              |
| 8:m:26:TYR:HB2    | 9:n:11:PHE:HE2    | 1.80                     | 0.46              |
| 9:n:157:SER:OG    | 9:n:159:TRP:NE1   | 2.49                     | 0.46              |
| 11:N:50:TYR:HA    | 11:N:58:ARG:HB2   | 1.96                     | 0.46              |
| 17:L:197:ILE:HG21 | 17:L:239:ILE:HD13 | 1.96                     | 0.46              |
| 20:W:110:ILE:O    | 20:W:140:ASP:N    | 2.40                     | 0.46              |
| 22:P:28:ALA:HB3   | 22:P:70:ASN:HB3   | 1.98                     | 0.46              |
| 8:E:32:LYS:HG2    | 8:E:174:SER:HA    | 1.98                     | 0.46              |
| 5:3:169:GLN:OE1   | 5:3:173:ASN:ND2   | 2.49                     | 0.46              |
| 28:5:94:ARG:HH11  | 28:5:101:VAL:HG11 | 1.81                     | 0.46              |
| 29:6:214:HIS:NE2  | 29:6:216:GLN:HB2  | 2.30                     | 0.46              |
| 32:Z:574:TYR:HB3  | 32:Z:581:VAL:HG22 | 1.98                     | 0.46              |
| 28:f:242:ARG:HH22 | 28:f:284:ASN:HD21 | 1.64                     | 0.46              |
| 27:g:37:GLN:O     | 27:g:61:GLN:NE2   | 2.43                     | 0.46              |
| 1:I:174:ASP:OD1   | 1:I:175:LYS:N     | 2.49                     | 0.46              |
| 2:K:113:THR:HG21  | 17:L:126:ARG:HD3  | 1.98                     | 0.46              |
| 7:l:134:ILE:O     | 7:l:145:LEU:N     | 2.43                     | 0.46              |
| 8:m:46:VAL:HG11   | 8:m:145:ALA:HB1   | 1.98                     | 0.46              |
| 8:m:141:ALA:HB1   | 8:m:157:HIS:CE1   | 2.51                     | 0.46              |
| 15:Q:39:SER:HB2   | 15:Q:88:PHE:HB3   | 1.98                     | 0.46              |
| 17:L:242:ASN:HB3  | 17:L:276:CYS:HA   | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:H:385:ARG:HH22 | 23:H:413:ASN:HA   | 1.80                     | 0.46              |
| 26:1:43:ALA:O     | 26:1:44:TYR:HB2   | 2.16                     | 0.46              |
| 5:3:93:SER:O      | 5:3:97:GLU:HG3    | 2.15                     | 0.46              |
| 5:3:125:ASP:OD1   | 5:3:129:CYS:N     | 2.46                     | 0.46              |
| 16:J:78:ILE:HD13  | 16:J:104:VAL:HB   | 1.97                     | 0.46              |
| 19:U:69:ASP:HB2   | 19:U:73:ILE:HG13  | 1.98                     | 0.46              |
| 23:H:105:ILE:HD12 | 23:H:146:VAL:HG13 | 1.98                     | 0.46              |
| 4:A:123:ASN:ND2   | 25:B:87:ASP:OD2   | 2.49                     | 0.46              |
| 3:2:64:HIS:N      | 3:2:72:CYS:O      | 2.45                     | 0.46              |
| 29:e:129:ILE:HG23 | 29:e:141:VAL:HG13 | 1.98                     | 0.46              |
| 2:K:244:HIS:ND1   | 2:K:249:GLU:HB3   | 2.29                     | 0.45              |
| 4:c:220:LYS:HD2   | 4:c:238:ALA:HB1   | 1.98                     | 0.45              |
| 8:m:70:ILE:HA     | 8:m:93:ARG:HG2    | 1.97                     | 0.45              |
| 11:N:337:GLY:HA2  | 11:N:374:ILE:HG13 | 1.98                     | 0.45              |
| 11:N:785:PRO:HD2  | 11:N:873:ARG:HH12 | 1.80                     | 0.45              |
| 19:U:35:GLY:HA3   | 19:U:93:TYR:CZ    | 2.52                     | 0.45              |
| 19:U:98:LYS:HB2   | 19:U:100:ARG:NH1  | 2.31                     | 0.45              |
| 19:U:211:LEU:HD13 | 21:O:363:ILE:HD13 | 1.99                     | 0.45              |
| 21:O:74:ASN:OD1   | 21:O:75:GLN:N     | 2.49                     | 0.45              |
| 4:A:218:PHE:HB3   | 4:A:222:ASP:HB2   | 1.98                     | 0.45              |
| 25:B:157:PHE:HB3  | 25:B:159:TRP:CD1  | 2.51                     | 0.45              |
| 28:5:237:LEU:HD11 | 28:5:272:PHE:HD1  | 1.80                     | 0.45              |
| 3:i:77:THR:HG22   | 3:i:79:ALA:H      | 1.81                     | 0.45              |
| 5:h:58:THR:HG23   | 27:g:89:ALA:HB1   | 1.98                     | 0.45              |
| 5:h:161:GLU:OE1   | 5:h:198:ARG:NH1   | 2.41                     | 0.45              |
| 16:J:321:VAL:HG22 | 16:J:324:ARG:HH22 | 1.81                     | 0.45              |
| 21:O:277:ILE:HG22 | 21:O:279:ILE:H    | 1.81                     | 0.45              |
| 22:P:245:TYR:CE1  | 22:P:261:LEU:HD13 | 2.52                     | 0.45              |
| 7:F:226:ASP:OD1   | 7:F:227:GLY:N     | 2.50                     | 0.45              |
| 31:X:117:LYS:HB3  | 31:X:120:GLU:HB3  | 1.98                     | 0.45              |
| 28:f:208:GLN:NE2  | 27:g:25:ILE:HD11  | 2.32                     | 0.45              |
| 2:K:347:ARG:HD3   | 15:Q:209:TYR:HD1  | 1.81                     | 0.45              |
| 6:k:95:GLU:HG3    | 6:k:115:ARG:HH21  | 1.80                     | 0.45              |
| 22:P:121:THR:O    | 22:P:123:ARG:NH1  | 2.48                     | 0.45              |
| 22:P:196:ALA:HA   | 22:P:199:LEU:HD12 | 1.99                     | 0.45              |
| 5:3:113:ASN:ND2   | 5:3:116:SER:OG    | 2.50                     | 0.45              |
| 32:Z:918:ASP:HB3  | 32:Z:921:GLU:HB2  | 1.97                     | 0.45              |
| 29:e:29:GLY:O     | 29:e:74:ASN:ND2   | 2.39                     | 0.45              |
| 2:K:106:ASN:HA    | 2:K:122:ILE:HB    | 1.99                     | 0.45              |
| 4:c:58:LYS:HG2    | 4:c:60:PRO:HD3    | 1.99                     | 0.45              |
| 5:h:126:LEU:HD12  | 5:h:127:ILE:HG23  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:S:381:VAL:HG13 | 13:T:150:ARG:HG3  | 1.99                     | 0.45              |
| 15:Q:165:PHE:HE2  | 15:Q:177:VAL:HG21 | 1.81                     | 0.45              |
| 19:U:228:LYS:HD3  | 22:P:425:HIS:HA   | 1.98                     | 0.45              |
| 7:F:143:HIS:ND1   | 7:F:155:GLU:OE2   | 2.36                     | 0.45              |
| 9:D:56:ASP:HB3    | 9:D:59:ILE:HG12   | 1.97                     | 0.45              |
| 25:B:140:ASP:N    | 25:B:144:GLY:O    | 2.41                     | 0.45              |
| 29:6:109:ALA:HB3  | 29:6:142:TYR:HD2  | 1.82                     | 0.45              |
| 31:X:91:PHE:H     | 31:X:96:ARG:NE    | 2.15                     | 0.45              |
| 32:Z:543:THR:OG1  | 32:Z:574:TYR:OH   | 2.21                     | 0.45              |
| 24:d:209:ASP:OD1  | 24:d:210:ARG:N    | 2.49                     | 0.45              |
| 26:b:54:THR:HB    | 26:b:62:CYS:HB3   | 1.97                     | 0.45              |
| 28:f:96:THR:HG21  | 28:f:245:TYR:HA   | 1.99                     | 0.45              |
| 27:g:40:PRO:O     | 27:g:189:ILE:HG13 | 2.17                     | 0.45              |
| 33:V:278:LYS:HA   | 33:V:282:GLU:HB3  | 1.98                     | 0.45              |
| 2:K:126:LEU:HD21  | 2:K:148:ASP:HA    | 1.99                     | 0.45              |
| 2:K:131:LEU:HD21  | 33:V:273:ARG:HE   | 1.82                     | 0.45              |
| 9:n:4:TYR:CD2     | 9:n:125:GLY:HA2   | 2.51                     | 0.45              |
| 11:N:288:ASN:HB3  | 11:N:293:LEU:HD12 | 1.98                     | 0.45              |
| 12:S:285:ASP:OD1  | 12:S:286:TYR:N    | 2.49                     | 0.45              |
| 17:L:183:ILE:HD12 | 17:L:227:GLY:HA2  | 1.99                     | 0.45              |
| 21:O:164:PRO:HB2  | 21:O:166:ARG:HG2  | 1.98                     | 0.45              |
| 8:E:159:GLU:OE2   | 8:E:167:TYR:OH    | 2.35                     | 0.45              |
| 32:Z:230:ILE:O    | 32:Z:267:THR:OG1  | 2.32                     | 0.45              |
| 32:Z:306:MET:HG3  | 32:Z:310:LEU:HG   | 1.98                     | 0.45              |
| 32:Z:741:LEU:HB3  | 32:Z:745:LEU:HD12 | 1.98                     | 0.45              |
| 12:S:232:MET:HA   | 12:S:235:ASN:HD22 | 1.80                     | 0.45              |
| 17:L:108:VAL:HA   | 17:L:119:VAL:HG22 | 1.99                     | 0.45              |
| 22:P:134:VAL:HG21 | 22:P:175:GLU:HB3  | 1.99                     | 0.45              |
| 6:G:108:PRO:HB2   | 6:G:110:PRO:HD2   | 1.99                     | 0.45              |
| 32:Z:406:TRP:CE3  | 32:Z:407:VAL:HG23 | 2.52                     | 0.45              |
| 25:j:140:ASP:N    | 25:j:144:GLY:O    | 2.42                     | 0.45              |
| 33:V:45:VAL:HB    | 33:V:46:PRO:HD2   | 1.99                     | 0.45              |
| 2:K:109:ILE:HA    | 2:K:119:VAL:HA    | 1.98                     | 0.45              |
| 2:K:356:ILE:HG22  | 2:K:387:MET:HE2   | 1.99                     | 0.45              |
| 11:N:775:CYS:SG   | 11:N:776:TYR:N    | 2.88                     | 0.45              |
| 12:S:306:SER:O    | 12:S:310:LEU:HB3  | 2.16                     | 0.45              |
| 14:R:137:LEU:HB3  | 14:R:141:TYR:CE2  | 2.51                     | 0.45              |
| 15:Q:267:LEU:HD21 | 15:Q:334:HIS:ND1  | 2.31                     | 0.45              |
| 18:M:351:LEU:HD13 | 18:M:385:GLU:HG2  | 1.98                     | 0.45              |
| 23:H:309:ASP:OD1  | 23:H:310:GLU:N    | 2.49                     | 0.45              |
| 32:Z:509:LEU:HD23 | 32:Z:512:ILE:HD12 | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:e:33:GLY:HA3   | 29:e:129:ILE:HG21 | 1.99                     | 0.45              |
| 33:V:25:GLU:HG2   | 33:V:60:ASP:HA    | 1.98                     | 0.45              |
| 1:I:117:HIS:HA    | 1:I:131:SER:HA    | 1.98                     | 0.45              |
| 1:I:288:GLY:HA2   | 1:I:306:MET:SD    | 2.57                     | 0.45              |
| 5:h:204:GLN:HB3   | 28:5:241:HIS:CE1  | 2.51                     | 0.45              |
| 12:S:284:LEU:HD23 | 12:S:382:ARG:NH2  | 2.31                     | 0.45              |
| 16:J:211:ILE:O    | 16:J:246:PHE:N    | 2.43                     | 0.45              |
| 20:W:132:LEU:HD12 | 20:W:161:VAL:HG21 | 1.99                     | 0.45              |
| 23:H:361:LEU:HB3  | 23:H:365:LEU:HD23 | 1.98                     | 0.45              |
| 6:G:47:VAL:HG13   | 6:G:218:TRP:HB3   | 1.99                     | 0.45              |
| 9:D:124:GLY:N     | 8:E:133:LEU:O     | 2.48                     | 0.45              |
| 24:C:141:ASP:OD1  | 24:C:142:ASP:N    | 2.50                     | 0.45              |
| 29:6:76:PHE:CE2   | 29:6:78:ALA:HB3   | 2.52                     | 0.45              |
| 32:Z:234:PRO:HB3  | 32:Z:271:ILE:HA   | 1.99                     | 0.45              |
| 32:Z:253:VAL:HG13 | 32:Z:264:PHE:CD2  | 2.48                     | 0.45              |
| 32:Z:927:VAL:HG11 | 32:Z:963:ALA:HB1  | 1.98                     | 0.45              |
| 28:f:188:TYR:HE1  | 28:f:198:LYS:HG3  | 1.81                     | 0.45              |
| 33:V:38:LEU:HD21  | 33:V:141:VAL:HG11 | 1.99                     | 0.45              |
| 33:V:134:SER:O    | 33:V:157:ARG:NH2  | 2.49                     | 0.45              |
| 4:c:29:GLU:O      | 4:c:33:LYS:N      | 2.46                     | 0.45              |
| 6:k:120:VAL:HG21  | 6:k:151:LEU:HD21  | 1.98                     | 0.45              |
| 11:N:762:ARG:HH11 | 11:N:765:ASP:H    | 1.65                     | 0.45              |
| 14:R:232:VAL:HG13 | 14:R:253:ALA:HA   | 1.99                     | 0.45              |
| 14:R:292:LEU:HD11 | 14:R:311:THR:HG21 | 1.99                     | 0.45              |
| 17:L:225:GLY:HA3  | 18:M:342:ARG:NH2  | 2.31                     | 0.45              |
| 18:M:70:LYS:O     | 18:M:74:GLN:HG2   | 2.16                     | 0.45              |
| 6:G:76:CYS:HA     | 6:G:138:PHE:HA    | 1.99                     | 0.45              |
| 4:A:29:GLU:O      | 4:A:33:LYS:HG3    | 2.17                     | 0.45              |
| 25:B:230:ASP:OD1  | 25:B:231:LYS:N    | 2.50                     | 0.45              |
| 27:4:35:THR:OG1   | 27:4:44:MET:O     | 2.28                     | 0.45              |
| 2:K:90:GLN:O      | 2:K:93:PRO:HD2    | 2.17                     | 0.45              |
| 4:c:54:ILE:HG12   | 4:c:225:VAL:HG13  | 1.99                     | 0.45              |
| 4:c:59:VAL:HG13   | 4:c:64:LEU:HD12   | 1.99                     | 0.45              |
| 5:h:21:VAL:HG11   | 5:h:110:ALA:HB1   | 1.98                     | 0.45              |
| 7:l:60:GLN:HE21   | 7:l:62:LYS:HZ3    | 1.65                     | 0.45              |
| 8:m:51:GLU:HG2    | 8:m:53:ARG:HG3    | 1.99                     | 0.45              |
| 14:R:203:ASP:HA   | 16:J:334:LYS:HA   | 1.98                     | 0.45              |
| 20:W:4:GLU:HG2    | 20:W:107:HIS:HB2  | 1.98                     | 0.45              |
| 21:O:329:MET:HA   | 21:O:332:ILE:HD12 | 1.99                     | 0.45              |
| 21:O:332:ILE:HG23 | 21:O:337:LEU:O    | 2.17                     | 0.45              |
| 4:A:141:LEU:O     | 4:A:157:THR:N     | 2.44                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:B:75:TYR:CE1   | 25:B:79:GLY:HA2   | 2.52                     | 0.45              |
| 3:2:48:ARG:NH2    | 29:e:212:GLU:OE1  | 2.50                     | 0.45              |
| 28:5:282:PHE:HA   | 27:g:145:ASP:HB3  | 1.98                     | 0.45              |
| 32:Z:391:ASN:HB2  | 32:Z:425:ILE:HG12 | 1.98                     | 0.45              |
| 32:Z:612:GLY:N    | 32:Z:747:ALA:HB2  | 2.32                     | 0.45              |
| 30:a:115:ASP:OD1  | 30:a:116:ALA:N    | 2.49                     | 0.45              |
| 1:I:122:SER:HB3   | 1:I:126:PRO:HD3   | 1.98                     | 0.44              |
| 3:i:102:GLU:HB3   | 3:i:134:PRO:HG3   | 1.98                     | 0.44              |
| 6:k:40:ILE:HB     | 6:k:47:VAL:HB     | 1.98                     | 0.44              |
| 8:m:133:LEU:HB3   | 9:n:124:GLY:N     | 2.33                     | 0.44              |
| 9:n:83:ARG:HD2    | 9:n:86:ILE:HD12   | 1.99                     | 0.44              |
| 11:N:608:LEU:HD21 | 16:J:45:GLU:HG2   | 1.99                     | 0.44              |
| 17:L:115:GLU:HB3  | 17:L:131:VAL:HG21 | 1.98                     | 0.44              |
| 20:W:10:ILE:HA    | 20:W:113:PHE:HB2  | 1.99                     | 0.44              |
| 25:B:190:HIS:HB3  | 25:B:250:LEU:HD21 | 1.99                     | 0.44              |
| 26:1:103:GLU:OE2  | 30:7:98:ARG:NH1   | 2.35                     | 0.44              |
| 3:2:196:LEU:HD11  | 29:e:49:ILE:HG21  | 1.99                     | 0.44              |
| 30:a:68:ARG:NH1   | 26:b:145:ILE:O    | 2.43                     | 0.44              |
| 29:e:214:HIS:NE2  | 29:e:216:GLN:HB2  | 2.32                     | 0.44              |
| 2:K:182:GLN:HG2   | 16:J:371:ARG:HH21 | 1.82                     | 0.44              |
| 8:m:107:ILE:HD13  | 8:m:112:LEU:HD13  | 1.99                     | 0.44              |
| 11:N:66:SER:OG    | 11:N:78:ALA:O     | 2.32                     | 0.44              |
| 16:J:116:ARG:HB2  | 16:J:121:MET:H    | 1.81                     | 0.44              |
| 16:J:226:GLY:HA2  | 16:J:229:MET:HB2  | 1.97                     | 0.44              |
| 20:W:53:SER:O     | 20:W:60:ARG:N     | 2.39                     | 0.44              |
| 7:F:232:LYS:HE3   | 7:F:233:TYR:CZ    | 2.52                     | 0.44              |
| 24:C:59:GLN:NE2   | 24:C:209:ASP:O    | 2.48                     | 0.44              |
| 27:4:55:GLN:HE22  | 28:5:160:ASN:HA   | 1.82                     | 0.44              |
| 32:Z:528:LEU:HD13 | 32:Z:565:PHE:HB3  | 1.98                     | 0.44              |
| 1:I:399:ALA:HB1   | 1:I:411:VAL:HG11  | 2.00                     | 0.44              |
| 2:K:292:VAL:HA    | 2:K:295:ILE:HD12  | 1.98                     | 0.44              |
| 4:c:141:LEU:O     | 4:c:157:THR:N     | 2.46                     | 0.44              |
| 6:k:135:SER:HB2   | 6:k:153:PRO:HD3   | 1.99                     | 0.44              |
| 13:T:201:PRO:HA   | 13:T:232:LYS:HG2  | 1.99                     | 0.44              |
| 14:R:382:ASP:OD1  | 14:R:383:ARG:N    | 2.50                     | 0.44              |
| 23:H:428:MET:HA   | 23:H:431:ILE:HD12 | 1.98                     | 0.44              |
| 24:C:74:ALA:HB2   | 24:C:227:GLN:HE22 | 1.83                     | 0.44              |
| 26:1:132:ILE:HG12 | 26:1:138:VAL:HA   | 2.00                     | 0.44              |
| 29:6:21:PHE:HB2   | 30:7:142:PRO:HB3  | 1.98                     | 0.44              |
| 31:X:91:PHE:HB3   | 31:X:94:ASN:HB2   | 1.99                     | 0.44              |
| 32:Z:378:GLN:HG3  | 32:Z:845:LEU:HD23 | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:a:68:ARG:HG3   | 30:a:69:PHE:CD1   | 2.52                     | 0.44              |
| 30:a:122:PRO:HG2  | 30:a:151:GLY:HA3  | 2.00                     | 0.44              |
| 26:b:18:LEU:HD11  | 26:b:68:ALA:HA    | 1.99                     | 0.44              |
| 27:g:22:THR:HG23  | 27:g:26:SER:O     | 2.18                     | 0.44              |
| 3:i:247:VAL:HG12  | 5:h:45:HIS:CD2    | 2.52                     | 0.44              |
| 5:h:5:SER:HA      | 5:h:56:LEU:HB2    | 1.99                     | 0.44              |
| 8:m:84:ASP:OD1    | 9:n:122:GLN:NE2   | 2.50                     | 0.44              |
| 15:Q:359:ILE:HD12 | 15:Q:395:GLY:HA2  | 2.00                     | 0.44              |
| 21:O:331:ALA:HB1  | 21:O:336:LEU:HD12 | 1.99                     | 0.44              |
| 23:H:163:VAL:CG2  | 23:H:185:LEU:HD11 | 2.44                     | 0.44              |
| 8:E:41:ALA:HB2    | 8:E:155:LEU:HB2   | 1.99                     | 0.44              |
| 24:C:108:VAL:O    | 24:C:112:VAL:HG23 | 2.17                     | 0.44              |
| 25:B:66:LEU:HD11  | 25:B:69:PRO:HA    | 1.99                     | 0.44              |
| 26:1:146:ALA:HB2  | 30:7:68:ARG:HH22  | 1.82                     | 0.44              |
| 32:Z:957:LEU:HD13 | 32:Z:961:GLU:HB2  | 2.00                     | 0.44              |
| 25:j:230:ASP:OD1  | 25:j:231:LYS:N    | 2.51                     | 0.44              |
| 1:I:331:ILE:HG13  | 1:I:334:LEU:HB2   | 1.98                     | 0.44              |
| 1:I:384:LYS:HE3   | 1:I:387:LEU:HD12  | 1.99                     | 0.44              |
| 2:K:244:HIS:CG    | 2:K:249:GLU:HB3   | 2.52                     | 0.44              |
| 11:N:630:ALA:HA   | 11:N:663:ILE:HA   | 1.98                     | 0.44              |
| 12:S:380:CYS:HA   | 12:S:383:LEU:HD12 | 1.98                     | 0.44              |
| 14:R:382:ASP:OD2  | 14:R:385:ASN:HB2  | 2.18                     | 0.44              |
| 15:Q:104:PHE:CE2  | 15:Q:114:GLN:HB2  | 2.53                     | 0.44              |
| 17:L:171:THR:HG22 | 17:L:173:PHE:H    | 1.82                     | 0.44              |
| 17:L:397:GLU:OE2  | 17:L:421:LYS:NZ   | 2.46                     | 0.44              |
| 18:M:309:LEU:HD22 | 18:M:342:ARG:HD3  | 1.98                     | 0.44              |
| 19:U:167:GLU:HG2  | 33:V:35:LEU:HD13  | 1.99                     | 0.44              |
| 21:O:114:GLN:NE2  | 21:O:126:ILE:HD12 | 2.32                     | 0.44              |
| 9:D:139:ASP:HB2   | 9:D:142:ASP:HB3   | 2.00                     | 0.44              |
| 26:1:44:TYR:HD1   | 30:a:179:PHE:HZ   | 1.65                     | 0.44              |
| 3:2:192:ILE:HG23  | 3:2:199:GLY:HA2   | 1.99                     | 0.44              |
| 29:6:83:LEU:O     | 29:6:87:PHE:N     | 2.45                     | 0.44              |
| 29:6:113:GLN:HB2  | 29:6:150:TYR:CE2  | 2.53                     | 0.44              |
| 31:X:35:ILE:HG22  | 31:X:46:TRP:CE3   | 2.52                     | 0.44              |
| 2:K:109:ILE:HD11  | 2:K:117:SER:HB3   | 1.99                     | 0.44              |
| 2:K:244:HIS:CB    | 2:K:249:GLU:HB3   | 2.47                     | 0.44              |
| 2:K:399:ARG:NH1   | 2:K:406:ASP:OD2   | 2.51                     | 0.44              |
| 11:N:775:CYS:SG   | 11:N:878:GLN:NE2  | 2.88                     | 0.44              |
| 19:U:195:LYS:O    | 19:U:199:GLY:N    | 2.45                     | 0.44              |
| 6:G:125:LEU:HA    | 4:A:135:ARG:HB3   | 1.99                     | 0.44              |
| 8:E:84:ASP:OD2    | 8:E:136:ARG:NH1   | 2.51                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:3:11:ILE:HG21   | 5:3:142:ALA:HB3   | 2.00                     | 0.44              |
| 30:7:88:GLY:HA3   | 30:7:145:ASN:HA   | 2.00                     | 0.44              |
| 30:7:179:PHE:HZ   | 26:b:44:TYR:HD1   | 1.64                     | 0.44              |
| 32:Z:228:GLU:HA   | 32:Z:264:PHE:CE1  | 2.52                     | 0.44              |
| 32:Z:857:LEU:HD21 | 32:Z:908:ILE:HD13 | 1.98                     | 0.44              |
| 30:a:48:LYS:HE3   | 30:a:160:LEU:HB3  | 2.00                     | 0.44              |
| 27:g:8:ARG:HA     | 27:g:13:VAL:HA    | 2.00                     | 0.44              |
| 33:V:54:LEU:HD23  | 33:V:104:VAL:HA   | 2.00                     | 0.44              |
| 2:K:249:GLU:HA    | 2:K:252:ARG:HG2   | 1.99                     | 0.44              |
| 2:K:367:ASP:OD1   | 2:K:368:LEU:N     | 2.51                     | 0.44              |
| 5:h:147:PHE:O     | 5:h:151:GLU:HG2   | 2.17                     | 0.44              |
| 7:l:38:LEU:HA     | 7:l:158:GLY:HA2   | 2.00                     | 0.44              |
| 14:R:213:TYR:HA   | 14:R:216:ILE:HD12 | 2.00                     | 0.44              |
| 16:J:226:GLY:O    | 16:J:230:VAL:HG23 | 2.18                     | 0.44              |
| 18:M:399:GLY:HA3  | 23:H:240:ILE:HG21 | 1.99                     | 0.44              |
| 4:A:211:ILE:O     | 4:A:215:GLY:N     | 2.51                     | 0.44              |
| 7:F:157:TYR:HB2   | 7:F:176:LEU:HD21  | 2.00                     | 0.44              |
| 24:C:86:ILE:HA    | 25:B:116:LYS:HE3  | 1.98                     | 0.44              |
| 26:1:78:VAL:HG21  | 26:1:101:PHE:CE1  | 2.53                     | 0.44              |
| 3:2:193:TRP:HB3   | 29:e:57:ARG:HH22  | 1.83                     | 0.44              |
| 5:3:8:ASN:ND2     | 5:3:30:GLY:O      | 2.40                     | 0.44              |
| 5:3:45:HIS:ND1    | 5:3:50:PHE:HD1    | 2.14                     | 0.44              |
| 28:5:148:ARG:HH11 | 28:5:180:THR:HA   | 1.82                     | 0.44              |
| 28:5:201:ILE:HD12 | 27:g:171:ARG:NH2  | 2.33                     | 0.44              |
| 32:Z:228:GLU:HA   | 32:Z:264:PHE:HE1  | 1.82                     | 0.44              |
| 2:K:296:LEU:HD23  | 2:K:299:LEU:HD12  | 2.00                     | 0.44              |
| 4:c:162:TYR:HB2   | 25:j:80:PRO:HD3   | 2.00                     | 0.44              |
| 12:S:289:ALA:HB1  | 12:S:320:ILE:HD13 | 1.99                     | 0.44              |
| 15:Q:335:PHE:HD1  | 15:Q:338:LEU:HD12 | 1.83                     | 0.44              |
| 15:Q:358:GLU:HG2  | 15:Q:360:SER:H    | 1.83                     | 0.44              |
| 9:D:68:ASP:OD1    | 9:D:69:SER:N      | 2.43                     | 0.44              |
| 5:3:56:LEU:O      | 5:3:60:VAL:HG23   | 2.18                     | 0.44              |
| 5:3:204:GLN:HB3   | 28:f:241:HIS:CE1  | 2.52                     | 0.44              |
| 32:Z:495:ILE:HG12 | 32:Z:903:MET:HA   | 2.00                     | 0.44              |
| 30:a:51:ASN:HA    | 30:a:235:LYS:HE2  | 2.00                     | 0.44              |
| 3:i:105:VAL:HG11  | 3:i:138:HIS:HB2   | 2.00                     | 0.44              |
| 4:c:46:ARG:HH21   | 4:c:167:LYS:HA    | 1.83                     | 0.44              |
| 8:m:71:ASP:HB3    | 8:m:74:ILE:HG12   | 2.00                     | 0.44              |
| 17:L:175:GLN:H    | 17:L:243:PHE:HB3  | 1.83                     | 0.44              |
| 21:O:175:ASN:HA   | 21:O:178:TYR:HB3  | 1.99                     | 0.44              |
| 8:E:117:CYS:HA    | 8:E:120:ALA:HB3   | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:1:176:HIS:CD2  | 26:1:215:LEU:HD13 | 2.52                     | 0.44              |
| 27:4:140:THR:O    | 27:4:143:LEU:N    | 2.51                     | 0.44              |
| 32:Z:347:ASN:HB3  | 32:Z:353:VAL:HG23 | 1.99                     | 0.44              |
| 1:I:172:LYS:HZ3   | 1:I:246:ARG:HB3   | 1.82                     | 0.43              |
| 15:Q:97:LEU:HD21  | 15:Q:137:LEU:HD11 | 2.00                     | 0.43              |
| 15:Q:338:LEU:HA   | 15:Q:341:THR:HB   | 2.00                     | 0.43              |
| 15:Q:373:VAL:HG22 | 15:Q:377:LEU:HG   | 2.00                     | 0.43              |
| 21:O:83:LEU:HD11  | 21:O:98:TYR:HB3   | 2.00                     | 0.43              |
| 21:O:189:TYR:HA   | 21:O:220:SER:HB2  | 1.99                     | 0.43              |
| 23:H:180:LYS:HD3  | 23:H:180:LYS:HA   | 1.78                     | 0.43              |
| 3:2:41:VAL:HG11   | 3:2:130:ALA:HB1   | 2.00                     | 0.43              |
| 29:6:105:ILE:HG12 | 29:6:133:LEU:H    | 1.83                     | 0.43              |
| 30:7:76:ILE:HG22  | 30:7:78:VAL:HG23  | 1.99                     | 0.43              |
| 32:Z:272:TYR:HB3  | 32:Z:277:GLU:H    | 1.82                     | 0.43              |
| 32:Z:924:LYS:HE2  | 32:Z:993:GLU:HG3  | 1.99                     | 0.43              |
| 29:e:221:LEU:N    | 29:e:236:TYR:O    | 2.44                     | 0.43              |
| 3:i:92:ILE:HD12   | 3:i:107:SER:HB3   | 1.98                     | 0.43              |
| 13:T:161:TRP:HH2  | 13:T:182:LYS:HE3  | 1.82                     | 0.43              |
| 14:R:346:LYS:HB2  | 15:Q:389:VAL:HB   | 2.00                     | 0.43              |
| 16:J:195:LYS:HG2  | 16:J:316:PHE:CE2  | 2.52                     | 0.43              |
| 16:J:248:ASP:C    | 16:J:250:ILE:H    | 2.26                     | 0.43              |
| 22:P:173:MET:O    | 22:P:177:ILE:HG13 | 2.18                     | 0.43              |
| 7:F:106:GLU:HG2   | 30:7:110:ASP:HB3  | 1.99                     | 0.43              |
| 27:4:41:HIS:NE2   | 27:4:186:LYS:O    | 2.47                     | 0.43              |
| 25:j:77:GLY:HA3   | 25:j:132:VAL:HG12 | 1.98                     | 0.43              |
| 30:a:69:PHE:HE2   | 26:b:133:PRO:HD3  | 1.82                     | 0.43              |
| 26:b:27:PHE:CE2   | 26:b:32:ILE:HG13  | 2.54                     | 0.43              |
| 27:g:141:PHE:HD1  | 27:g:144:LEU:HD12 | 1.82                     | 0.43              |
| 6:k:52:LYS:NZ     | 6:k:60:VAL:O      | 2.51                     | 0.43              |
| 11:N:4:THR:HG23   | 11:N:8:PRO:HG2    | 2.01                     | 0.43              |
| 11:N:779:GLU:HA   | 11:N:783:SER:HB2  | 1.99                     | 0.43              |
| 12:S:453:ASP:OD1  | 12:S:454:SER:N    | 2.48                     | 0.43              |
| 8:E:88:MET:O      | 8:E:92:ALA:N      | 2.51                     | 0.43              |
| 25:B:70:ASP:HB2   | 25:B:104:TYR:OH   | 2.18                     | 0.43              |
| 27:4:29:LYS:HB2   | 28:5:202:PHE:CE1  | 2.53                     | 0.43              |
| 31:X:37:PRO:HD3   | 31:X:46:TRP:CZ3   | 2.52                     | 0.43              |
| 28:f:237:LEU:HD11 | 28:f:272:PHE:HD1  | 1.83                     | 0.43              |
| 33:V:135:ARG:HA   | 33:V:157:ARG:HH22 | 1.82                     | 0.43              |
| 7:l:232:LYS:HE3   | 7:l:233:TYR:CZ    | 2.52                     | 0.43              |
| 8:m:86:ARG:HA     | 8:m:89:ILE:HD12   | 1.99                     | 0.43              |
| 14:R:227:ALA:HB1  | 14:R:231:LEU:HB3  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:J:189:GLY:H    | 16:J:195:LYS:HZ2  | 1.66                     | 0.43              |
| 20:W:16:SER:OG    | 20:W:115:CYS:SG   | 2.76                     | 0.43              |
| 21:O:23:HIS:CG    | 21:O:24:PRO:HD2   | 2.53                     | 0.43              |
| 21:O:116:ASN:ND2  | 21:O:160:LYS:HD3  | 2.33                     | 0.43              |
| 22:P:283:LYS:HB2  | 22:P:286:ASN:CG   | 2.43                     | 0.43              |
| 6:G:50:VAL:HG21   | 6:G:66:LYS:HB2    | 1.99                     | 0.43              |
| 8:E:107:ILE:HD13  | 8:E:112:LEU:HD13  | 2.00                     | 0.43              |
| 3:2:185:SER:HB3   | 3:2:220:LEU:HD11  | 1.98                     | 0.43              |
| 5:3:68:ARG:HA     | 5:3:71:THR:HB     | 2.01                     | 0.43              |
| 27:4:61:GLN:HG2   | 27:4:65:GLN:HG2   | 2.00                     | 0.43              |
| 31:X:16:GLU:N     | 31:X:24:CYS:SG    | 2.91                     | 0.43              |
| 31:X:32:GLU:HB2   | 31:X:51:ARG:HB3   | 2.00                     | 0.43              |
| 32:Z:785:VAL:HG23 | 32:Z:817:LEU:HB3  | 1.99                     | 0.43              |
| 33:V:176:ASN:HD21 | 33:V:200:ASN:ND2  | 2.16                     | 0.43              |
| 2:K:109:ILE:HB    | 2:K:119:VAL:HG22  | 1.99                     | 0.43              |
| 11:N:142:GLU:HA   | 11:N:145:LEU:HB2  | 2.00                     | 0.43              |
| 12:S:403:SER:HB3  | 14:R:384:VAL:HG11 | 2.00                     | 0.43              |
| 14:R:346:LYS:O    | 14:R:389:GLU:HA   | 2.19                     | 0.43              |
| 17:L:125:PRO:HG2  | 17:L:127:TYR:CZ   | 2.54                     | 0.43              |
| 17:L:149:ASP:HB2  | 17:L:156:MET:HE2  | 1.98                     | 0.43              |
| 22:P:145:GLU:HA   | 22:P:148:LYS:HD3  | 1.99                     | 0.43              |
| 23:H:275:ILE:HA   | 23:H:309:ASP:HB3  | 1.99                     | 0.43              |
| 26:1:14:GLY:HA3   | 3:2:145:HIS:ND1   | 2.34                     | 0.43              |
| 27:4:61:GLN:HA    | 27:4:64:ILE:HB    | 2.00                     | 0.43              |
| 28:5:86:GLY:HA3   | 28:5:254:HIS:CE1  | 2.54                     | 0.43              |
| 29:e:128:THR:HB   | 29:e:144:PHE:CD2  | 2.53                     | 0.43              |
| 1:I:340:ARG:HD3   | 1:I:343:ARG:CG    | 2.49                     | 0.43              |
| 2:K:96:ILE:HD12   | 17:L:126:ARG:HB3  | 2.00                     | 0.43              |
| 8:m:84:ASP:OD2    | 8:m:136:ARG:NH1   | 2.52                     | 0.43              |
| 9:n:4:TYR:CZ      | 9:n:6:ARG:HB2     | 2.54                     | 0.43              |
| 21:O:226:LYS:HG2  | 21:O:227:ILE:HG13 | 2.01                     | 0.43              |
| 23:H:179:SER:C    | 23:H:181:TYR:H    | 2.26                     | 0.43              |
| 4:A:13:ASP:HB3    | 4:A:27:GLN:NE2    | 2.33                     | 0.43              |
| 4:A:53:VAL:HG11   | 4:A:144:VAL:HG21  | 1.99                     | 0.43              |
| 27:4:171:ARG:NH2  | 28:f:201:ILE:HD12 | 2.34                     | 0.43              |
| 31:X:85:ARG:HD2   | 31:X:101:LEU:HB3  | 2.00                     | 0.43              |
| 33:V:27:VAL:HG11  | 33:V:201:ILE:HG12 | 2.01                     | 0.43              |
| 2:K:157:SER:HB2   | 17:L:109:MET:HB3  | 2.00                     | 0.43              |
| 11:N:203:ARG:HG2  | 11:N:232:LEU:HD21 | 2.01                     | 0.43              |
| 14:R:38:VAL:HG12  | 14:R:39:SER:N     | 2.32                     | 0.43              |
| 18:M:151:ASP:OD1  | 18:M:152:SER:N    | 2.50                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:M:228:LYS:HG3  | 18:M:326:ALA:HB1  | 2.01                     | 0.43              |
| 8:E:156:PHE:HE1   | 8:E:166:ARG:HG3   | 1.84                     | 0.43              |
| 28:5:130:TRP:O    | 28:5:134:LEU:N    | 2.50                     | 0.43              |
| 32:Z:415:MET:HG3  | 32:Z:446:GLU:HB2  | 2.01                     | 0.43              |
| 25:j:33:THR:HA    | 25:j:165:GLY:HA3  | 2.00                     | 0.43              |
| 30:a:192:VAL:HG13 | 30:a:197:ASP:HB2  | 2.00                     | 0.43              |
| 27:g:99:GLN:HG3   | 27:g:121:TYR:CG   | 2.53                     | 0.43              |
| 2:K:150:LEU:HB3   | 2:K:154:SER:HB2   | 2.00                     | 0.43              |
| 4:c:78:THR:HG22   | 4:c:231:ASP:HA    | 2.00                     | 0.43              |
| 7:l:41:ASN:HD22   | 7:l:183:ASP:CG    | 2.25                     | 0.43              |
| 8:m:56:SER:OG     | 9:n:172:ARG:NH1   | 2.41                     | 0.43              |
| 11:N:548:ARG:HD2  | 11:N:583:VAL:HG22 | 2.00                     | 0.43              |
| 12:S:434:ALA:HB2  | 12:S:445:THR:HG22 | 2.00                     | 0.43              |
| 14:R:195:ASN:O    | 14:R:206:ARG:NH2  | 2.51                     | 0.43              |
| 16:J:84:VAL:O     | 16:J:96:VAL:N     | 2.41                     | 0.43              |
| 4:A:78:THR:HG22   | 4:A:231:ASP:HA    | 2.01                     | 0.43              |
| 7:F:132:LEU:HB2   | 7:F:147:PHE:HB3   | 2.01                     | 0.43              |
| 9:D:111:ARG:O     | 9:D:115:GLY:N     | 2.52                     | 0.43              |
| 29:6:161:ALA:HB2  | 29:6:214:HIS:CD2  | 2.53                     | 0.43              |
| 31:X:55:LYS:HE2   | 31:X:63:PRO:HD3   | 2.01                     | 0.43              |
| 32:Z:372:ALA:O    | 32:Z:374:LEU:HG   | 2.18                     | 0.43              |
| 29:e:76:PHE:HE2   | 29:e:78:ALA:HB3   | 1.84                     | 0.43              |
| 5:h:56:LEU:O      | 5:h:60:VAL:HG23   | 2.18                     | 0.43              |
| 6:k:167:LYS:HD3   | 6:k:207:ASN:HD21  | 1.83                     | 0.43              |
| 6:k:194:LYS:HE2   | 6:k:238:GLU:HG2   | 2.01                     | 0.43              |
| 9:n:187:THR:HG22  | 9:n:189:GLU:H     | 1.84                     | 0.43              |
| 11:N:312:GLY:HA2  | 11:N:315:ASN:HB3  | 2.01                     | 0.43              |
| 15:Q:219:ASP:HB3  | 15:Q:238:TYR:HB3  | 2.01                     | 0.43              |
| 7:F:91:GLN:HA     | 7:F:94:TYR:HB3    | 2.01                     | 0.43              |
| 25:B:39:ALA:C     | 25:B:41:ASN:H     | 2.26                     | 0.43              |
| 3:2:217:ARG:HG2   | 3:2:218:ASN:ND2   | 2.33                     | 0.43              |
| 28:5:96:THR:HG21  | 28:5:245:TYR:HA   | 2.01                     | 0.43              |
| 2:K:371:LEU:O     | 2:K:375:ASN:ND2   | 2.24                     | 0.43              |
| 11:N:33:ASP:HB3   | 11:N:71:ASN:HD21  | 1.84                     | 0.43              |
| 11:N:419:THR:HB   | 11:N:423:LEU:HD13 | 2.01                     | 0.43              |
| 12:S:208:ILE:HB   | 13:T:44:LEU:HD11  | 2.01                     | 0.43              |
| 12:S:226:ASP:HB3  | 12:S:230:LYS:HB2  | 2.01                     | 0.43              |
| 9:D:32:CYS:O      | 9:D:63:LYS:NZ     | 2.52                     | 0.43              |
| 24:C:89:ASN:ND2   | 5:3:77:LYS:HE2    | 2.34                     | 0.43              |
| 3:2:50:THR:HG21   | 3:2:197:GLY:HA2   | 2.01                     | 0.43              |
| 32:Z:269:TYR:OH   | 32:Z:276:ASN:OD1  | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:d:108:VAL:O    | 24:d:112:VAL:HG23 | 2.19                     | 0.43              |
| 30:a:58:ASP:HA    | 30:a:228:PHE:HA   | 2.01                     | 0.43              |
| 27:g:158:LEU:HD13 | 27:g:198:GLN:HE22 | 1.84                     | 0.43              |
| 33:V:111:HIS:CD2  | 33:V:118:LEU:HB3  | 2.54                     | 0.43              |
| 3:i:113:LYS:HD3   | 26:b:73:ALA:HB2   | 2.00                     | 0.42              |
| 3:i:217:ARG:HG2   | 3:i:218:ASN:ND2   | 2.34                     | 0.42              |
| 12:S:286:TYR:HE1  | 12:S:382:ARG:HD3  | 1.84                     | 0.42              |
| 14:R:239:THR:HG23 | 14:R:241:ILE:H    | 1.83                     | 0.42              |
| 17:L:420:ARG:HD3  | 6:G:170:GLN:HB3   | 2.00                     | 0.42              |
| 22:P:280:LEU:HA   | 22:P:283:LYS:HE2  | 2.01                     | 0.42              |
| 4:A:13:ASP:HB2    | 4:A:26:TYR:HB2    | 2.00                     | 0.42              |
| 8:E:49:GLY:HA2    | 8:E:219:LEU:HA    | 1.99                     | 0.42              |
| 8:E:70:ILE:HA     | 8:E:93:ARG:HG2    | 2.00                     | 0.42              |
| 27:4:126:VAL:HG22 | 27:4:128:LEU:HG   | 2.00                     | 0.42              |
| 28:5:188:TYR:HE1  | 28:5:198:LYS:HG3  | 1.83                     | 0.42              |
| 32:Z:277:GLU:OE1  | 32:Z:974:THR:OG1  | 2.36                     | 0.42              |
| 2:K:244:HIS:HB2   | 2:K:249:GLU:HB3   | 2.01                     | 0.42              |
| 11:N:770:LYS:HA   | 11:N:870:ASN:ND2  | 2.28                     | 0.42              |
| 14:R:154:LEU:HD21 | 14:R:170:VAL:HA   | 2.01                     | 0.42              |
| 16:J:84:VAL:N     | 16:J:96:VAL:O     | 2.43                     | 0.42              |
| 17:L:90:LYS:HB3   | 18:M:133:GLY:HA3  | 2.01                     | 0.42              |
| 18:M:70:LYS:HA    | 18:M:73:ARG:HB3   | 2.01                     | 0.42              |
| 21:O:306:ARG:HH12 | 21:O:349:THR:HG23 | 1.84                     | 0.42              |
| 23:H:357:ARG:HH21 | 23:H:466:TYR:H    | 1.67                     | 0.42              |
| 26:1:40:THR:HG22  | 26:1:44:TYR:O     | 2.18                     | 0.42              |
| 3:2:123:ILE:HG12  | 5:3:99:ARG:HE     | 1.84                     | 0.42              |
| 5:3:176:ASP:O     | 28:f:104:GLN:NE2  | 2.52                     | 0.42              |
| 28:5:119:THR:OG1  | 28:5:175:MET:N    | 2.46                     | 0.42              |
| 32:Z:407:VAL:HG12 | 32:Z:409:LYS:H    | 1.84                     | 0.42              |
| 26:b:147:GLY:O    | 26:b:154:TYR:OH   | 2.31                     | 0.42              |
| 29:e:76:PHE:CE2   | 29:e:78:ALA:HB3   | 2.54                     | 0.42              |
| 33:V:67:ASP:HA    | 33:V:100:ARG:NH2  | 2.34                     | 0.42              |
| 2:K:241:GLU:HG3   | 2:K:245:LYS:HE2   | 2.01                     | 0.42              |
| 2:K:392:LEU:HD11  | 17:L:215:PRO:HG3  | 2.01                     | 0.42              |
| 11:N:769:PRO:HG2  | 11:N:771:PHE:CE2  | 2.54                     | 0.42              |
| 12:S:475:TYR:CE2  | 19:U:291:LEU:HB2  | 2.55                     | 0.42              |
| 13:T:267:ALA:HA   | 13:T:270:ILE:HD12 | 2.01                     | 0.42              |
| 26:1:152:PHE:CZ   | 30:a:66:LEU:HD23  | 2.54                     | 0.42              |
| 25:j:39:ALA:C     | 25:j:41:ASN:H     | 2.27                     | 0.42              |
| 25:j:66:LEU:O     | 25:j:90:ARG:NH2   | 2.53                     | 0.42              |
| 25:j:146:SER:HB2  | 25:j:148:TYR:CE2  | 2.54                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:e:110:ARG:HA   | 29:e:150:TYR:OH   | 2.18                     | 0.42              |
| 1:I:306:MET:HG3   | 1:I:338:LEU:HD21  | 2.02                     | 0.42              |
| 2:K:306:PHE:CE1   | 2:K:312:VAL:HB    | 2.54                     | 0.42              |
| 4:c:17:THR:O      | 25:j:128:ARG:NE   | 2.53                     | 0.42              |
| 5:h:188:TYR:HE1   | 5:h:197:LYS:HG3   | 1.83                     | 0.42              |
| 11:N:768:ILE:O    | 11:N:917:ILE:HG22 | 2.19                     | 0.42              |
| 17:L:219:LEU:HD13 | 17:L:343:LEU:HD13 | 2.01                     | 0.42              |
| 18:M:146:VAL:HA   | 18:M:159:LEU:H    | 1.85                     | 0.42              |
| 18:M:166:ARG:HB3  | 18:M:269:LEU:HD22 | 2.01                     | 0.42              |
| 18:M:170:MET:HE3  | 23:H:180:LYS:HZ3  | 1.83                     | 0.42              |
| 21:O:371:VAL:O    | 21:O:375:ASP:N    | 2.50                     | 0.42              |
| 22:P:234:TYR:CD2  | 22:P:270:LEU:HD13 | 2.54                     | 0.42              |
| 23:H:225:VAL:HA   | 23:H:350:LYS:HE3  | 2.02                     | 0.42              |
| 26:1:193:ARG:HH11 | 26:1:206:ILE:HD12 | 1.82                     | 0.42              |
| 29:6:98:HIS:HB3   | 29:6:101:LYS:HB3  | 2.01                     | 0.42              |
| 32:Z:246:CYS:HB2  | 32:Z:272:TYR:OH   | 2.19                     | 0.42              |
| 32:Z:493:LEU:HD12 | 32:Z:496:ALA:HB3  | 2.00                     | 0.42              |
| 24:d:79:GLY:HA3   | 24:d:133:VAL:HG22 | 2.00                     | 0.42              |
| 1:I:129:TYR:HB3   | 23:H:171:GLY:C    | 2.45                     | 0.42              |
| 13:T:3:SER:HA     | 13:T:9:LYS:HB3    | 2.01                     | 0.42              |
| 13:T:85:LEU:HA    | 13:T:88:TYR:CD2   | 2.54                     | 0.42              |
| 19:U:16:LEU:HB3   | 33:V:32:ILE:HG12  | 2.02                     | 0.42              |
| 19:U:21:HIS:CD2   | 33:V:100:ARG:HB2  | 2.54                     | 0.42              |
| 20:W:21:PHE:HB2   | 20:W:25:ARG:CZ    | 2.49                     | 0.42              |
| 21:O:258:LEU:HB3  | 21:O:291:ILE:HG12 | 2.00                     | 0.42              |
| 6:G:60:VAL:HG21   | 7:F:39:ARG:NH2    | 2.33                     | 0.42              |
| 9:D:117:GLN:HA    | 9:D:120:TYR:CD2   | 2.55                     | 0.42              |
| 9:D:138:PHE:HE1   | 9:D:145:PRO:HB3   | 1.84                     | 0.42              |
| 8:E:40:ILE:O      | 8:E:47:VAL:N      | 2.49                     | 0.42              |
| 8:E:89:ILE:O      | 8:E:93:ARG:HB2    | 2.20                     | 0.42              |
| 32:Z:494:GLY:HA2  | 32:Z:497:PHE:CD2  | 2.55                     | 0.42              |
| 32:Z:562:TRP:HA   | 32:Z:565:PHE:CD2  | 2.55                     | 0.42              |
| 29:e:160:ALA:HB3  | 29:e:214:HIS:CE1  | 2.54                     | 0.42              |
| 1:I:183:ASP:HB3   | 1:I:365:HIS:HE2   | 1.84                     | 0.42              |
| 2:K:112:SER:OG    | 2:K:116:MET:O     | 2.35                     | 0.42              |
| 5:h:18:LYS:HD2    | 5:h:157:ASN:HB3   | 2.02                     | 0.42              |
| 6:k:100:LYS:O     | 30:a:98:ARG:HD2   | 2.19                     | 0.42              |
| 7:l:4:ASN:HA      | 7:l:7:ASP:HB3     | 2.01                     | 0.42              |
| 8:m:49:GLY:HA2    | 8:m:219:LEU:HA    | 2.01                     | 0.42              |
| 8:m:156:PHE:HE1   | 8:m:166:ARG:HG3   | 1.84                     | 0.42              |
| 9:n:68:ASP:OD1    | 9:n:69:SER:N      | 2.43                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:M:357:ARG:NH2  | 18:M:383:THR:O    | 2.53                     | 0.42              |
| 21:O:50:ASP:OD1   | 21:O:51:ASP:N     | 2.52                     | 0.42              |
| 6:G:7:GLY:HA2     | 4:A:15:HIS:CE1    | 2.54                     | 0.42              |
| 6:G:167:LYS:HG2   | 6:G:207:ASN:HD21  | 1.85                     | 0.42              |
| 5:3:151:GLU:HB3   | 29:e:209:SER:HB3  | 2.02                     | 0.42              |
| 28:5:96:THR:HA    | 28:5:101:VAL:HA   | 2.02                     | 0.42              |
| 29:6:109:ALA:HB2  | 29:6:130:ILE:HD13 | 2.01                     | 0.42              |
| 32:Z:283:ALA:HB2  | 32:Z:317:GLN:OE1  | 2.19                     | 0.42              |
| 2:K:246:TYR:CG    | 2:K:247:LEU:N     | 2.88                     | 0.42              |
| 5:h:120:PHE:CE2   | 5:h:122:ALA:HB2   | 2.54                     | 0.42              |
| 11:N:9:LEU:HD21   | 13:T:80:ASN:ND2   | 2.35                     | 0.42              |
| 15:Q:262:LEU:HD11 | 15:Q:281:ILE:HG21 | 2.01                     | 0.42              |
| 6:G:69:VAL:HG21   | 6:G:228:HIS:CE1   | 2.54                     | 0.42              |
| 24:C:136:ILE:HG12 | 24:C:150:THR:HG23 | 2.02                     | 0.42              |
| 5:3:58:THR:HG23   | 27:4:89:ALA:HB1   | 2.01                     | 0.42              |
| 32:Z:896:LYS:O    | 32:Z:897:HIS:CG   | 2.72                     | 0.42              |
| 24:d:59:GLN:NE2   | 24:d:209:ASP:O    | 2.47                     | 0.42              |
| 30:a:183:MET:C    | 30:a:186:PRO:HD2  | 2.44                     | 0.42              |
| 1:I:147:VAL:HG12  | 1:I:159:VAL:HG23  | 2.01                     | 0.42              |
| 7:l:39:ARG:NH1    | 7:l:142:ALA:O     | 2.52                     | 0.42              |
| 7:l:60:GLN:HE21   | 7:l:62:LYS:NZ     | 2.16                     | 0.42              |
| 13:T:136:LEU:HD23 | 13:T:142:LEU:HD13 | 2.01                     | 0.42              |
| 19:U:72:TYR:H     | 20:W:64:THR:HG21  | 1.84                     | 0.42              |
| 19:U:174:LEU:O    | 33:V:205:LYS:NZ   | 2.41                     | 0.42              |
| 3:2:206:VAL:HB    | 3:2:214:GLU:HB2   | 2.02                     | 0.42              |
| 32:Z:494:GLY:HA2  | 32:Z:497:PHE:CE2  | 2.55                     | 0.42              |
| 24:d:98:TYR:CD2   | 24:d:106:ILE:HB   | 2.54                     | 0.42              |
| 25:j:32:VAL:O     | 25:j:76:SER:OG    | 2.32                     | 0.42              |
| 1:I:433:GLU:HB3   | 1:I:436:TYR:HE2   | 1.85                     | 0.42              |
| 2:K:285:GLN:O     | 2:K:289:ASP:HB3   | 2.20                     | 0.42              |
| 2:K:349:ARG:HG2   | 2:K:383:ILE:HD11  | 2.02                     | 0.42              |
| 2:K:421:VAL:HG11  | 4:A:33:LYS:HA     | 2.01                     | 0.42              |
| 7:l:45:VAL:HG11   | 7:l:190:ILE:HA    | 2.01                     | 0.42              |
| 12:S:345:TYR:HD1  | 12:S:348:LEU:HD12 | 1.84                     | 0.42              |
| 16:J:97:ASP:OD1   | 16:J:98:VAL:N     | 2.53                     | 0.42              |
| 18:M:432:PHE:HD2  | 7:F:77:LEU:HD13   | 1.84                     | 0.42              |
| 7:F:19:LEU:HG     | 7:F:21:GLN:H      | 1.83                     | 0.42              |
| 7:F:101:ARG:HG2   | 30:7:124:TYR:OH   | 2.20                     | 0.42              |
| 32:Z:166:ASN:HD21 | 32:Z:226:GLU:C    | 2.28                     | 0.42              |
| 32:Z:376:SER:O    | 32:Z:379:GLN:N    | 2.53                     | 0.42              |
| 30:a:62:SER:HA    | 30:a:68:ARG:HB3   | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:h:104:PHE:HD1   | 5:h:126:LEU:HD22  | 1.84                     | 0.42              |
| 15:Q:37:GLN:HB2   | 15:Q:48:ASP:HB3   | 2.02                     | 0.42              |
| 19:U:188:ILE:HG21 | 33:V:218:LYS:NZ   | 2.34                     | 0.42              |
| 23:H:311:ILE:HG12 | 23:H:354:ALA:O    | 2.20                     | 0.42              |
| 4:A:54:ILE:HG12   | 4:A:225:VAL:HG13  | 2.01                     | 0.42              |
| 26:1:54:THR:O     | 26:1:62:CYS:N     | 2.52                     | 0.42              |
| 28:5:200:ASP:OD1  | 28:5:201:ILE:N    | 2.48                     | 0.42              |
| 30:7:49:TYR:HE1   | 30:7:51:ASN:HB2   | 1.84                     | 0.42              |
| 30:7:225:SER:OG   | 30:7:226:ARG:N    | 2.53                     | 0.42              |
| 32:Z:442:VAL:HG12 | 32:Z:443:ASP:N    | 2.34                     | 0.42              |
| 32:Z:785:VAL:HG11 | 32:Z:881:ILE:HD13 | 2.01                     | 0.42              |
| 25:j:157:PHE:HB3  | 25:j:159:TRP:CD1  | 2.55                     | 0.42              |
| 26:b:113:THR:HB   | 26:b:134:LEU:HD11 | 2.02                     | 0.42              |
| 26:b:179:SER:HB3  | 26:b:212:TYR:HB2  | 2.02                     | 0.42              |
| 28:f:103:SER:HB3  | 28:f:106:VAL:HG23 | 2.01                     | 0.42              |
| 27:g:18:SER:HA    | 27:g:179:VAL:HG12 | 2.02                     | 0.42              |
| 1:I:170:VAL:HG23  | 16:J:231:ARG:HD3  | 2.01                     | 0.41              |
| 1:I:231:LEU:HD23  | 1:I:234:LYS:HD2   | 2.02                     | 0.41              |
| 2:K:250:GLY:O     | 2:K:254:VAL:HG23  | 2.20                     | 0.41              |
| 6:k:93:ARG:NH1    | 30:a:109:TYR:HB3  | 2.34                     | 0.41              |
| 9:n:117:GLN:HA    | 9:n:120:TYR:CD2   | 2.54                     | 0.41              |
| 12:S:404:LEU:HB2  | 12:S:441:GLY:HA3  | 2.02                     | 0.41              |
| 13:T:162:ASP:O    | 13:T:166:SER:OG   | 2.33                     | 0.41              |
| 18:M:82:VAL:O     | 18:M:143:ASN:N    | 2.53                     | 0.41              |
| 22:P:277:GLN:HA   | 22:P:280:LEU:HD12 | 2.02                     | 0.41              |
| 23:H:98:GLN:HA    | 23:H:194:SER:HB2  | 2.02                     | 0.41              |
| 23:H:403:ARG:HH22 | 8:E:206:GLN:HA    | 1.85                     | 0.41              |
| 4:A:40:ILE:HG12   | 4:A:71:TYR:HE2    | 1.85                     | 0.41              |
| 7:F:46:LEU:HB2    | 7:F:214:ALA:HB3   | 2.01                     | 0.41              |
| 25:B:71:ILE:HG23  | 25:B:137:ALA:O    | 2.20                     | 0.41              |
| 28:5:82:ARG:NE    | 28:5:200:ASP:HB3  | 2.34                     | 0.41              |
| 30:7:115:ASP:OD1  | 30:7:116:ALA:N    | 2.53                     | 0.41              |
| 32:Z:180:ASP:OD1  | 32:Z:181:GLY:N    | 2.53                     | 0.41              |
| 25:j:71:ILE:HG23  | 25:j:137:ALA:O    | 2.20                     | 0.41              |
| 29:e:128:THR:HB   | 29:e:144:PHE:HD2  | 1.85                     | 0.41              |
| 33:V:42:ARG:CZ    | 33:V:147:VAL:HG12 | 2.50                     | 0.41              |
| 1:I:225:PRO:HG2   | 16:J:306:ARG:NH2  | 2.34                     | 0.41              |
| 1:I:268:PHE:HE1   | 1:I:279:VAL:HG21  | 1.85                     | 0.41              |
| 5:h:35:GLY:HA3    | 5:h:183:TRP:CH2   | 2.55                     | 0.41              |
| 8:m:134:MET:HE3   | 8:m:137:PRO:HA    | 2.01                     | 0.41              |
| 9:n:7:ALA:HA      | 9:n:124:GLY:HA3   | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:N:371:LEU:HB3  | 11:N:375:HIS:HD2  | 1.85                     | 0.41              |
| 11:N:378:ASN:OD1  | 11:N:924:LYS:NZ   | 2.41                     | 0.41              |
| 13:T:73:PHE:CE1   | 13:T:176:SER:HB3  | 2.55                     | 0.41              |
| 17:L:263:ILE:HG23 | 17:L:266:MET:HE2  | 2.01                     | 0.41              |
| 17:L:327:THR:HG21 | 17:L:333:LEU:HD11 | 2.01                     | 0.41              |
| 18:M:82:VAL:HB    | 18:M:144:ASP:HB3  | 2.02                     | 0.41              |
| 22:P:60:ALA:HA    | 22:P:96:MET:HG2   | 2.01                     | 0.41              |
| 23:H:95:HIS:HD2   | 23:H:189:PRO:HB3  | 1.86                     | 0.41              |
| 23:H:365:LEU:O    | 23:H:370:ARG:HD2  | 2.20                     | 0.41              |
| 6:G:102:LEU:HA    | 26:1:103:GLU:HG3  | 2.00                     | 0.41              |
| 24:C:48:ALA:N     | 24:C:212:GLU:O    | 2.53                     | 0.41              |
| 32:Z:474:LEU:HD21 | 32:Z:509:LEU:HD21 | 2.02                     | 0.41              |
| 32:Z:809:MET:HE1  | 32:Z:892:SER:HB2  | 2.01                     | 0.41              |
| 26:b:132:ILE:HG12 | 26:b:138:VAL:HA   | 2.03                     | 0.41              |
| 26:b:151:THR:HA   | 26:b:154:TYR:CD2  | 2.55                     | 0.41              |
| 26:b:152:PHE:HE2  | 26:b:184:TRP:HB2  | 1.83                     | 0.41              |
| 29:e:31:ILE:HG22  | 29:e:44:GLY:HA3   | 2.02                     | 0.41              |
| 28:f:107:LYS:HE2  | 28:f:109:VAL:HB   | 2.01                     | 0.41              |
| 28:f:200:ASP:OD1  | 28:f:201:ILE:N    | 2.47                     | 0.41              |
| 33:V:273:ARG:HG3  | 33:V:274:GLN:N    | 2.34                     | 0.41              |
| 2:K:368:LEU:HD23  | 2:K:407:LEU:HD13  | 2.01                     | 0.41              |
| 4:c:13:ASP:HB2    | 4:c:26:TYR:HB2    | 2.03                     | 0.41              |
| 5:h:30:GLY:HA2    | 5:h:36:VAL:HG23   | 2.01                     | 0.41              |
| 7:l:41:ASN:ND2    | 7:l:183:ASP:OD2   | 2.43                     | 0.41              |
| 11:N:20:VAL:HG23  | 11:N:21:LYS:H     | 1.86                     | 0.41              |
| 16:J:216:ALA:N    | 16:J:249:GLU:OE1  | 2.51                     | 0.41              |
| 17:L:301:ILE:HG13 | 18:M:299:ARG:HD3  | 2.01                     | 0.41              |
| 20:W:179:ARG:HG2  | 20:W:180:LEU:N    | 2.33                     | 0.41              |
| 23:H:434:ARG:CZ   | 32:Z:956:LEU:HB2  | 2.51                     | 0.41              |
| 4:A:114:CYS:HG    | 4:A:153:SER:HG    | 1.53                     | 0.41              |
| 24:C:235:ILE:HA   | 24:C:238:ILE:HD12 | 2.02                     | 0.41              |
| 29:e:156:ARG:HA   | 29:e:166:MET:SD   | 2.61                     | 0.41              |
| 4:c:79:ILE:HD11   | 4:c:112:MET:O     | 2.20                     | 0.41              |
| 5:h:8:ASN:HA      | 5:h:30:GLY:O      | 2.20                     | 0.41              |
| 11:N:399:PHE:HA   | 11:N:441:VAL:HG22 | 2.01                     | 0.41              |
| 15:Q:227:CYS:HB3  | 15:Q:334:HIS:CE1  | 2.56                     | 0.41              |
| 17:L:88:TYR:CE1   | 18:M:61:LYS:HD3   | 2.55                     | 0.41              |
| 17:L:248:ALA:HB2  | 17:L:283:VAL:HG22 | 2.03                     | 0.41              |
| 17:L:285:ALA:HB1  | 18:M:299:ARG:NE   | 2.35                     | 0.41              |
| 18:M:253:GLN:HB2  | 18:M:258:GLU:HB3  | 2.02                     | 0.41              |
| 19:U:69:ASP:HB3   | 19:U:72:TYR:HB3   | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:G:9:ASP:OD1     | 6:G:10:LEU:N      | 2.53                     | 0.41              |
| 4:A:98:LYS:HD3    | 26:1:88:GLN:HG2   | 2.02                     | 0.41              |
| 7:F:47:VAL:HG22   | 7:F:213:ILE:HG12  | 2.03                     | 0.41              |
| 7:F:50:LYS:NZ     | 7:F:62:LYS:H      | 2.18                     | 0.41              |
| 9:D:66:LYS:HB3    | 27:4:69:ILE:HG23  | 2.02                     | 0.41              |
| 25:B:138:GLY:O    | 25:B:146:SER:N    | 2.53                     | 0.41              |
| 27:4:29:LYS:HB2   | 28:5:202:PHE:HE1  | 1.85                     | 0.41              |
| 27:4:104:ILE:HD12 | 27:4:119:ILE:HD12 | 2.03                     | 0.41              |
| 32:Z:158:ALA:HB1  | 32:Z:223:LEU:HD11 | 2.02                     | 0.41              |
| 33:V:36:LYS:NZ    | 33:V:69:PHE:HA    | 2.35                     | 0.41              |
| 2:K:90:GLN:HB3    | 2:K:147:VAL:HG22  | 2.01                     | 0.41              |
| 4:c:135:ARG:HB2   | 6:k:13:SER:HA     | 2.02                     | 0.41              |
| 9:n:66:LYS:O      | 9:n:90:ARG:NE     | 2.52                     | 0.41              |
| 9:n:77:GLY:HA3    | 9:n:131:VAL:HG22  | 2.01                     | 0.41              |
| 11:N:479:GLU:HB2  | 11:N:512:ASN:HB3  | 2.01                     | 0.41              |
| 16:J:118:ASP:OD1  | 16:J:119:SER:N    | 2.53                     | 0.41              |
| 17:L:137:ARG:HA   | 17:L:140:LEU:HD12 | 2.02                     | 0.41              |
| 21:O:76:LEU:HB3   | 21:O:123:GLY:N    | 2.35                     | 0.41              |
| 6:G:52:LYS:NZ     | 6:G:60:VAL:O      | 2.53                     | 0.41              |
| 4:A:141:LEU:HB2   | 4:A:157:THR:HB    | 2.03                     | 0.41              |
| 9:D:72:VAL:HG21   | 9:D:221:ILE:HG12  | 2.01                     | 0.41              |
| 9:D:149:GLN:O     | 9:D:156:TYR:HA    | 2.20                     | 0.41              |
| 8:E:201:LEU:HB3   | 8:E:243:LEU:HD22  | 2.02                     | 0.41              |
| 24:C:112:VAL:HG22 | 24:C:137:TYR:CD2  | 2.55                     | 0.41              |
| 25:B:105:PRO:HG2  | 25:B:110:LEU:HD13 | 2.02                     | 0.41              |
| 26:1:38:ARG:NH2   | 26:1:189:GLY:HA3  | 2.36                     | 0.41              |
| 28:5:82:ARG:H     | 28:5:200:ASP:HB2  | 1.85                     | 0.41              |
| 31:X:10:PHE:CE2   | 31:X:12:ALA:HB2   | 2.56                     | 0.41              |
| 32:Z:382:ALA:O    | 32:Z:849:ARG:NH1  | 2.54                     | 0.41              |
| 24:d:160:TRP:CD1  | 24:d:163:ILE:HD13 | 2.55                     | 0.41              |
| 25:j:146:SER:HB2  | 25:j:148:TYR:HE2  | 1.85                     | 0.41              |
| 30:a:36:GLN:HE21  | 30:a:38:ILE:HD11  | 1.85                     | 0.41              |
| 30:a:44:VAL:H     | 30:a:177:THR:HB   | 1.85                     | 0.41              |
| 33:V:271:VAL:HB   | 33:V:275:ASP:HB2  | 2.02                     | 0.41              |
| 1:I:391:ASP:OD1   | 16:J:307:PRO:HG3  | 2.20                     | 0.41              |
| 2:K:425:ASP:OD1   | 4:A:24:ARG:NH1    | 2.53                     | 0.41              |
| 4:c:136:PRO:HG2   | 6:k:15:PHE:CZ     | 2.55                     | 0.41              |
| 6:k:50:VAL:HG21   | 6:k:66:LYS:HB2    | 2.03                     | 0.41              |
| 11:N:785:PRO:HD2  | 11:N:873:ARG:NH1  | 2.34                     | 0.41              |
| 16:J:116:ARG:HG3  | 16:J:121:MET:HB3  | 2.03                     | 0.41              |
| 22:P:393:VAL:HG13 | 22:P:400:VAL:HG22 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 23:H:451:ILE:O   | 23:H:455:LYS:HB3  | 2.20                     | 0.41              |
| 6:G:38:ILE:HG12  | 6:G:200:ILE:HD11  | 2.02                     | 0.41              |
| 9:D:72:VAL:HB    | 9:D:215:VAL:HG22  | 2.02                     | 0.41              |
| 24:C:137:TYR:N   | 24:C:149:TYR:O    | 2.49                     | 0.41              |
| 25:B:49:LYS:HD2  | 25:B:210:GLU:HB2  | 2.03                     | 0.41              |
| 26:1:133:PRO:HD3 | 30:7:69:PHE:HE2   | 1.86                     | 0.41              |
| 5:3:21:VAL:HB    | 5:3:190:ILE:HB    | 2.02                     | 0.41              |
| 27:4:175:ASP:HB3 | 27:4:177:LYS:HE2  | 2.02                     | 0.41              |
| 24:d:232:PRO:HA  | 24:d:235:ILE:HD12 | 2.02                     | 0.41              |
| 25:j:231:LYS:HD3 | 25:j:234:ARG:HH21 | 1.84                     | 0.41              |
| 28:f:166:LYS:NZ  | 28:f:193:ASP:OD1  | 2.54                     | 0.41              |
| 1:I:181:TYR:CD1  | 1:I:184:ILE:HD11  | 2.55                     | 0.41              |
| 2:K:345:ASP:OD1  | 2:K:346:ARG:N     | 2.43                     | 0.41              |
| 3:i:192:ILE:HG23 | 3:i:199:GLY:HA2   | 2.02                     | 0.41              |
| 4:c:64:LEU:HD22  | 6:k:158:TRP:HE1   | 1.86                     | 0.41              |
| 5:h:2:SER:OG     | 5:h:3:ASP:N       | 2.51                     | 0.41              |
| 5:h:109:VAL:HB   | 5:h:122:ALA:HB3   | 2.01                     | 0.41              |
| 13:T:57:ILE:O    | 13:T:61:ILE:HG13  | 2.20                     | 0.41              |
| 16:J:51:LEU:HD23 | 16:J:54:LYS:HD2   | 2.01                     | 0.41              |
| 17:L:400:PHE:HB3 | 18:M:195:GLU:OE1  | 2.20                     | 0.41              |
| 18:M:63:LYS:HA   | 18:M:66:LYS:HD2   | 2.02                     | 0.41              |
| 18:M:228:LYS:NZ  | 18:M:328:ASN:OD1  | 2.53                     | 0.41              |
| 21:O:169:ASN:OD1 | 21:O:198:THR:OG1  | 2.21                     | 0.41              |
| 22:P:56:LYS:HD2  | 22:P:92:SER:HB3   | 2.01                     | 0.41              |
| 24:C:94:HIS:HB3  | 24:C:114:ARG:HH11 | 1.85                     | 0.41              |
| 26:1:27:PHE:CE2  | 26:1:32:ILE:HG13  | 2.56                     | 0.41              |
| 27:4:145:ASP:HA  | 27:4:148:TYR:HB3  | 2.02                     | 0.41              |
| 29:6:221:LEU:N   | 29:6:236:TYR:O    | 2.52                     | 0.41              |
| 31:X:15:CYS:SG   | 31:X:16:GLU:N     | 2.94                     | 0.41              |
| 32:Z:813:PHE:CE1 | 32:Z:847:ILE:HG23 | 2.55                     | 0.41              |
| 2:K:275:ASP:HB3  | 2:K:318:THR:OG1   | 2.20                     | 0.41              |
| 4:c:218:PHE:HB3  | 4:c:222:ASP:HB2   | 2.03                     | 0.41              |
| 6:k:204:HIS:O    | 6:k:208:LYS:HB2   | 2.20                     | 0.41              |
| 7:l:2:PHE:CE2    | 7:l:4:ASN:HB2     | 2.55                     | 0.41              |
| 7:l:62:LYS:HD2   | 7:l:74:LEU:HD11   | 2.03                     | 0.41              |
| 8:m:83:ALA:HB3   | 8:m:136:ARG:NH2   | 2.36                     | 0.41              |
| 15:Q:66:VAL:HA   | 15:Q:71:LYS:HG3   | 2.03                     | 0.41              |
| 19:U:32:ARG:HG3  | 19:U:95:SER:HB2   | 2.02                     | 0.41              |
| 23:H:177:ASP:C   | 23:H:179:SER:N    | 2.78                     | 0.41              |
| 23:H:210:ASP:OD1 | 23:H:388:ILE:HD11 | 2.21                     | 0.41              |
| 6:G:194:LYS:HE2  | 6:G:238:GLU:HG2   | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:E:71:ASP:HB3    | 8:E:74:ILE:HG12   | 2.01                     | 0.41              |
| 25:B:231:LYS:HD3  | 25:B:234:ARG:HH21 | 1.86                     | 0.41              |
| 28:5:205:GLY:N    | 28:5:208:GLN:HB3  | 2.36                     | 0.41              |
| 30:7:39:VAL:O     | 30:7:89:ASP:HA    | 2.21                     | 0.41              |
| 32:Z:208:VAL:O    | 32:Z:212:LEU:HG   | 2.21                     | 0.41              |
| 1:I:331:ILE:O     | 1:I:335:ASP:N     | 2.54                     | 0.41              |
| 2:K:248:GLY:O     | 2:K:252:ARG:HG2   | 2.20                     | 0.41              |
| 3:i:113:LYS:NZ    | 26:b:72:GLN:O     | 2.42                     | 0.41              |
| 6:k:23:GLN:NE2    | 7:l:11:VAL:O      | 2.54                     | 0.41              |
| 8:m:133:LEU:O     | 9:n:124:GLY:N     | 2.51                     | 0.41              |
| 11:N:55:PHE:CZ    | 11:N:57:ASP:HB2   | 2.56                     | 0.41              |
| 11:N:120:ASP:OD1  | 11:N:121:GLU:N    | 2.53                     | 0.41              |
| 12:S:234:ILE:O    | 12:S:238:LEU:N    | 2.43                     | 0.41              |
| 12:S:241:PHE:HA   | 12:S:244:ASN:O    | 2.21                     | 0.41              |
| 12:S:293:ILE:HD13 | 12:S:320:ILE:HD12 | 2.03                     | 0.41              |
| 20:W:113:PHE:HE1  | 20:W:142:ILE:HD13 | 1.86                     | 0.41              |
| 21:O:81:TYR:HA    | 21:O:84:ALA:HB3   | 2.03                     | 0.41              |
| 22:P:268:LEU:HB3  | 22:P:277:GLN:NE2  | 2.36                     | 0.41              |
| 22:P:307:GLU:C    | 22:P:309:MET:H    | 2.28                     | 0.41              |
| 7:F:67:ASP:OD1    | 7:F:68:GLU:N      | 2.43                     | 0.41              |
| 24:C:122:TYR:HD2  | 24:C:130:PRO:HA   | 1.86                     | 0.41              |
| 27:4:34:LYS:HD3   | 27:4:53:THR:HG21  | 2.02                     | 0.41              |
| 29:6:124:TYR:HE1  | 30:7:137:ARG:HH12 | 1.67                     | 0.41              |
| 30:7:44:VAL:H     | 30:7:177:THR:HB   | 1.85                     | 0.41              |
| 32:Z:243:GLN:HE21 | 32:Z:277:GLU:CD   | 2.28                     | 0.41              |
| 32:Z:243:GLN:O    | 32:Z:247:GLN:HG3  | 2.21                     | 0.41              |
| 32:Z:407:VAL:C    | 32:Z:409:LYS:H    | 2.29                     | 0.41              |
| 24:d:101:THR:HG23 | 27:g:83:PHE:HD1   | 1.85                     | 0.41              |
| 29:e:161:ALA:HB2  | 29:e:214:HIS:CD2  | 2.56                     | 0.41              |
| 28:f:82:ARG:H     | 28:f:200:ASP:HB2  | 1.85                     | 0.41              |
| 28:f:82:ARG:NE    | 28:f:200:ASP:HB3  | 2.35                     | 0.41              |
| 33:V:284:ALA:O    | 33:V:287:THR:OG1  | 2.34                     | 0.41              |
| 4:c:40:ILE:HG12   | 4:c:71:TYR:CE2    | 2.56                     | 0.41              |
| 8:m:31:ILE:HD12   | 8:m:141:ALA:HB2   | 2.03                     | 0.41              |
| 11:N:893:VAL:HG22 | 11:N:906:ARG:HH11 | 1.85                     | 0.41              |
| 15:Q:145:HIS:HA   | 15:Q:148:LYS:HB3  | 2.02                     | 0.41              |
| 17:L:329:ARG:HH11 | 17:L:331:ASP:HB3  | 1.85                     | 0.41              |
| 19:U:32:ARG:HA    | 19:U:95:SER:HB2   | 2.02                     | 0.41              |
| 23:H:176:VAL:H    | 23:H:190:ARG:HB2  | 1.86                     | 0.41              |
| 23:H:316:GLY:HA2  | 23:H:360:THR:O    | 2.21                     | 0.41              |
| 4:A:164:VAL:HG23  | 25:B:61:LEU:HB2   | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:1:155:GLY:HA3  | 26:b:152:PHE:HB3  | 2.03                     | 0.41              |
| 3:2:33:VAL:HG22   | 3:2:188:ILE:HD11  | 2.03                     | 0.41              |
| 3:2:38:ASN:HD21   | 3:2:174:ASP:HA    | 1.86                     | 0.41              |
| 27:4:141:PHE:HD1  | 27:4:144:LEU:HD12 | 1.86                     | 0.41              |
| 28:5:128:GLN:NE2  | 29:6:150:TYR:O    | 2.53                     | 0.41              |
| 28:5:253:TYR:HE1  | 28:5:262:TYR:HD1  | 1.69                     | 0.41              |
| 30:7:183:MET:C    | 30:7:186:PRO:HD2  | 2.45                     | 0.41              |
| 33:V:189:ILE:HG12 | 33:V:196:TYR:CE2  | 2.55                     | 0.41              |
| 1:I:371:LEU:HD21  | 1:I:377:LEU:HD21  | 2.03                     | 0.40              |
| 4:c:25:LEU:HB2    | 4:c:28:VAL:HG23   | 2.03                     | 0.40              |
| 5:h:178:ASP:OD1   | 5:h:179:ALA:N     | 2.54                     | 0.40              |
| 6:k:150:MET:HB3   | 6:k:160:TYR:CD2   | 2.56                     | 0.40              |
| 11:N:894:ARG:NH1  | 11:N:896:PHE:HB3  | 2.35                     | 0.40              |
| 14:R:36:SER:O     | 14:R:43:ARG:HD3   | 2.21                     | 0.40              |
| 14:R:271:ILE:HA   | 14:R:276:LEU:HD23 | 2.02                     | 0.40              |
| 16:J:113:VAL:HG12 | 16:J:125:VAL:HG22 | 2.03                     | 0.40              |
| 20:W:56:GLY:HA2   | 20:W:83:GLY:HA3   | 2.03                     | 0.40              |
| 20:W:111:VAL:HG22 | 20:W:140:ASP:HB3  | 2.04                     | 0.40              |
| 21:O:239:MET:O    | 21:O:242:ILE:HG13 | 2.21                     | 0.40              |
| 22:P:63:VAL:HG11  | 22:P:79:LEU:HD21  | 2.02                     | 0.40              |
| 23:H:198:MET:HE1  | 23:H:294:LEU:HB2  | 2.03                     | 0.40              |
| 6:G:47:VAL:HG11   | 6:G:193:VAL:HG22  | 2.02                     | 0.40              |
| 9:D:25:GLU:HG2    | 9:D:28:LYS:HD2    | 2.03                     | 0.40              |
| 26:1:73:ALA:HB2   | 3:2:113:LYS:HD3   | 2.03                     | 0.40              |
| 3:2:79:ALA:HB2    | 5:3:130:ILE:HG13  | 2.02                     | 0.40              |
| 5:3:84:PRO:HB2    | 5:3:120:PHE:HD2   | 1.86                     | 0.40              |
| 32:Z:92:LEU:HG    | 32:Z:122:LEU:HD22 | 2.03                     | 0.40              |
| 33:V:50:MET:HG3   | 33:V:71:MET:HG3   | 2.03                     | 0.40              |
| 33:V:159:ILE:HG23 | 33:V:164:LEU:HD13 | 2.02                     | 0.40              |
| 33:V:278:LYS:HE3  | 33:V:279:HIS:NE2  | 2.36                     | 0.40              |
| 1:I:380:LEU:HD22  | 1:I:420:LYS:NZ    | 2.36                     | 0.40              |
| 2:K:123:LEU:HG    | 2:K:125:THR:H     | 1.86                     | 0.40              |
| 2:K:145:ALA:HB1   | 16:J:65:LEU:HD13  | 2.03                     | 0.40              |
| 8:m:134:MET:HA    | 9:n:122:GLN:O     | 2.21                     | 0.40              |
| 11:N:124:TYR:OH   | 11:N:164:ASP:OD2  | 2.29                     | 0.40              |
| 11:N:720:ALA:H    | 11:N:900:ASN:HD21 | 1.69                     | 0.40              |
| 22:P:95:TYR:CD1   | 22:P:99:LYS:HE3   | 2.57                     | 0.40              |
| 23:H:184:GLU:O    | 23:H:188:PRO:HD3  | 2.22                     | 0.40              |
| 23:H:249:TYR:CD2  | 23:H:358:PRO:HB3  | 2.56                     | 0.40              |
| 23:H:447:VAL:HG13 | 23:H:451:ILE:HD12 | 2.03                     | 0.40              |
| 4:A:110:TYR:CG    | 4:A:111:ASP:N     | 2.90                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:F:92:CYS:HA     | 7:F:103:LEU:HD22  | 2.02                     | 0.40              |
| 9:D:66:LYS:H      | 9:D:90:ARG:HH21   | 1.69                     | 0.40              |
| 8:E:148:ASP:HB3   | 8:E:152:GLY:H     | 1.86                     | 0.40              |
| 26:1:139:HIS:HE1  | 30:7:90:ILE:HG21  | 1.85                     | 0.40              |
| 32:Z:85:VAL:HG21  | 32:Z:90:LYS:HB2   | 2.03                     | 0.40              |
| 32:Z:207:ILE:HG23 | 32:Z:211:PHE:CD2  | 2.56                     | 0.40              |
| 32:Z:319:THR:HG21 | 32:Z:535:VAL:HG12 | 2.02                     | 0.40              |
| 32:Z:380:ASN:ND2  | 32:Z:407:VAL:HG22 | 2.37                     | 0.40              |
| 1:I:86:GLU:HA     | 1:I:89:GLN:HB3    | 2.03                     | 0.40              |
| 1:I:113:ILE:HD11  | 23:H:96:PRO:HD2   | 2.04                     | 0.40              |
| 2:K:56:LYS:O      | 2:K:60:LEU:HG     | 2.22                     | 0.40              |
| 2:K:66:ASP:HB3    | 11:N:573:HIS:HE1  | 1.86                     | 0.40              |
| 9:n:39:LYS:HD2    | 9:n:186:ALA:HA    | 2.02                     | 0.40              |
| 11:N:258:ALA:HA   | 11:N:261:LEU:HD12 | 2.04                     | 0.40              |
| 11:N:302:PHE:CZ   | 11:N:873:ARG:HG2  | 2.56                     | 0.40              |
| 12:S:155:LEU:O    | 12:S:159:ASN:N    | 2.51                     | 0.40              |
| 12:S:404:LEU:HA   | 12:S:407:ILE:HD12 | 2.04                     | 0.40              |
| 18:M:338:LEU:HD21 | 18:M:346:LYS:HE3  | 2.02                     | 0.40              |
| 21:O:83:LEU:HD23  | 21:O:132:GLU:HG3  | 2.03                     | 0.40              |
| 6:G:15:PHE:CZ     | 4:A:136:PRO:HG2   | 2.56                     | 0.40              |
| 9:D:55:GLN:HB3    | 24:C:159:GLY:O    | 2.21                     | 0.40              |
| 24:C:232:PRO:HA   | 24:C:235:ILE:HD12 | 2.03                     | 0.40              |
| 26:1:55:ARG:HB2   | 26:1:61:TRP:CZ3   | 2.56                     | 0.40              |
| 27:4:41:HIS:HB2   | 27:4:74:GLU:OE2   | 2.22                     | 0.40              |
| 24:d:112:VAL:HG22 | 24:d:137:TYR:CD2  | 2.57                     | 0.40              |
| 27:g:44:MET:HE2   | 27:g:46:PHE:HE1   | 1.87                     | 0.40              |
| 1:I:120:VAL:HG11  | 1:I:128:TYR:HD2   | 1.86                     | 0.40              |
| 1:I:169:SER:HB3   | 1:I:263:LEU:HD13  | 2.02                     | 0.40              |
| 11:N:145:LEU:HD21 | 11:N:153:ALA:HB2  | 2.03                     | 0.40              |
| 12:S:224:LYS:HE3  | 12:S:225:HIS:CE1  | 2.57                     | 0.40              |
| 13:T:62:LEU:HD12  | 13:T:85:LEU:HD13  | 2.04                     | 0.40              |
| 13:T:67:LEU:HD23  | 13:T:105:LEU:HD21 | 2.02                     | 0.40              |
| 16:J:112:ARG:NE   | 16:J:128:ASN:O    | 2.51                     | 0.40              |
| 17:L:338:LEU:HD23 | 17:L:343:LEU:HD12 | 2.03                     | 0.40              |
| 21:O:16:MET:HG3   | 21:O:20:PRO:HG3   | 2.03                     | 0.40              |
| 6:G:204:HIS:O     | 6:G:208:LYS:HB2   | 2.21                     | 0.40              |
| 32:Z:796:LEU:HA   | 32:Z:799:PHE:CE2  | 2.57                     | 0.40              |
| 30:a:226:ARG:NE   | 30:a:246:GLN:HB3  | 2.31                     | 0.40              |
| 26:b:184:TRP:O    | 26:b:185:ASP:HB2  | 2.21                     | 0.40              |
| 29:e:133:LEU:HD11 | 29:e:226:VAL:HG12 | 2.03                     | 0.40              |
| 3:i:64:HIS:N      | 3:i:72:CYS:O      | 2.52                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:c:164:VAL:HG23  | 25:j:61:LEU:HB2   | 2.04                     | 0.40              |
| 10:Y:65:ASP:HB3   | 14:R:328:PHE:CE1  | 2.57                     | 0.40              |
| 11:N:588:VAL:HA   | 11:N:591:LEU:HD12 | 2.03                     | 0.40              |
| 15:Q:302:VAL:HA   | 15:Q:305:ALA:HB3  | 2.03                     | 0.40              |
| 15:Q:343:LEU:HG   | 15:Q:366:ILE:HD11 | 2.04                     | 0.40              |
| 15:Q:377:LEU:HB3  | 15:Q:390:LEU:HD11 | 2.02                     | 0.40              |
| 17:L:104:LEU:HD23 | 18:M:127:VAL:HG12 | 2.02                     | 0.40              |
| 23:H:388:ILE:HD13 | 23:H:416:GLY:HA2  | 2.03                     | 0.40              |
| 6:G:100:LYS:O     | 30:7:98:ARG:HD2   | 2.21                     | 0.40              |
| 7:F:168:ALA:HB1   | 7:F:196:ALA:HB1   | 2.04                     | 0.40              |
| 8:E:31:ILE:HG13   | 8:E:160:PRO:HG3   | 2.02                     | 0.40              |
| 3:2:102:GLU:HB3   | 3:2:134:PRO:HG3   | 2.03                     | 0.40              |
| 31:X:92:SER:H     | 31:X:94:ASN:HD22  | 1.67                     | 0.40              |
| 28:f:86:GLY:HA3   | 28:f:254:HIS:CE1  | 2.57                     | 0.40              |
| 28:f:189:TYR:CE1  | 28:f:204:VAL:HG21 | 2.56                     | 0.40              |
| 27:g:135:TYR:HB3  | 27:g:172:MET:HE1  | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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   | I     | 360/437 (82%) | 315 (88%) | 44 (12%) | 1 (0%)   | 36          | 72  |
| 2   | K     | 379/428 (89%) | 326 (86%) | 53 (14%) | 0        | 100         | 100 |
| 3   | 2     | 220/261 (84%) | 210 (96%) | 10 (4%)  | 0        | 100         | 100 |
| 3   | i     | 220/261 (84%) | 209 (95%) | 11 (5%)  | 0        | 100         | 100 |
| 4   | A     | 241/252 (96%) | 228 (95%) | 13 (5%)  | 0        | 100         | 100 |
| 4   | c     | 241/252 (96%) | 227 (94%) | 14 (6%)  | 0        | 100         | 100 |
| 5   | 3     | 202/205 (98%) | 190 (94%) | 12 (6%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 5   | h     | 202/205 (98%) | 188 (93%) | 13 (6%)  | 1 (0%)   | 24          | 63  |
| 6   | G     | 243/288 (84%) | 235 (97%) | 8 (3%)   | 0        | 100         | 100 |
| 6   | k     | 243/288 (84%) | 233 (96%) | 10 (4%)  | 0        | 100         | 100 |
| 7   | F     | 231/234 (99%) | 221 (96%) | 10 (4%)  | 0        | 100         | 100 |
| 7   | l     | 231/234 (99%) | 221 (96%) | 10 (4%)  | 0        | 100         | 100 |
| 8   | E     | 241/260 (93%) | 226 (94%) | 15 (6%)  | 0        | 100         | 100 |
| 8   | m     | 241/260 (93%) | 227 (94%) | 14 (6%)  | 0        | 100         | 100 |
| 9   | D     | 240/254 (94%) | 222 (92%) | 18 (8%)  | 0        | 100         | 100 |
| 9   | n     | 240/254 (94%) | 226 (94%) | 14 (6%)  | 0        | 100         | 100 |
| 10  | Y     | 25/89 (28%)   | 23 (92%)  | 2 (8%)   | 0        | 100         | 100 |
| 11  | N     | 843/945 (89%) | 786 (93%) | 57 (7%)  | 0        | 100         | 100 |
| 12  | S     | 351/523 (67%) | 313 (89%) | 37 (10%) | 1 (0%)   | 36          | 72  |
| 13  | T     | 270/274 (98%) | 231 (86%) | 39 (14%) | 0        | 100         | 100 |
| 14  | R     | 398/429 (93%) | 357 (90%) | 40 (10%) | 1 (0%)   | 36          | 72  |
| 15  | Q     | 429/434 (99%) | 393 (92%) | 36 (8%)  | 0        | 100         | 100 |
| 16  | J     | 371/405 (92%) | 335 (90%) | 35 (9%)  | 1 (0%)   | 36          | 72  |
| 17  | L     | 359/437 (82%) | 320 (89%) | 38 (11%) | 1 (0%)   | 36          | 72  |
| 18  | M     | 363/434 (84%) | 331 (91%) | 31 (8%)  | 1 (0%)   | 36          | 72  |
| 19  | U     | 278/338 (82%) | 260 (94%) | 18 (6%)  | 0        | 100         | 100 |
| 20  | W     | 195/268 (73%) | 182 (93%) | 13 (7%)  | 0        | 100         | 100 |
| 21  | O     | 385/393 (98%) | 341 (89%) | 43 (11%) | 1 (0%)   | 36          | 72  |
| 22  | P     | 430/445 (97%) | 386 (90%) | 44 (10%) | 0        | 100         | 100 |
| 23  | H     | 364/467 (78%) | 311 (85%) | 52 (14%) | 1 (0%)   | 36          | 72  |
| 24  | C     | 243/258 (94%) | 228 (94%) | 15 (6%)  | 0        | 100         | 100 |
| 24  | d     | 243/258 (94%) | 227 (93%) | 16 (7%)  | 0        | 100         | 100 |
| 25  | B     | 248/250 (99%) | 234 (94%) | 14 (6%)  | 0        | 100         | 100 |
| 25  | j     | 248/250 (99%) | 232 (94%) | 16 (6%)  | 0        | 100         | 100 |
| 26  | 1     | 203/215 (94%) | 185 (91%) | 17 (8%)  | 1 (0%)   | 24          | 63  |
| 26  | b     | 203/215 (94%) | 184 (91%) | 18 (9%)  | 1 (0%)   | 24          | 63  |
| 27  | 4     | 196/198 (99%) | 186 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 27  | g     | 196/198 (99%) | 182 (93%) | 14 (7%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 28  | 5     | 210/287 (73%)     | 200 (95%)   | 10 (5%)   | 0        | 100         | 100 |
| 28  | f     | 210/287 (73%)     | 198 (94%)   | 12 (6%)   | 0        | 100         | 100 |
| 29  | 6     | 220/241 (91%)     | 204 (93%)   | 16 (7%)   | 0        | 100         | 100 |
| 29  | e     | 220/241 (91%)     | 205 (93%)   | 15 (7%)   | 0        | 100         | 100 |
| 30  | 7     | 231/266 (87%)     | 215 (93%)   | 16 (7%)   | 0        | 100         | 100 |
| 30  | a     | 231/266 (87%)     | 216 (94%)   | 15 (6%)   | 0        | 100         | 100 |
| 31  | X     | 125/156 (80%)     | 113 (90%)   | 12 (10%)  | 0        | 100         | 100 |
| 32  | Z     | 807/993 (81%)     | 716 (89%)   | 90 (11%)  | 1 (0%)   | 48          | 83  |
| 33  | V     | 282/306 (92%)     | 234 (83%)   | 45 (16%)  | 3 (1%)   | 11          | 46  |
| All | All   | 13352/15139 (88%) | 12232 (92%) | 1105 (8%) | 15 (0%)  | 49          | 83  |

All (15) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | L     | 332 | THR  |
| 5   | h     | 105 | VAL  |
| 14  | R     | 241 | ILE  |
| 33  | V     | 305 | ILE  |
| 16  | J     | 134 | VAL  |
| 32  | Z     | 442 | VAL  |
| 33  | V     | 273 | ARG  |
| 26  | 1     | 28  | LYS  |
| 26  | b     | 28  | LYS  |
| 18  | M     | 167 | VAL  |
| 1   | I     | 168 | VAL  |
| 21  | O     | 357 | ILE  |
| 12  | S     | 163 | VAL  |
| 23  | H     | 105 | ILE  |
| 33  | V     | 303 | VAL  |

### 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   | I     | 319/385 (83%)  | 319 (100%) | 0        | 100         | 100 |
| 2   | K     | 334/374 (89%)  | 334 (100%) | 0        | 100         | 100 |
| 3   | 2     | 181/214 (85%)  | 181 (100%) | 0        | 100         | 100 |
| 3   | i     | 181/214 (85%)  | 181 (100%) | 0        | 100         | 100 |
| 4   | A     | 207/210 (99%)  | 207 (100%) | 0        | 100         | 100 |
| 4   | c     | 207/210 (99%)  | 207 (100%) | 0        | 100         | 100 |
| 5   | 3     | 172/173 (99%)  | 172 (100%) | 0        | 100         | 100 |
| 5   | h     | 172/173 (99%)  | 172 (100%) | 0        | 100         | 100 |
| 6   | G     | 201/239 (84%)  | 201 (100%) | 0        | 100         | 100 |
| 6   | k     | 201/239 (84%)  | 201 (100%) | 0        | 100         | 100 |
| 7   | F     | 192/193 (100%) | 192 (100%) | 0        | 100         | 100 |
| 7   | l     | 192/193 (100%) | 192 (100%) | 0        | 100         | 100 |
| 8   | E     | 199/215 (93%)  | 199 (100%) | 0        | 100         | 100 |
| 8   | m     | 199/215 (93%)  | 199 (100%) | 0        | 100         | 100 |
| 9   | D     | 214/226 (95%)  | 214 (100%) | 0        | 100         | 100 |
| 9   | n     | 214/226 (95%)  | 214 (100%) | 0        | 100         | 100 |
| 10  | Y     | 26/81 (32%)    | 26 (100%)  | 0        | 100         | 100 |
| 11  | N     | 713/797 (90%)  | 713 (100%) | 0        | 100         | 100 |
| 12  | S     | 330/489 (68%)  | 330 (100%) | 0        | 100         | 100 |
| 13  | T     | 254/256 (99%)  | 254 (100%) | 0        | 100         | 100 |
| 14  | R     | 351/379 (93%)  | 351 (100%) | 0        | 100         | 100 |
| 15  | Q     | 388/391 (99%)  | 388 (100%) | 0        | 100         | 100 |
| 16  | J     | 325/352 (92%)  | 325 (100%) | 0        | 100         | 100 |
| 17  | L     | 308/377 (82%)  | 308 (100%) | 0        | 100         | 100 |
| 18  | M     | 315/375 (84%)  | 315 (100%) | 0        | 100         | 100 |
| 19  | U     | 256/308 (83%)  | 256 (100%) | 0        | 100         | 100 |
| 20  | W     | 171/230 (74%)  | 171 (100%) | 0        | 100         | 100 |
| 21  | O     | 363/368 (99%)  | 363 (100%) | 0        | 100         | 100 |
| 22  | P     | 405/415 (98%)  | 405 (100%) | 0        | 100         | 100 |
| 23  | H     | 314/399 (79%)  | 313 (100%) | 1 (0%)   | 86          | 85  |
| 24  | C     | 204/216 (94%)  | 204 (100%) | 0        | 100         | 100 |
| 24  | d     | 204/216 (94%)  | 204 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 25  | B     | 209/209 (100%)    | 209 (100%)   | 0        | 100         | 100 |
| 25  | j     | 209/209 (100%)    | 209 (100%)   | 0        | 100         | 100 |
| 26  | 1     | 169/178 (95%)     | 169 (100%)   | 0        | 100         | 100 |
| 26  | b     | 168/178 (94%)     | 168 (100%)   | 0        | 100         | 100 |
| 27  | 4     | 175/175 (100%)    | 175 (100%)   | 0        | 100         | 100 |
| 27  | g     | 175/175 (100%)    | 175 (100%)   | 0        | 100         | 100 |
| 28  | 5     | 169/235 (72%)     | 169 (100%)   | 0        | 100         | 100 |
| 28  | f     | 169/235 (72%)     | 169 (100%)   | 0        | 100         | 100 |
| 29  | 6     | 185/201 (92%)     | 185 (100%)   | 0        | 100         | 100 |
| 29  | e     | 185/201 (92%)     | 185 (100%)   | 0        | 100         | 100 |
| 30  | 7     | 199/224 (89%)     | 199 (100%)   | 0        | 100         | 100 |
| 30  | a     | 199/224 (89%)     | 199 (100%)   | 0        | 100         | 100 |
| 31  | X     | 116/144 (81%)     | 116 (100%)   | 0        | 100         | 100 |
| 32  | Z     | 692/850 (81%)     | 692 (100%)   | 0        | 100         | 100 |
| 33  | V     | 249/268 (93%)     | 249 (100%)   | 0        | 100         | 100 |
| All | All   | 11580/13054 (89%) | 11579 (100%) | 1 (0%)   | 100         | 100 |

All (1) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | H     | 185 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (189) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 89  | GLN  |
| 1   | I     | 95  | GLN  |
| 1   | I     | 117 | HIS  |
| 1   | I     | 151 | HIS  |
| 1   | I     | 238 | ASN  |
| 1   | I     | 303 | GLN  |
| 1   | I     | 431 | ASN  |
| 2   | K     | 64  | GLN  |
| 2   | K     | 83  | GLN  |
| 2   | K     | 200 | GLN  |
| 2   | K     | 228 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | K     | 244 | HIS  |
| 2   | K     | 388 | GLN  |
| 2   | K     | 414 | GLN  |
| 2   | K     | 419 | ASN  |
| 3   | i     | 110 | GLN  |
| 3   | i     | 138 | HIS  |
| 3   | i     | 170 | HIS  |
| 3   | i     | 189 | GLN  |
| 4   | c     | 92  | ASN  |
| 4   | c     | 185 | HIS  |
| 5   | h     | 48  | HIS  |
| 5   | h     | 169 | GLN  |
| 5   | h     | 173 | ASN  |
| 6   | k     | 23  | GLN  |
| 6   | k     | 121 | GLN  |
| 6   | k     | 183 | HIS  |
| 6   | k     | 207 | ASN  |
| 6   | k     | 225 | ASN  |
| 6   | k     | 228 | HIS  |
| 7   | l     | 21  | GLN  |
| 7   | l     | 43  | HIS  |
| 7   | l     | 60  | GLN  |
| 7   | l     | 93  | ASN  |
| 7   | l     | 117 | GLN  |
| 7   | l     | 121 | GLN  |
| 8   | m     | 99  | HIS  |
| 8   | m     | 100 | ASN  |
| 8   | m     | 157 | HIS  |
| 8   | m     | 168 | ASN  |
| 9   | n     | 16  | HIS  |
| 9   | n     | 19  | GLN  |
| 9   | n     | 40  | ASN  |
| 9   | n     | 96  | HIS  |
| 9   | n     | 118 | GLN  |
| 11  | N     | 34  | GLN  |
| 11  | N     | 71  | ASN  |
| 11  | N     | 176 | GLN  |
| 11  | N     | 256 | GLN  |
| 11  | N     | 306 | ASN  |
| 11  | N     | 529 | GLN  |
| 11  | N     | 691 | GLN  |
| 11  | N     | 703 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | S     | 154 | GLN  |
| 12  | S     | 235 | ASN  |
| 12  | S     | 314 | ASN  |
| 12  | S     | 469 | ASN  |
| 12  | S     | 472 | HIS  |
| 13  | T     | 80  | ASN  |
| 13  | T     | 127 | GLN  |
| 13  | T     | 272 | ASN  |
| 14  | R     | 76  | GLN  |
| 14  | R     | 325 | HIS  |
| 14  | R     | 397 | ASN  |
| 15  | Q     | 226 | HIS  |
| 15  | Q     | 361 | HIS  |
| 15  | Q     | 418 | GLN  |
| 16  | J     | 25  | GLN  |
| 16  | J     | 123 | HIS  |
| 17  | L     | 311 | GLN  |
| 18  | M     | 238 | GLN  |
| 18  | M     | 364 | HIS  |
| 18  | M     | 387 | ASN  |
| 19  | U     | 5   | HIS  |
| 19  | U     | 21  | HIS  |
| 19  | U     | 107 | ASN  |
| 19  | U     | 127 | GLN  |
| 19  | U     | 201 | GLN  |
| 19  | U     | 230 | GLN  |
| 20  | W     | 12  | ASN  |
| 20  | W     | 100 | HIS  |
| 20  | W     | 102 | GLN  |
| 20  | W     | 136 | ASN  |
| 20  | W     | 163 | ASN  |
| 21  | O     | 114 | GLN  |
| 21  | O     | 229 | ASN  |
| 21  | O     | 343 | GLN  |
| 21  | O     | 376 | GLN  |
| 22  | P     | 78  | GLN  |
| 22  | P     | 88  | GLN  |
| 22  | P     | 128 | ASN  |
| 22  | P     | 242 | GLN  |
| 22  | P     | 282 | HIS  |
| 22  | P     | 425 | HIS  |
| 23  | H     | 51  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | H     | 151 | GLN  |
| 23  | H     | 217 | GLN  |
| 23  | H     | 281 | GLN  |
| 23  | H     | 330 | GLN  |
| 23  | H     | 356 | ASN  |
| 6   | G     | 121 | GLN  |
| 6   | G     | 123 | HIS  |
| 6   | G     | 207 | ASN  |
| 6   | G     | 225 | ASN  |
| 6   | G     | 228 | HIS  |
| 4   | A     | 37  | GLN  |
| 4   | A     | 92  | ASN  |
| 4   | A     | 130 | GLN  |
| 4   | A     | 185 | HIS  |
| 4   | A     | 221 | ASN  |
| 7   | F     | 21  | GLN  |
| 7   | F     | 43  | HIS  |
| 7   | F     | 60  | GLN  |
| 7   | F     | 93  | ASN  |
| 7   | F     | 117 | GLN  |
| 7   | F     | 166 | GLN  |
| 9   | D     | 19  | GLN  |
| 9   | D     | 40  | ASN  |
| 9   | D     | 118 | GLN  |
| 9   | D     | 162 | GLN  |
| 8   | E     | 100 | ASN  |
| 24  | C     | 21  | GLN  |
| 24  | C     | 89  | ASN  |
| 25  | B     | 119 | GLN  |
| 25  | B     | 123 | GLN  |
| 26  | 1     | 57  | HIS  |
| 26  | 1     | 180 | GLN  |
| 3   | 2     | 64  | HIS  |
| 3   | 2     | 95  | HIS  |
| 3   | 2     | 114 | GLN  |
| 3   | 2     | 138 | HIS  |
| 3   | 2     | 170 | HIS  |
| 3   | 2     | 189 | GLN  |
| 5   | 3     | 48  | HIS  |
| 5   | 3     | 169 | GLN  |
| 5   | 3     | 173 | ASN  |
| 5   | 3     | 204 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | 4     | 86  | GLN  |
| 27  | 4     | 101 | ASN  |
| 27  | 4     | 112 | ASN  |
| 27  | 4     | 146 | HIS  |
| 27  | 4     | 147 | HIS  |
| 27  | 4     | 198 | GLN  |
| 28  | 5     | 251 | ASN  |
| 28  | 5     | 254 | HIS  |
| 28  | 5     | 266 | HIS  |
| 29  | 6     | 55  | ASN  |
| 29  | 6     | 89  | ASN  |
| 29  | 6     | 171 | ASN  |
| 29  | 6     | 172 | GLN  |
| 29  | 6     | 178 | GLN  |
| 30  | 7     | 36  | GLN  |
| 30  | 7     | 59  | ASN  |
| 30  | 7     | 111 | ASN  |
| 31  | X     | 94  | ASN  |
| 32  | Z     | 168 | GLN  |
| 32  | Z     | 307 | HIS  |
| 32  | Z     | 327 | GLN  |
| 32  | Z     | 338 | HIS  |
| 32  | Z     | 396 | ASN  |
| 32  | Z     | 593 | HIS  |
| 32  | Z     | 833 | GLN  |
| 32  | Z     | 898 | HIS  |
| 32  | Z     | 899 | GLN  |
| 32  | Z     | 958 | ASN  |
| 24  | d     | 31  | HIS  |
| 24  | d     | 177 | GLN  |
| 24  | d     | 227 | GLN  |
| 25  | j     | 20  | GLN  |
| 25  | j     | 119 | GLN  |
| 25  | j     | 123 | GLN  |
| 30  | a     | 36  | GLN  |
| 30  | a     | 59  | ASN  |
| 26  | b     | 57  | HIS  |
| 26  | b     | 180 | GLN  |
| 29  | e     | 171 | ASN  |
| 29  | e     | 172 | GLN  |
| 29  | e     | 178 | GLN  |
| 28  | f     | 104 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | f     | 241 | HIS  |
| 28  | f     | 254 | HIS  |
| 28  | f     | 266 | HIS  |
| 27  | g     | 86  | GLN  |
| 27  | g     | 198 | GLN  |
| 33  | V     | 97  | GLN  |
| 33  | V     | 184 | ASN  |
| 33  | V     | 200 | ASN  |
| 33  | V     | 274 | GLN  |
| 33  | V     | 301 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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-6693. These allow visual inspection of the internal detail of the map and identification of artifacts.

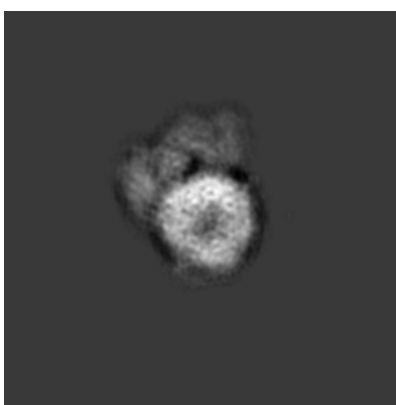
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

#### 6.1.1 Primary map



X



Y

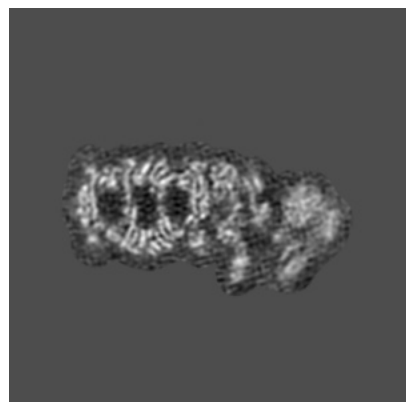


Z

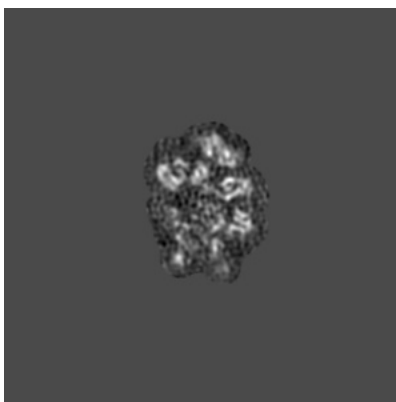
The images above show the map projected in three orthogonal directions.

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

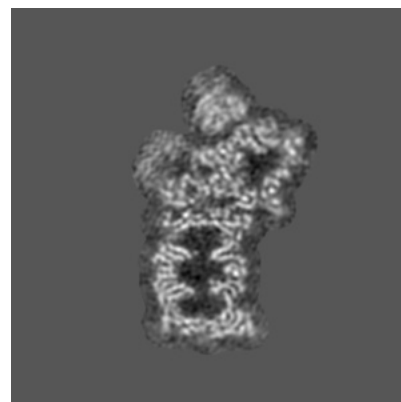
#### 6.2.1 Primary map



X Index: 180



Y Index: 180



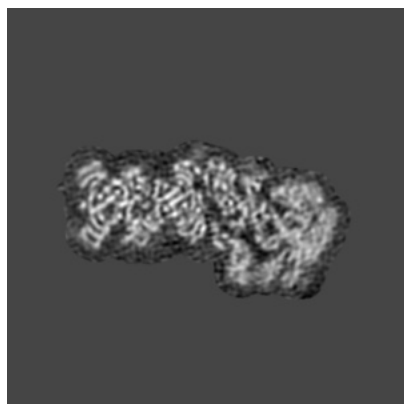
Z Index: 180



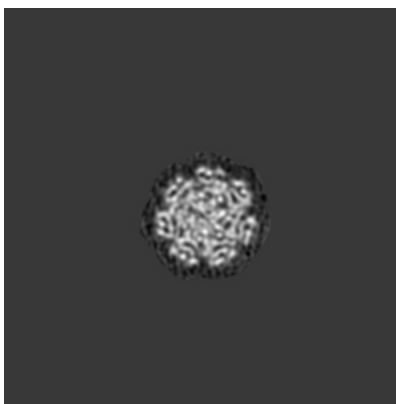
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 192



Y Index: 77

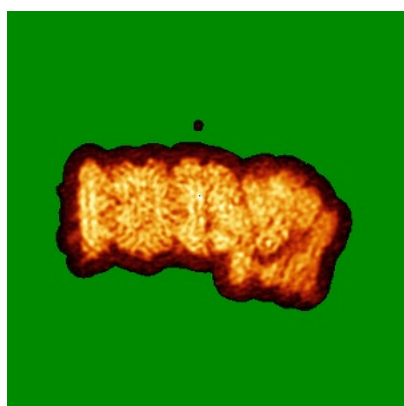


Z Index: 182

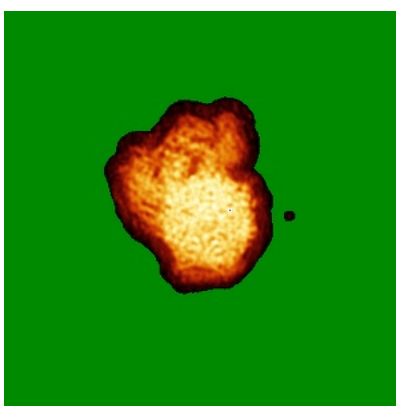
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X



Y

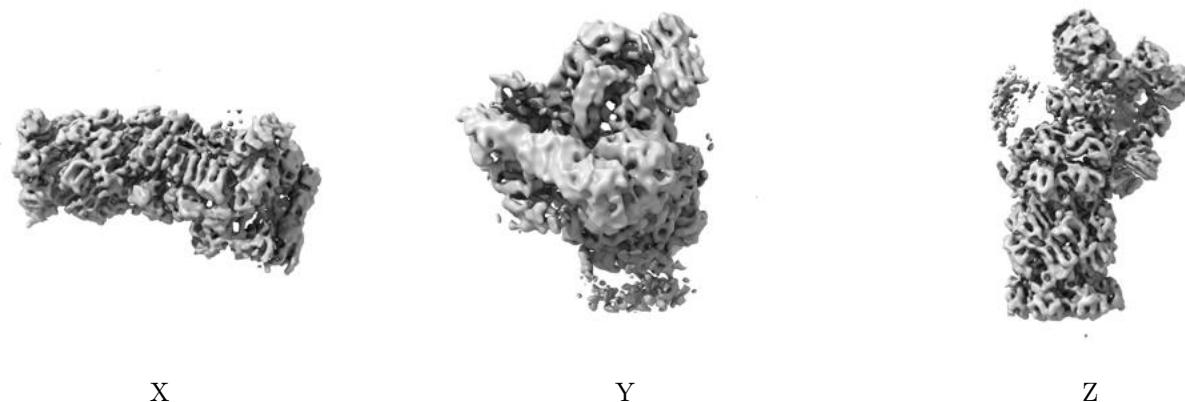


Z

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 0.755. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

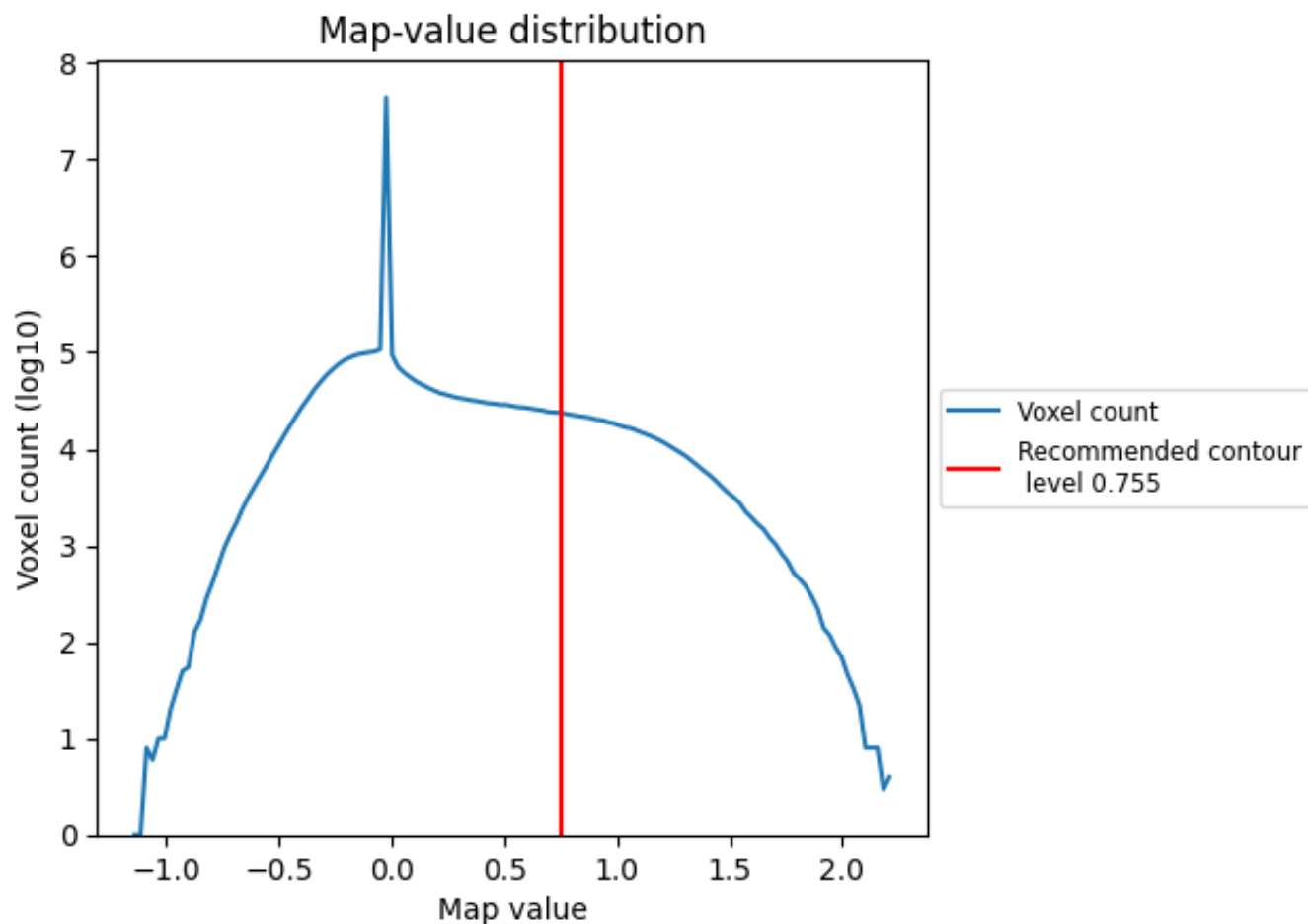
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

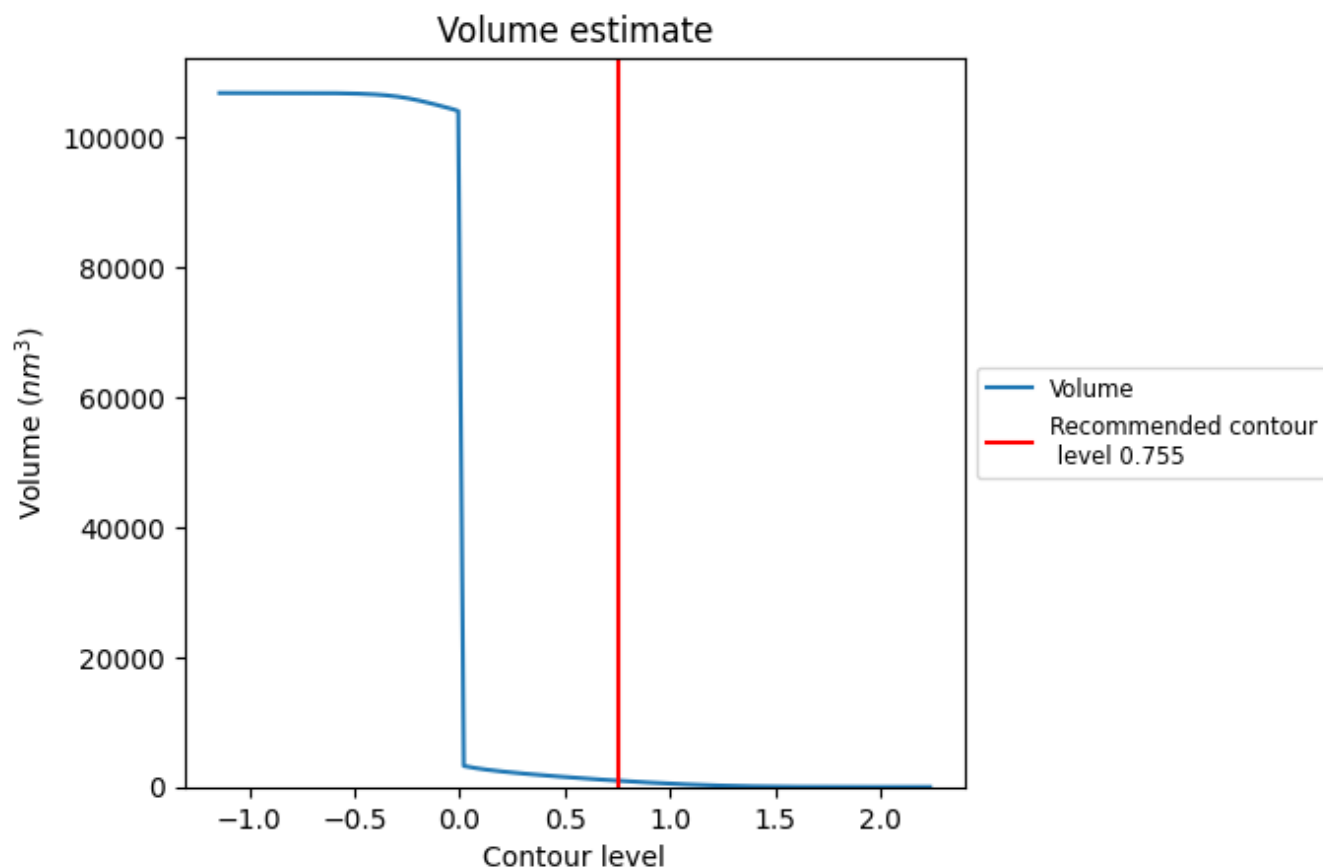
This section contains the results of statistical analysis of the map.

### 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.

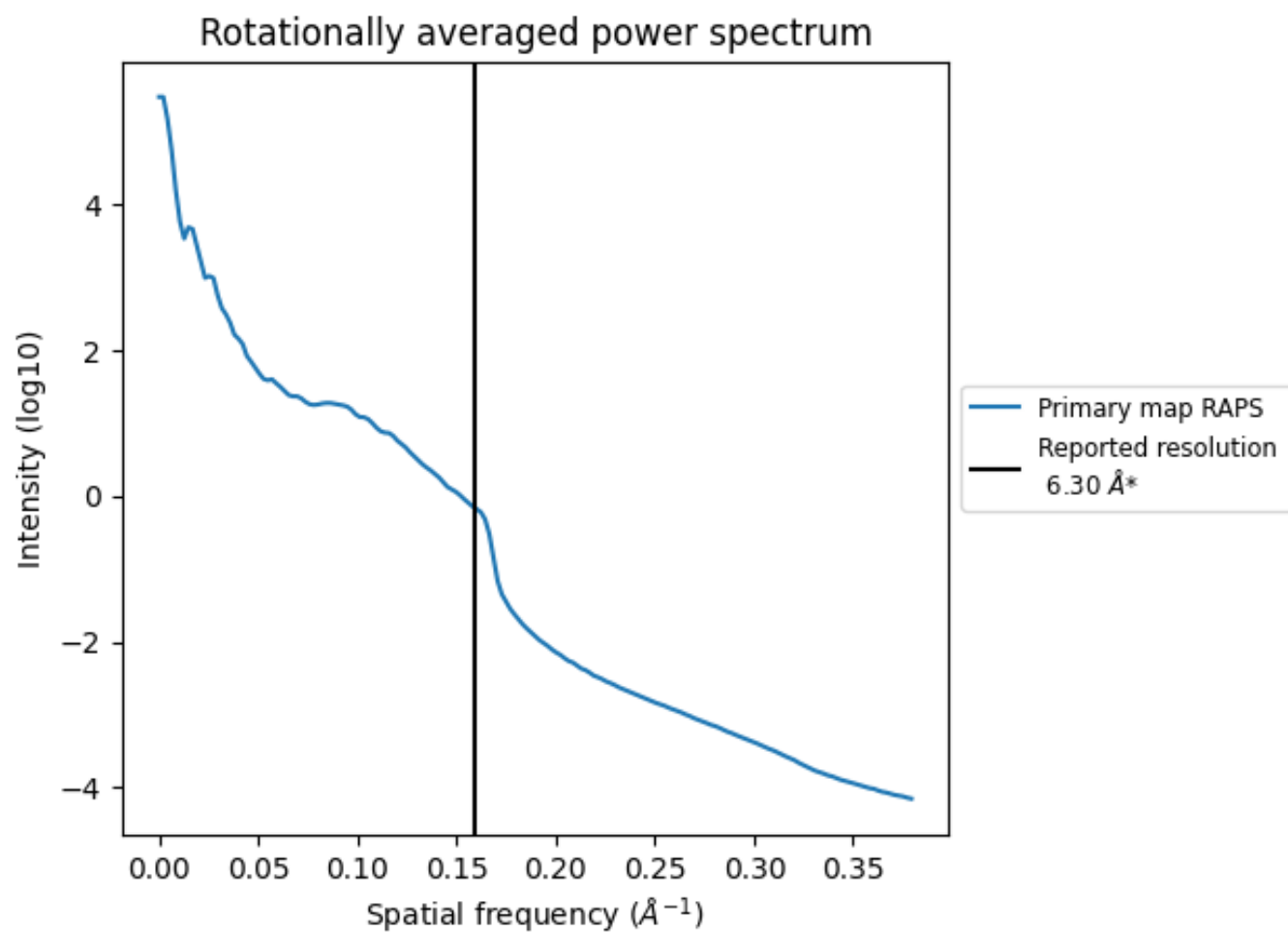
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 959 nm<sup>3</sup>; this corresponds to an approximate mass of 866 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 0.159 Å<sup>-1</sup>

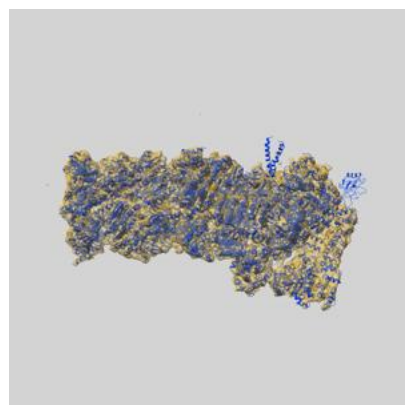
## 8 Fourier-Shell correlation

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

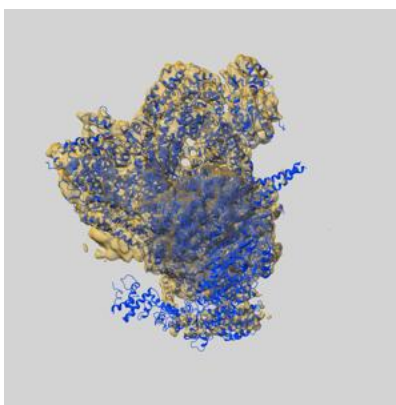
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6693 and PDB model 5WVI. Per-residue inclusion information can be found in section 3 on page 11.

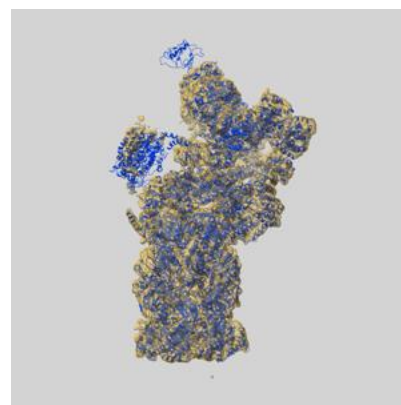
### 9.1 Map-model overlay [i](#)



X



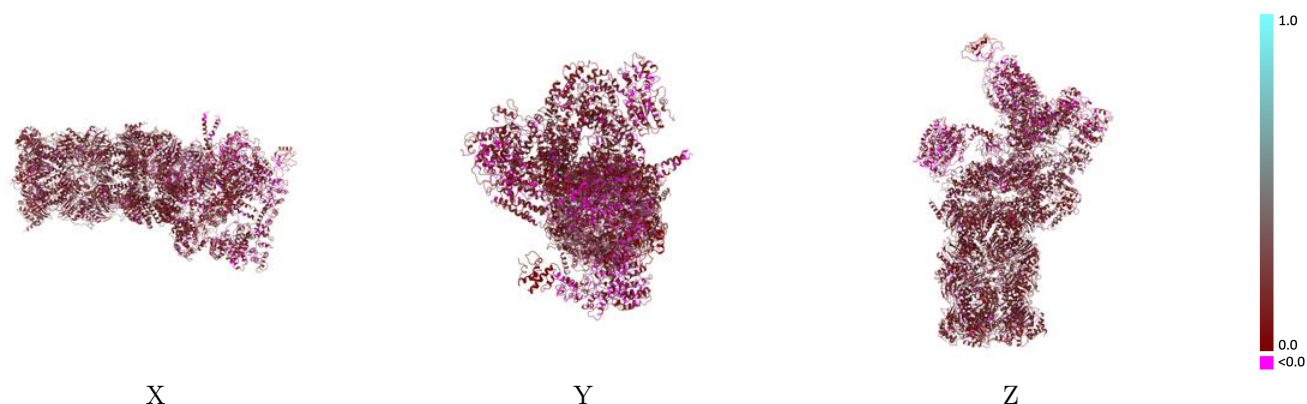
Y



Z

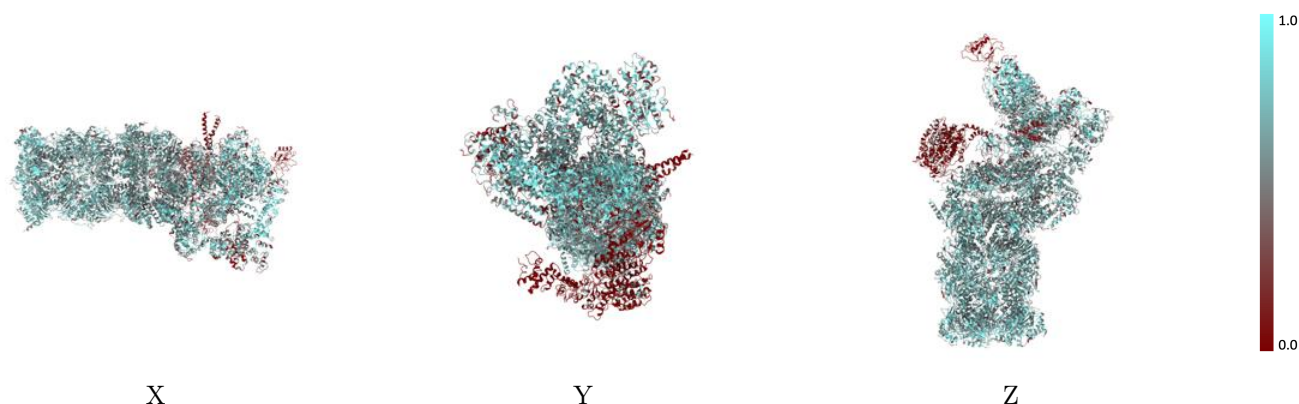
The images above show the 3D surface view of the map at the recommended contour level 0.755 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



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

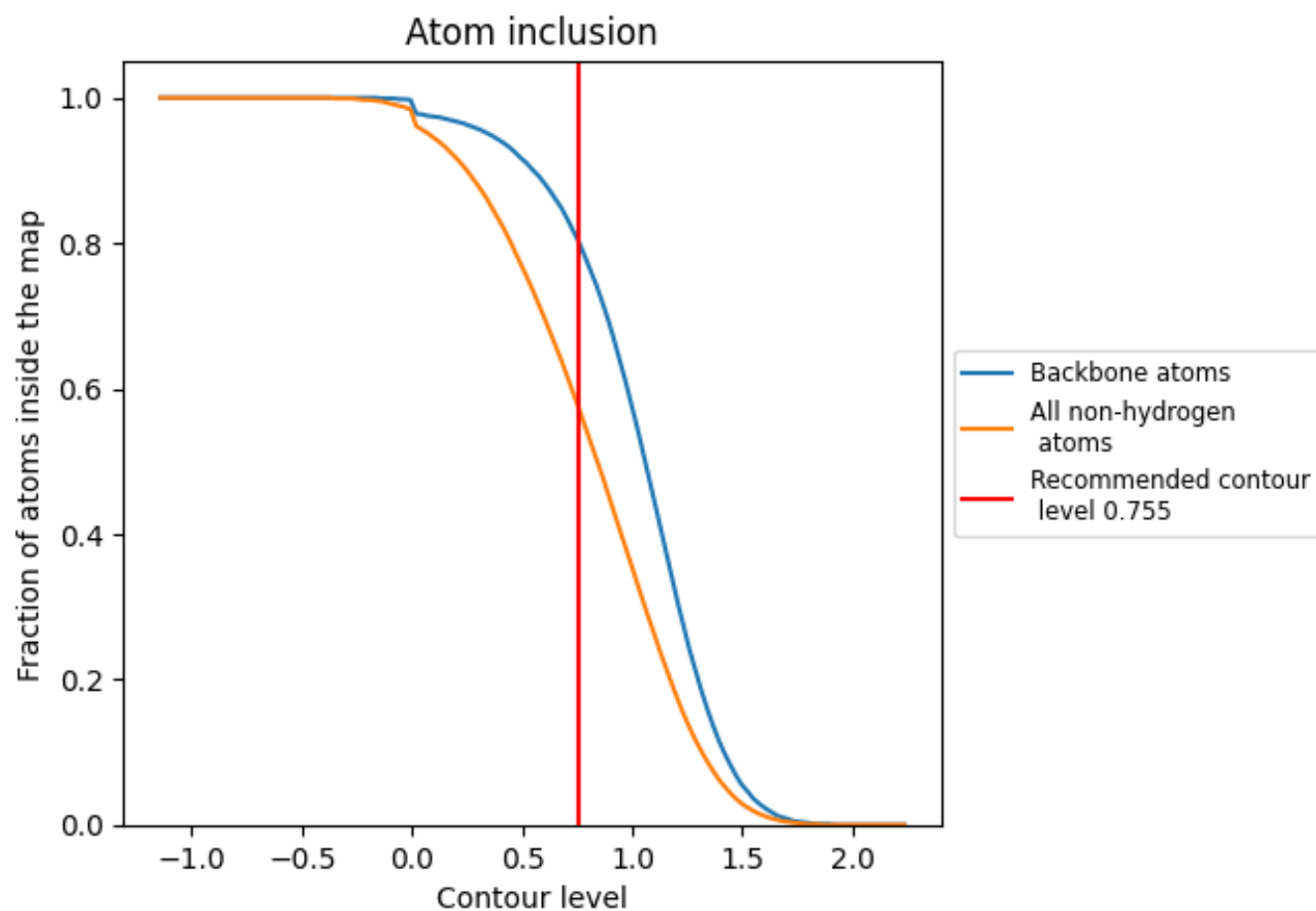
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.755).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 57% 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 (0.755) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.5750   |  0.1400   |
| 1     |  0.6150   |  0.1510   |
| 2     |  0.6520   |  0.1760   |
| 3     |  0.6420   |  0.1510   |
| 4     |  0.6490   |  0.1670   |
| 5     |  0.6430   |  0.1550   |
| 6     |  0.6460   |  0.1600   |
| 7     |  0.6290   |  0.1730   |
| A     |  0.6070   |  0.1720   |
| B     |  0.5830   |  0.1580   |
| C     |  0.6190   |  0.1490   |
| D     |  0.6500   |  0.1610   |
| E     |  0.6190   |  0.1520   |
| F     |  0.6280   |  0.1530   |
| G     |  0.6110  |  0.1600  |
| H     |  0.5320 |  0.1330 |
| I     |  0.5360 |  0.1430 |
| J     |  0.5500 |  0.1370 |
| K     |  0.5560 |  0.1460 |
| L     |  0.5420 |  0.1380 |
| M     |  0.5480 |  0.1460 |
| N     |  0.6810 |  0.1050 |
| O     |  0.6000 |  0.1270 |
| P     |  0.5960 |  0.1430 |
| Q     |  0.6190 |  0.1520 |
| R     |  0.6010 |  0.1280 |
| S     |  0.5630 |  0.1330 |
| T     |  0.3940 |  0.1160 |
| U     |  0.6130 |  0.1370 |
| V     |  0.5800 |  0.1280 |
| W     |  0.6060 |  0.1200 |
| X     |  0.0000 |  0.0040 |
| Y     |  0.5830 |  0.1600 |
| Z     |  0.0600 |  0.0640 |
| a     |  0.6350 |  0.1700 |



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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| b     |  0.6300 |  0.1500 |
| c     |  0.6810 |  0.1640 |
| d     |  0.6780 |  0.1490 |
| e     |  0.6680 |  0.1670 |
| f     |  0.6680 |  0.1560 |
| g     |  0.6530 |  0.1580 |
| h     |  0.6710 |  0.1500 |
| i     |  0.6710 |  0.1860 |
| j     |  0.6740 |  0.1650 |
| k     |  0.6660 |  0.1550 |
| l     |  0.6720 |  0.1540 |
| m     |  0.6670 |  0.1530 |
| n     |  0.6880 |  0.1530 |