



## Full wwPDB EM Validation Report ⓘ

Apr 20, 2026 – 03:33 PM JST

PDB ID : 9K54 / pdb\_00009k54  
EMDB ID : EMD-62080  
Title : Structure of substrate-engaged human 26S proteasome RP-CP subcomplex in state ED2.2  
Authors : Wu, Z.; Chen, E.; Mao, Y.  
Deposited on : 2024-10-21  
Resolution : 3.70 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:

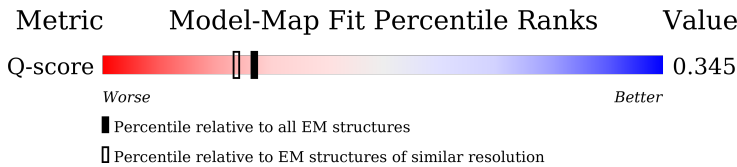
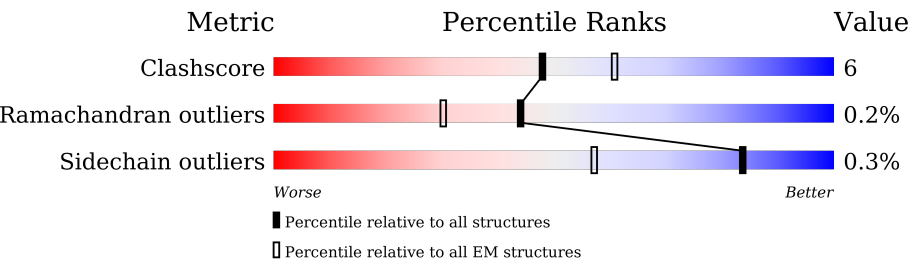
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.70 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                       | 11569 ( 3.20 - 4.20 )                                    |

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

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | A     | 433    | <div><div>22%</div><div>78%</div><div>17%</div><div>5%</div></div> |
| 2   | B     | 440    | <div><div>20%</div><div>75%</div><div>19%</div><div>7%</div></div> |
| 3   | C     | 398    | <div><div>10%</div><div>79%</div><div>20%</div><div>..</div></div> |
| 4   | D     | 418    | <div><div>12%</div><div>75%</div><div>15%</div><div>9%</div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | E     | 403    |                  |
| 6   | F     | 439    |                  |
| 7   | G     | 246    |                  |
| 7   | g     | 246    |                  |
| 8   | H     | 234    |                  |
| 8   | h     | 234    |                  |
| 9   | I     | 261    |                  |
| 9   | i     | 261    |                  |
| 10  | J     | 248    |                  |
| 10  | j     | 248    |                  |
| 11  | K     | 241    |                  |
| 11  | k     | 241    |                  |
| 12  | L     | 263    |                  |
| 12  | l     | 263    |                  |
| 13  | M     | 255    |                  |
| 13  | m     | 255    |                  |
| 14  | N     | 239    |                  |
| 14  | n     | 239    |                  |
| 15  | O     | 277    |                  |
| 15  | o     | 277    |                  |
| 16  | P     | 205    |                  |
| 16  | p     | 205    |                  |
| 17  | Q     | 201    |                  |
| 17  | q     | 201    |                  |
| 18  | R     | 263    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 18  | r     | 263    |                  |
| 19  | S     | 241    |                  |
| 19  | s     | 241    |                  |
| 20  | T     | 264    |                  |
| 20  | t     | 264    |                  |
| 21  | U     | 953    |                  |
| 22  | V     | 534    |                  |
| 23  | W     | 456    |                  |
| 24  | X     | 422    |                  |
| 25  | Y     | 389    |                  |
| 26  | Z     | 324    |                  |
| 27  | a     | 376    |                  |
| 28  | b     | 377    |                  |
| 29  | c     | 310    |                  |
| 30  | d     | 350    |                  |
| 31  | e     | 70     |                  |
| 32  | f     | 908    |                  |
| 33  | v     | 36     |                  |
| 34  | w     | 76     |                  |
| 34  | x     | 76     |                  |
| 34  | y     | 76     |                  |
| 34  | z     | 76     |                  |

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 108712 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 proteasome regulatory subunit 7.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 413      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3229  | 2034 | 566 | 611 | 18 |         |       |

- Molecule 2 is a protein called 26S proteasome regulatory subunit 4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | B     | 411      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3207  | 2022 | 548 | 622 | 15 |         |       |

- Molecule 3 is a protein called 26S proteasome regulatory subunit 8.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | C     | 396      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3105  | 1954 | 558 | 576 | 17 |         |       |

- Molecule 4 is a protein called 26S proteasome regulatory subunit 6B.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | D     | 380      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3040  | 1923 | 524 | 580 | 13 |         |       |

- Molecule 5 is a protein called Proteasome 26S subunit, ATPase 6.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | E     | 389      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3097  | 1947 | 552 | 581 | 17 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | F     | 395      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3098  | 1951 | 533 | 596 | 18 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | G     | 240      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1867  | 1187 | 312 | 355 | 13 |         |       |
| 7   | g     | 244      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1879  | 1193 | 318 | 355 | 13 |         |       |

- Molecule 8 is a protein called Proteasome subunit alpha type-2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8   | H     | 232      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1801  | 1149 | 304 | 342 | 6 |         |       |
| 8   | h     | 232      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1805  | 1154 | 307 | 338 | 6 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9   | I     | 248      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1933  | 1222 | 330 | 371 | 10 |         |       |
| 9   | i     | 250      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1955  | 1234 | 336 | 375 | 10 |         |       |

- Molecule 10 is a protein called Proteasome subunit alpha type-7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10  | J     | 239      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1861  | 1166 | 327 | 363 | 5 |         |       |
| 10  | j     | 239      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1861  | 1168 | 332 | 356 | 5 |         |       |

- Molecule 11 is a protein called Proteasome subunit alpha type-5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 11  | K     | 238      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1813  | 1139 | 302 | 361 | 11 |         |       |
| 11  | k     | 234      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1782  | 1119 | 295 | 357 | 11 |         |       |

- Molecule 12 is a protein called Proteasome subunit alpha type-1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12  | L     | 240      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1876  | 1175 | 338 | 352 | 11 |         |       |
| 12  | l     | 238      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1861  | 1165 | 335 | 350 | 11 |         |       |

- Molecule 13 is a protein called Proteasome subunit alpha type-3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 13  | M     | 242      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 1893  | 1202 | 323 | 356 | 12 |         |       |
| 13  | m     | 240      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1881  | 1193 | 321 | 356 | 11 |         |       |

- Molecule 14 is a protein called Proteasome subunit beta type-6.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 14  | N     | 203      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1521  | 954 | 259 | 296 | 12 |         |       |
| 14  | n     | 202      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1510  | 947 | 258 | 293 | 12 |         |       |

- Molecule 15 is a protein called Proteasome subunit beta type-7.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 15  | O     | 220      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1645  | 1035 | 278 | 320 | 12 |         |       |
| 15  | o     | 220      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1659  | 1044 | 283 | 320 | 12 |         |       |

- Molecule 16 is a protein called Proteasome subunit beta type-3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 16  | P     | 204      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1587  | 1010 | 264 | 294 | 19 |         |       |
| 16  | p     | 204      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1591  | 1013 | 265 | 294 | 19 |         |       |

- Molecule 17 is a protein called Proteasome subunit beta type-2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 17  | Q     | 199      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 1591  | 1019 | 270 | 292 | 10 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 17  | q     | 199      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1578  | 1012 | 267 | 290 | 9 |         |       |

- Molecule 18 is a protein called Proteasome subunit beta type-5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | R     | 201      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1559  | 982 | 274 | 294 | 9 |         |       |
| 18  | r     | 201      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1549  | 977 | 270 | 293 | 9 |         |       |

- Molecule 19 is a protein called Proteasome subunit beta type-1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 19  | S     | 213      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1641  | 1041 | 281 | 309 | 10 |         |       |
| 19  | s     | 213      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1650  | 1044 | 283 | 313 | 10 |         |       |

- Molecule 20 is a protein called Proteasome subunit beta type-4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 20  | T     | 216      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1683  | 1062 | 291 | 318 | 12 |         |       |
| 20  | t     | 216      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1687  | 1064 | 291 | 320 | 12 |         |       |

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 21  | U     | 878      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6867  | 4352 | 1163 | 1306 | 46 |         |       |

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 22  | V     | 444      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3612  | 2301 | 645 | 653 | 13 |         |       |

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 12.



| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 23  | W     | 441      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3596  | 2277 | 613 | 682 | 24 |         |       |

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 24  | X     | 422      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3335  | 2116 | 567 | 639 | 13 |         |       |

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 25  | Y     | 389      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3202  | 2041 | 545 | 598 | 18 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 26  | Z     | 286      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2281  | 1457 | 392 | 427 | 5 |         |       |

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 27  | a     | 373      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2995  | 1911 | 510 | 559 | 15 |         |       |

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | b     | 191      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1458  | 910 | 261 | 279 | 8 |         |       |

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 29  | c     | 287      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2260  | 1430 | 389 | 422 | 19 |         |       |

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 30  | d     | 257      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2116  | 1371 | 346 | 390 | 9 |         |       |

- Molecule 31 is a protein called 26S proteasome complex subunit SEM1.

| Mol | Chain | Residues | Atoms |     |    |     | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---------|-------|
| 31  | e     | 50       | Total | C   | N  | O   | 0       | 0     |
|     |       |          | 425   | 260 | 65 | 100 |         |       |

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 32  | f     | 844      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6529  | 4126 | 1108 | 1250 | 45 |         |       |

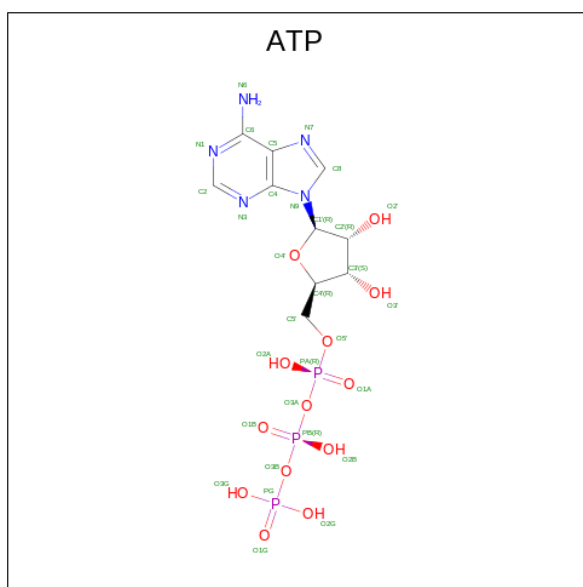
- Molecule 33 is a protein called Substrate.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 33  | v     | 36       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 180   | 108 | 36 | 36 |         |       |

- Molecule 34 is a protein called Ubiquitin.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | w     | 76       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 601   | 378 | 105 | 117 | 1 |         |       |
| 34  | x     | 76       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 601   | 378 | 105 | 117 | 1 |         |       |
| 34  | y     | 76       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 601   | 378 | 105 | 117 | 1 |         |       |
| 34  | z     | 76       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 601   | 378 | 105 | 117 | 1 |         |       |

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 35  | A     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 35  | B     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 35  | C     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 35  | F     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 36  | A     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 36  | B     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 36  | C     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 36  | D     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 36  | F     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms       |         |        |                   | AltConf |
|-----|-------|----------|-------------|---------|--------|-------------------|---------|
| 37  | D     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10<br>P<br>2 | 0       |

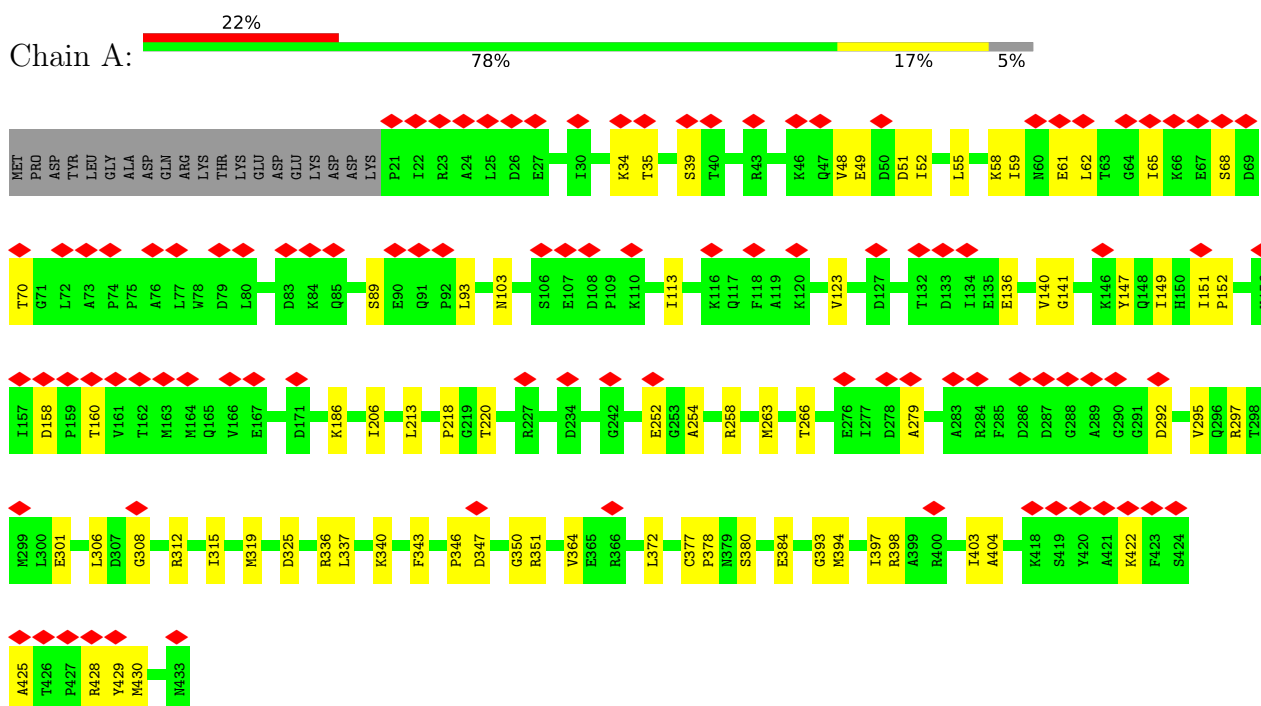
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms           | AltConf |
|-----|-------|----------|-----------------|---------|
| 38  | c     | 1        | Total Zn<br>1 1 | 0       |

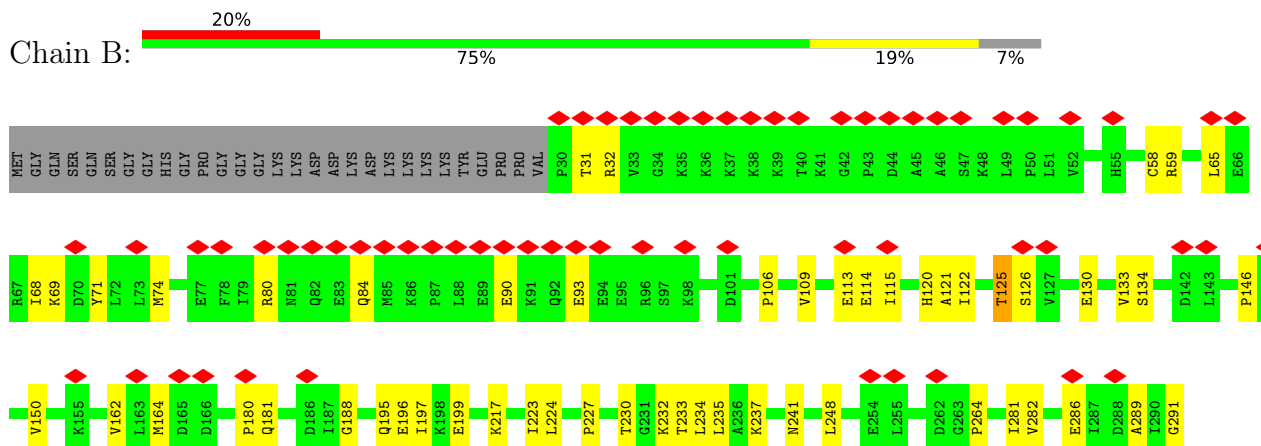
### 3 Residue-property plots

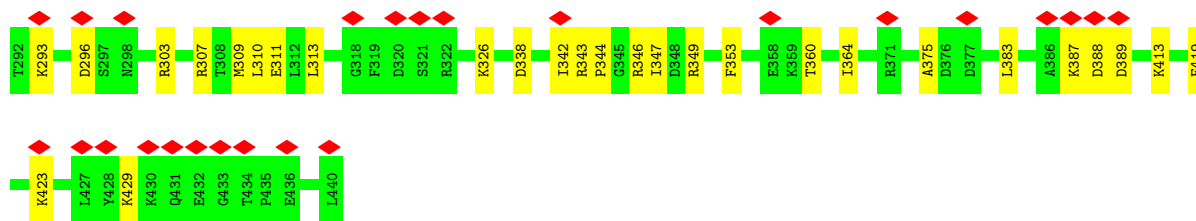
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 proteasome regulatory subunit 7

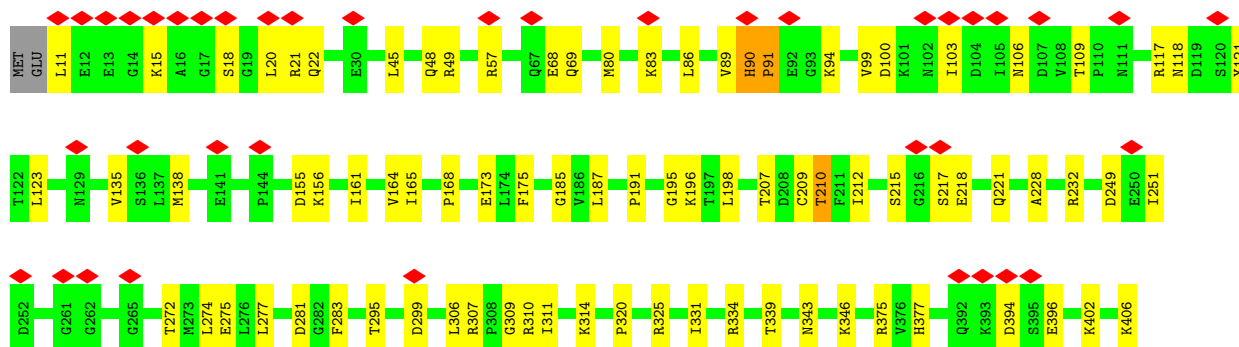
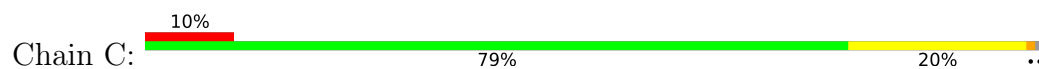


- Molecule 2: 26S proteasome regulatory subunit 4

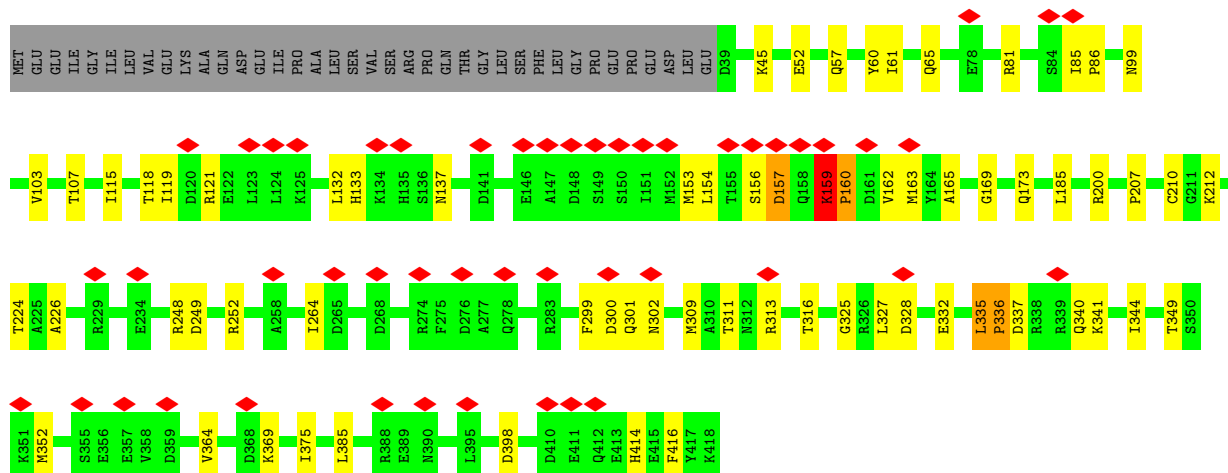
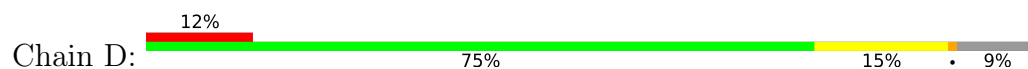




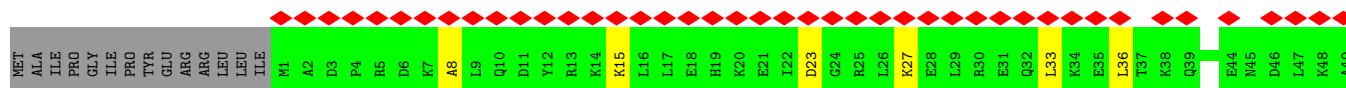
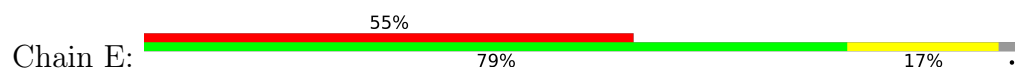
• Molecule 3: 26S proteasome regulatory subunit 8

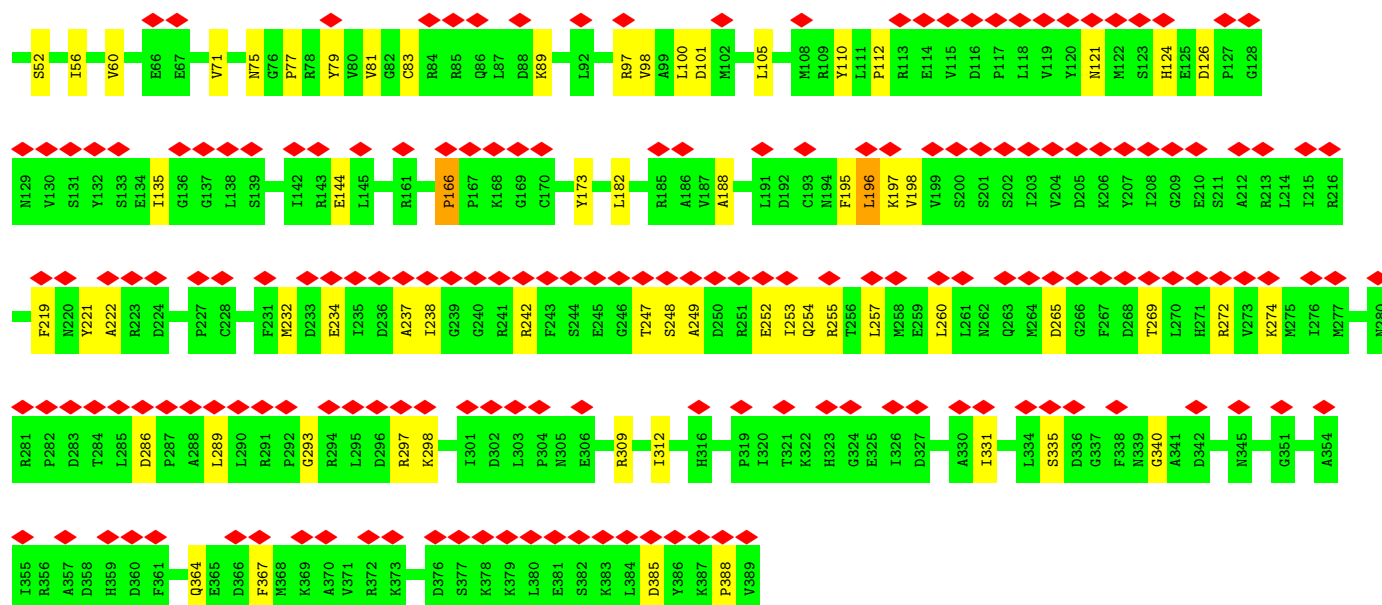


• Molecule 4: 26S proteasome regulatory subunit 6B

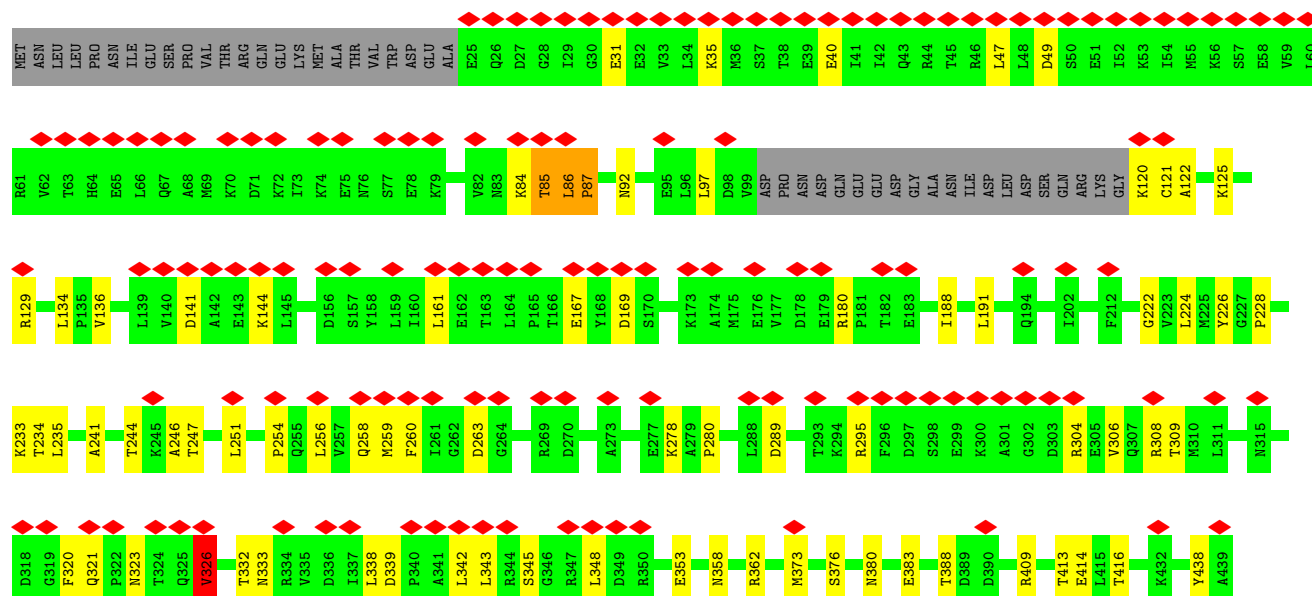
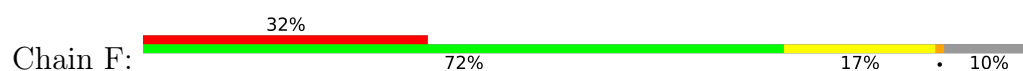


• Molecule 5: Proteasome 26S subunit, ATPase 6

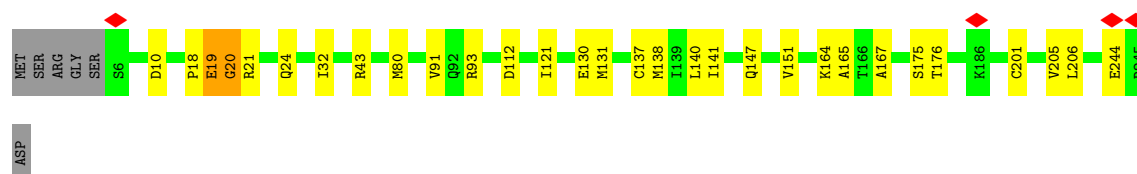
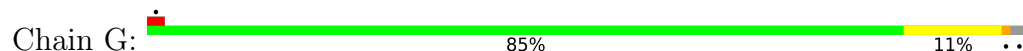




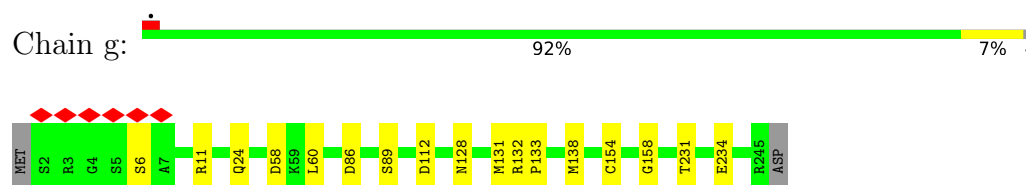
• Molecule 6: 26S proteasome regulatory subunit 6A



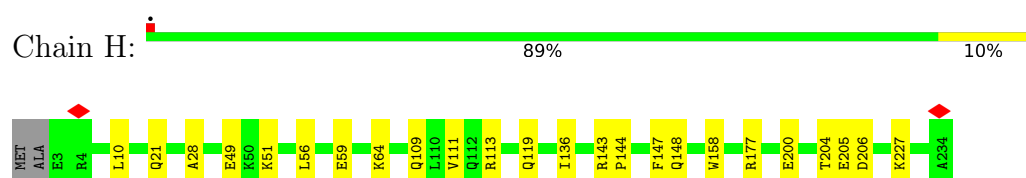
• Molecule 7: Proteasome subunit alpha type-6



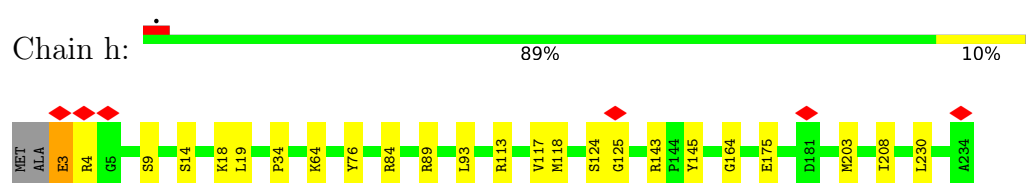
- Molecule 7: Proteasome subunit alpha type-6



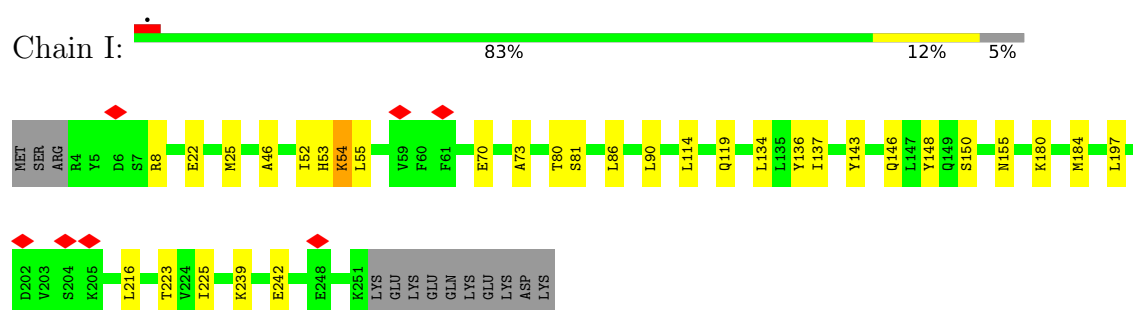
- Molecule 8: Proteasome subunit alpha type-2



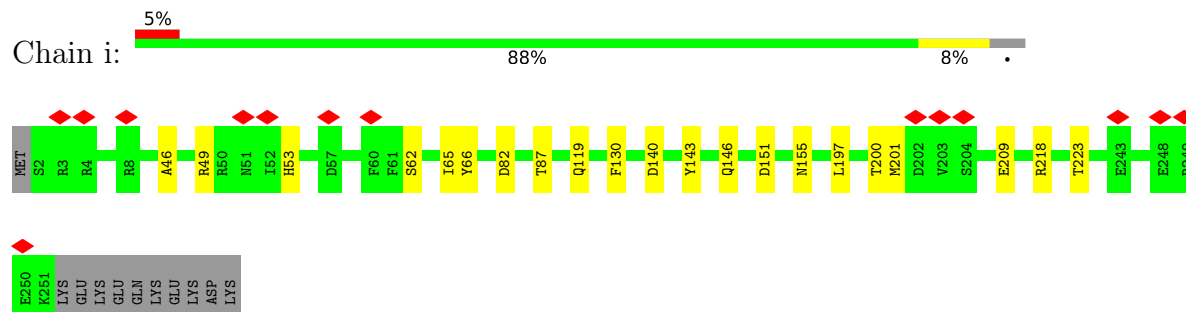
- Molecule 8: Proteasome subunit alpha type-2



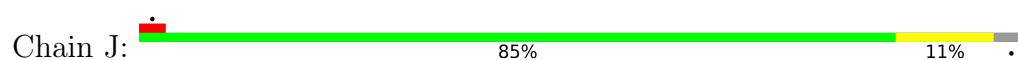
- Molecule 9: Proteasome subunit alpha type-4



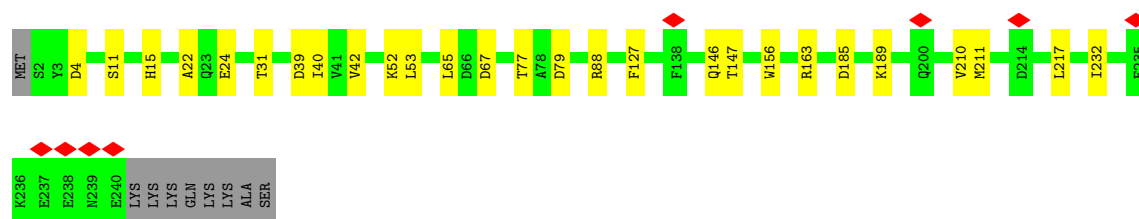
- Molecule 9: Proteasome subunit alpha type-4



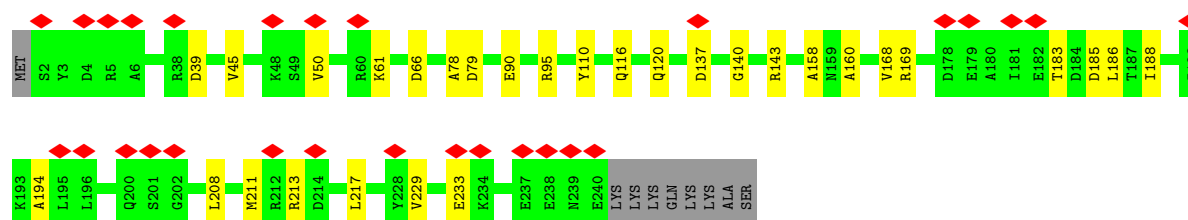
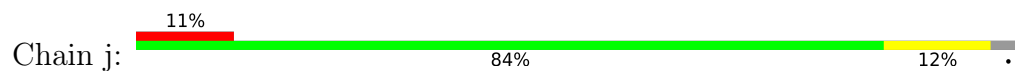
- Molecule 10: Proteasome subunit alpha type-7



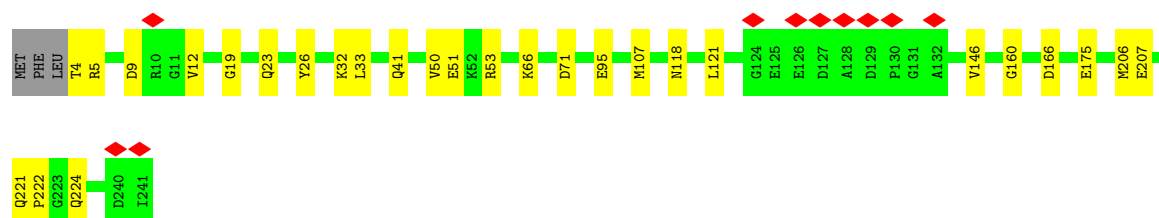
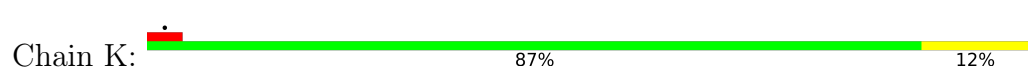




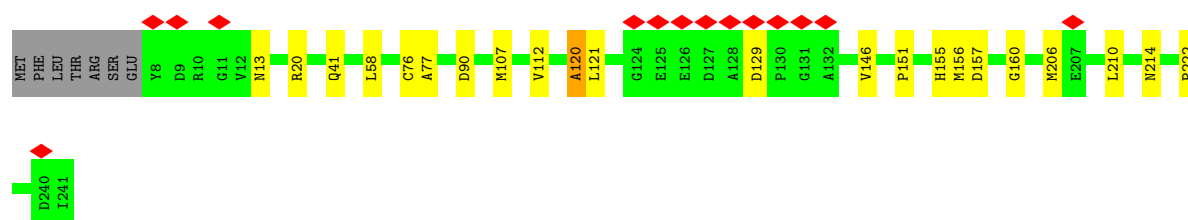
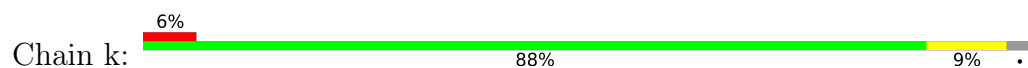
- Molecule 10: Proteasome subunit alpha type-7



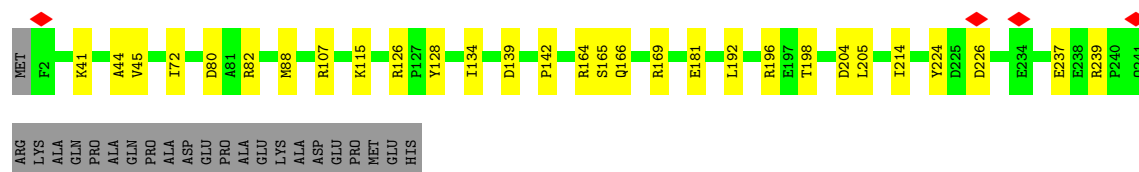
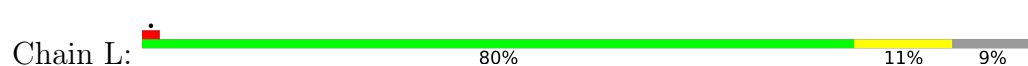
- Molecule 11: Proteasome subunit alpha type-5



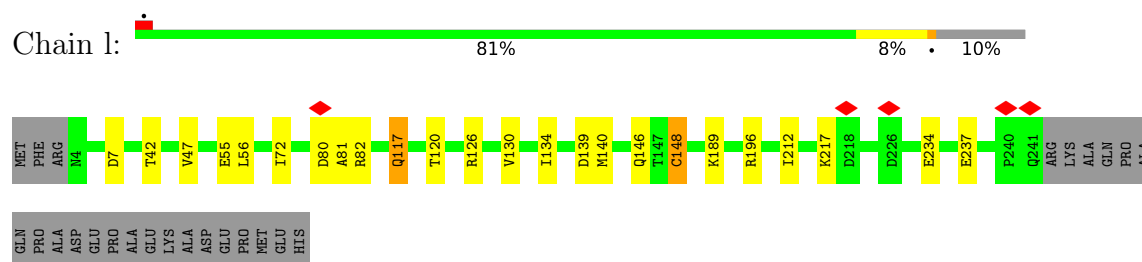
- Molecule 11: Proteasome subunit alpha type-5



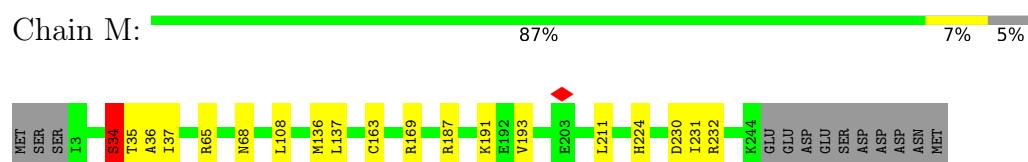
- Molecule 12: Proteasome subunit alpha type-1



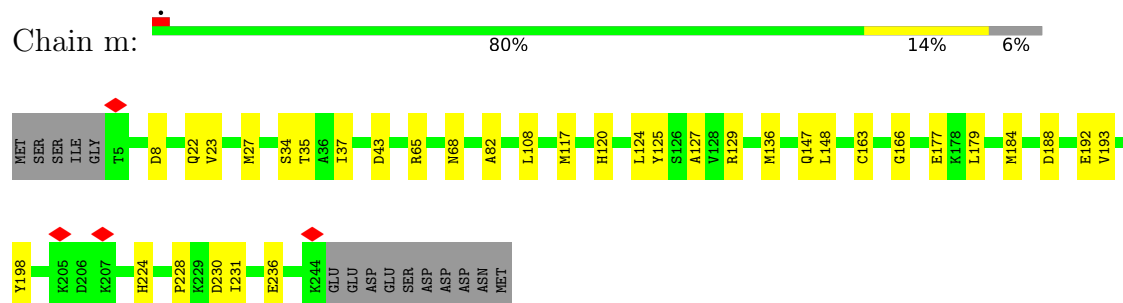
- Molecule 12: Proteasome subunit alpha type-1



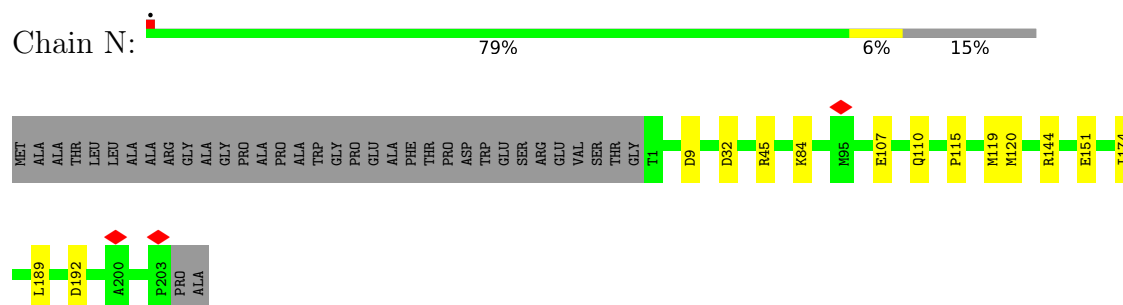
- Molecule 13: Proteasome subunit alpha type-3



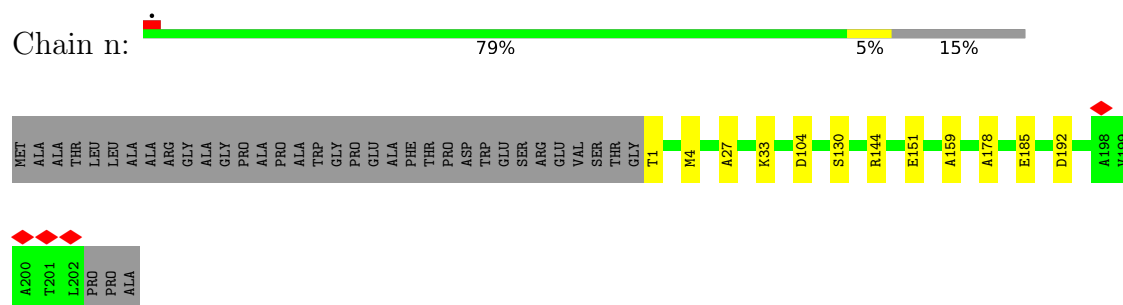
- Molecule 13: Proteasome subunit alpha type-3



- Molecule 14: Proteasome subunit beta type-6

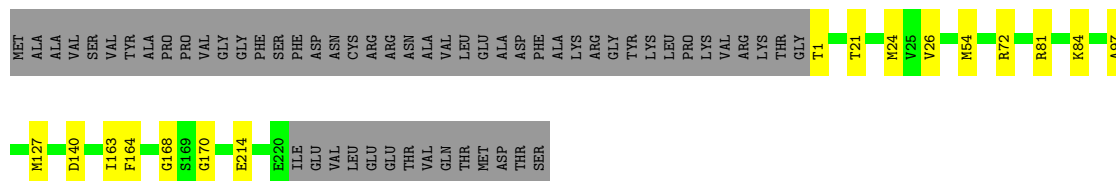


- Molecule 14: Proteasome subunit beta type-6



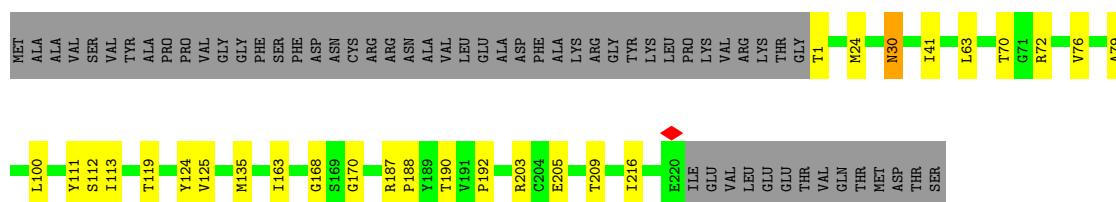
- Molecule 15: Proteasome subunit beta type-7

Chain O:  74% 6% 21%



- Molecule 15: Proteasome subunit beta type-7

Chain o:  69% 10% 21%




- Molecule 16: Proteasome subunit beta type-3

Chain P:  91% 8%




- Molecule 16: Proteasome subunit beta type-3

Chain p:  85% 14%




- Molecule 17: Proteasome subunit beta type-2

Chain Q:  89% 10%



- Molecule 17: Proteasome subunit beta type-2

Chain q:  85% 14%



- Molecule 18: Proteasome subunit beta type-5

Chain R:  67% 10% 24%

MET ALA LEU LEU SER VAL LEU GLU ARG PRO LEU PRO VAL ASN GLN ARG GLY PHE PHE GLY LEU GLY ARG ALA ASP LEU LEU ASP LEU LEU GLY PRO GLY SER LEU SER ASP GLY LEU SER LEU ALA ALA PRO GLY TRP VAL PRO GLU GLU PRO GLY ILE GLU MET LEU HIS GLY T1

T2 T3 K7 V12 A16 T21 I26 I37 R39 P39 Y40 L41 A46 A60 R64 E67 M93 G98 G103 P109 S122 G123 Y136 R166 D182 G183 W184 N191 V192 G201 SER THR PRO


- Molecule 18: Proteasome subunit beta type-5

Chain r:  70% 7% 24%

MET ALA LEU LEU SER VAL LEU GLU ARG PRO LEU PRO VAL ASN GLN ARG GLY PHE PHE GLY LEU GLY ARG ALA ASP LEU LEU ASP LEU LEU GLY PRO GLY SER LEU SER ASP GLY LEU SER LEU ALA ALA PRO GLY TRP VAL PRO GLU GLU PRO GLY ILE GLU MET LEU HIS GLY T1

F6 K7 G11 K32 D61 C63 R69 R70 K71 I74 A78 Y88 W104 P109 A135 M139 D140 R141 R166 V192 G201 SER THR PRO

- Molecule 19: Proteasome subunit beta type-1

Chain S:  78% 10% 12%

MET LEU SER THR ALA MET SER PRO ALA ARG ASP LEU MET GLU PRO HIS ARG ALA ALA GLY PRO LEU GLN LEU R1 P4 G10 A16 I22 T27 S40 P41 K42 C43 L92 V121 F124 D125 S129 L145 D150 M157 M158

Q159 N160 V161 V178 A182 V187 R194 I197 V198 I203 I213

- Molecule 19: Proteasome subunit beta type-1

Chain s:  76% 12% 12%

MET LEU SER THR ALA MET TYR SER PRO ALA ARG ASP LEU MET GLU PRO HIS ARG ALA ALA GLY PRO LEU GLN LEU R1 P4 A16 D19 T27 R38 R39 S40 K45 L64 I68 E69 L92 I95 S98 R99 R100 V121 D125

S129 L145 L148 L149 D150 E162 E163 V178 E184 V187 I195 I203 R204 E205 E206 R211 R212 D213

- Molecule 20: Proteasome subunit beta type-4

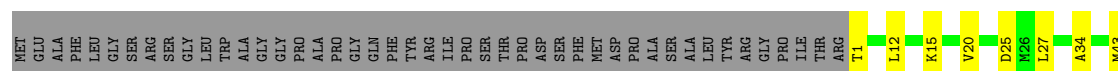
Chain T:  70% 11% 18%

MET GLU ALA PHE LEU GLY SER ARG GLY LEU TRP ALA GLY GLY PRO PRO GLY GLN PHE TYR ARG ILE PRO SER THR ASP PHE MET ASP PRO ALA ALA ALA LEU TYR ARG GLY PRO ILE THR ARG T1 V20 D25 M26 L27 A34 R41 I42 M43 R44



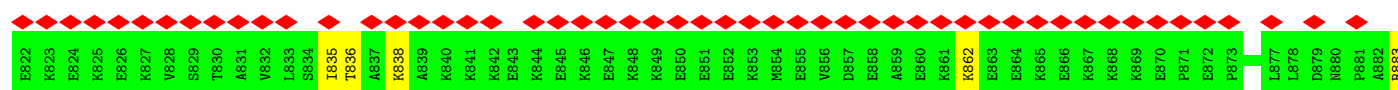
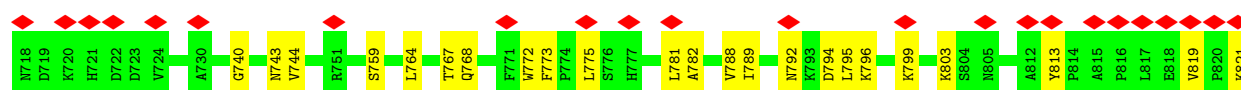
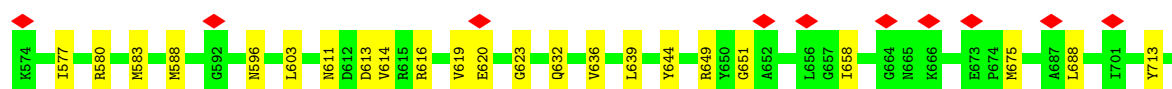
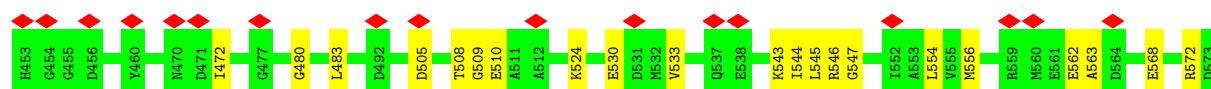
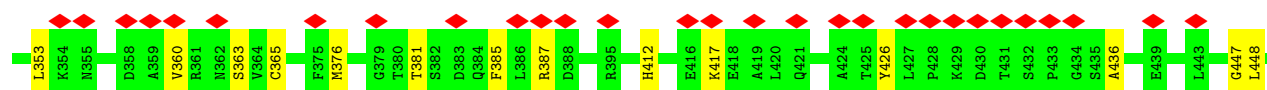
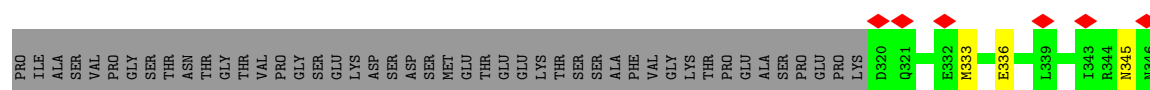
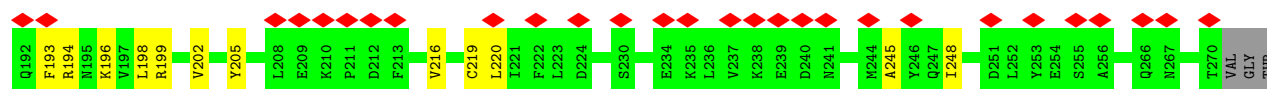
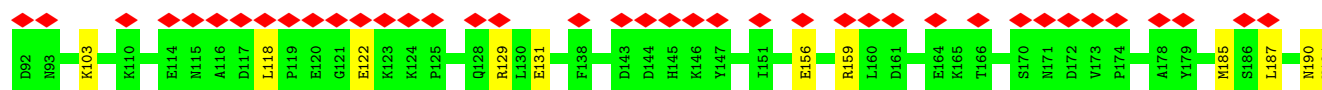
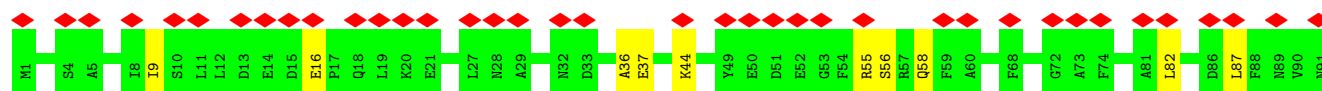
- Molecule 20: Proteasome subunit beta type-4

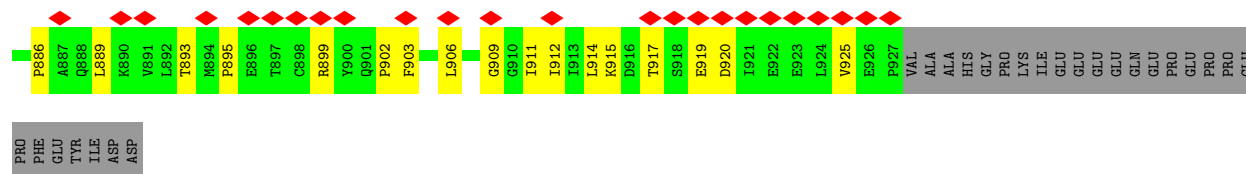
Chain t: 70% 12% 18%



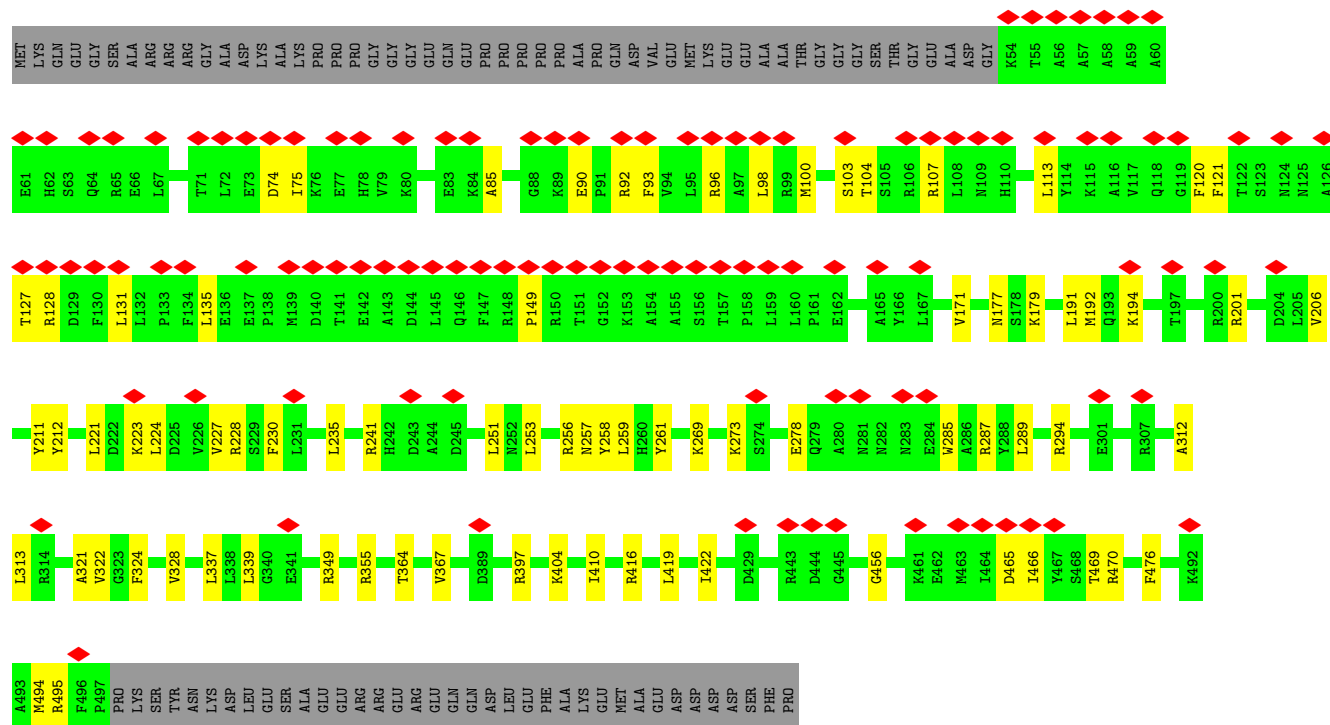
- Molecule 21: 26S proteasome non-ATPase regulatory subunit 1

Chain U: 28% 78% 15% 8%

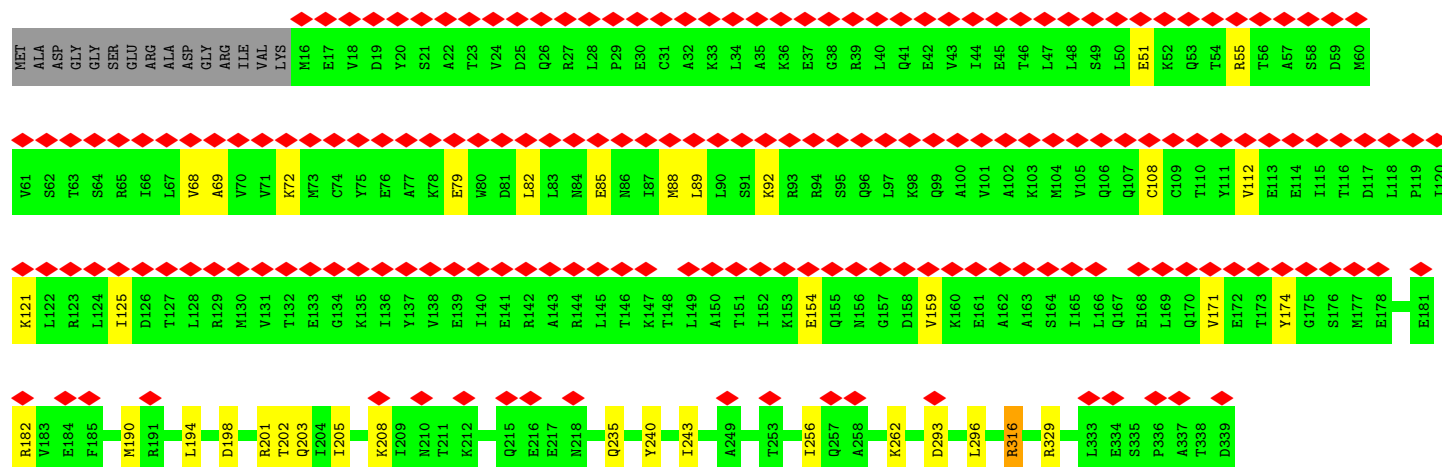
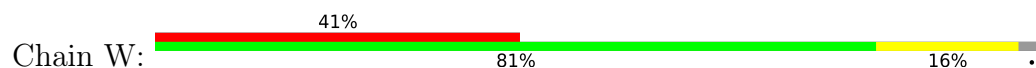


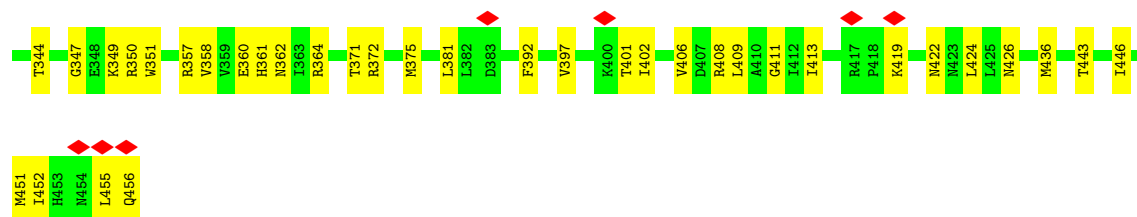


• Molecule 22: 26S proteasome non-ATPase regulatory subunit 3

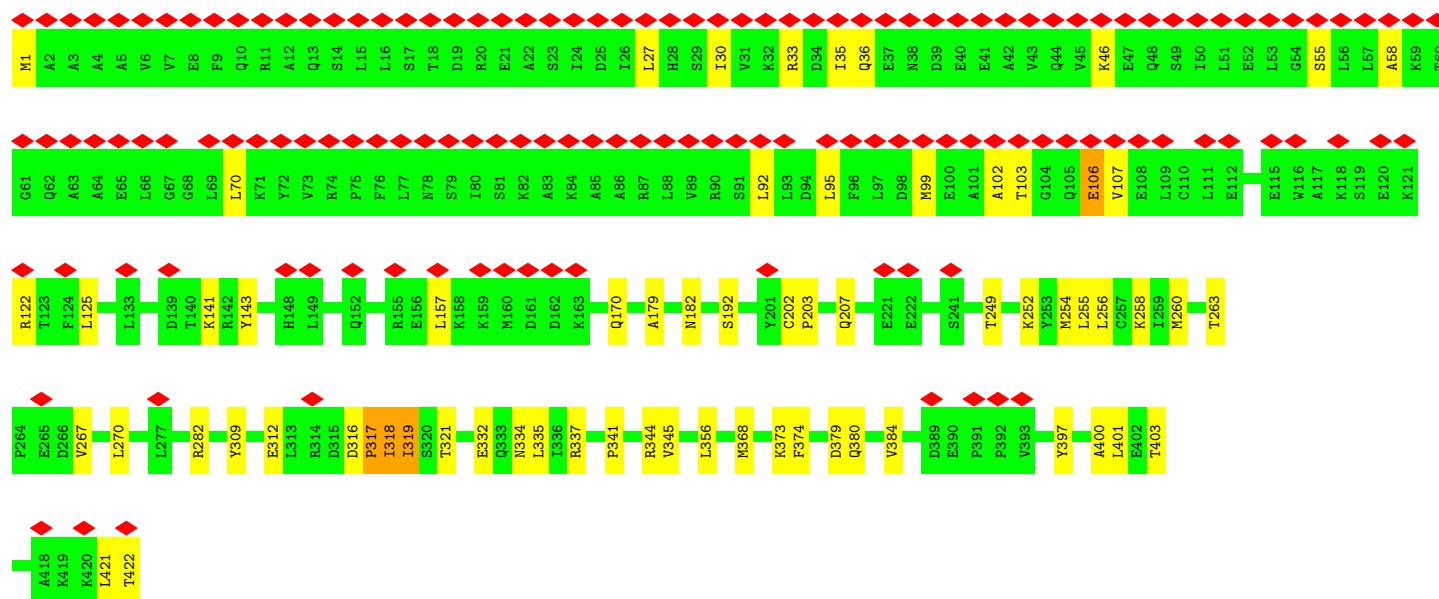
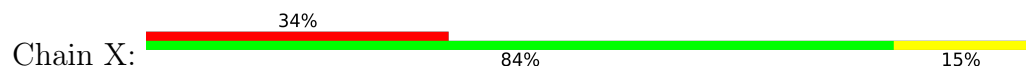


• Molecule 23: 26S proteasome non-ATPase regulatory subunit 12

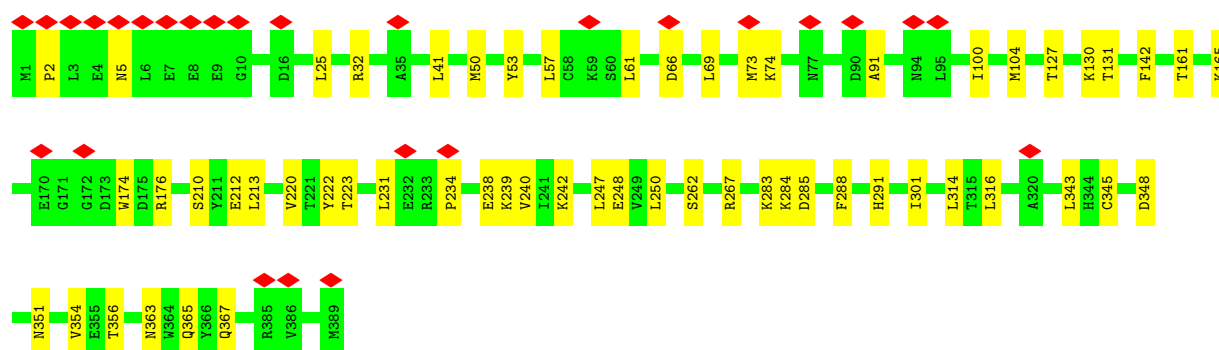
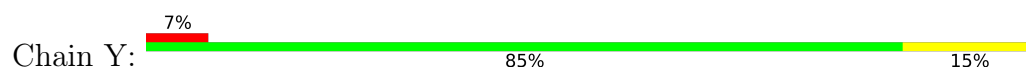




- Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

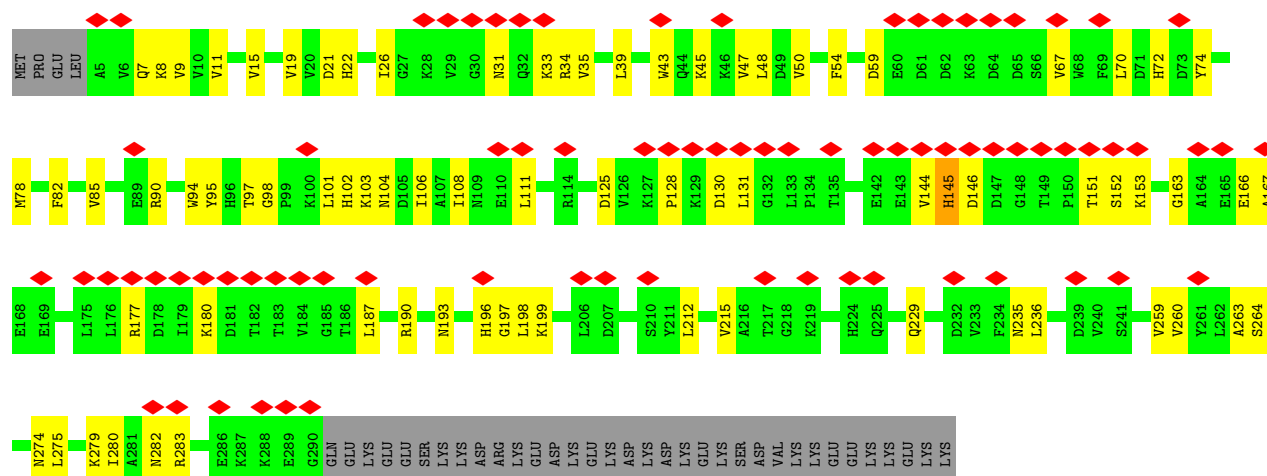


- Molecule 25: 26S proteasome non-ATPase regulatory subunit 6



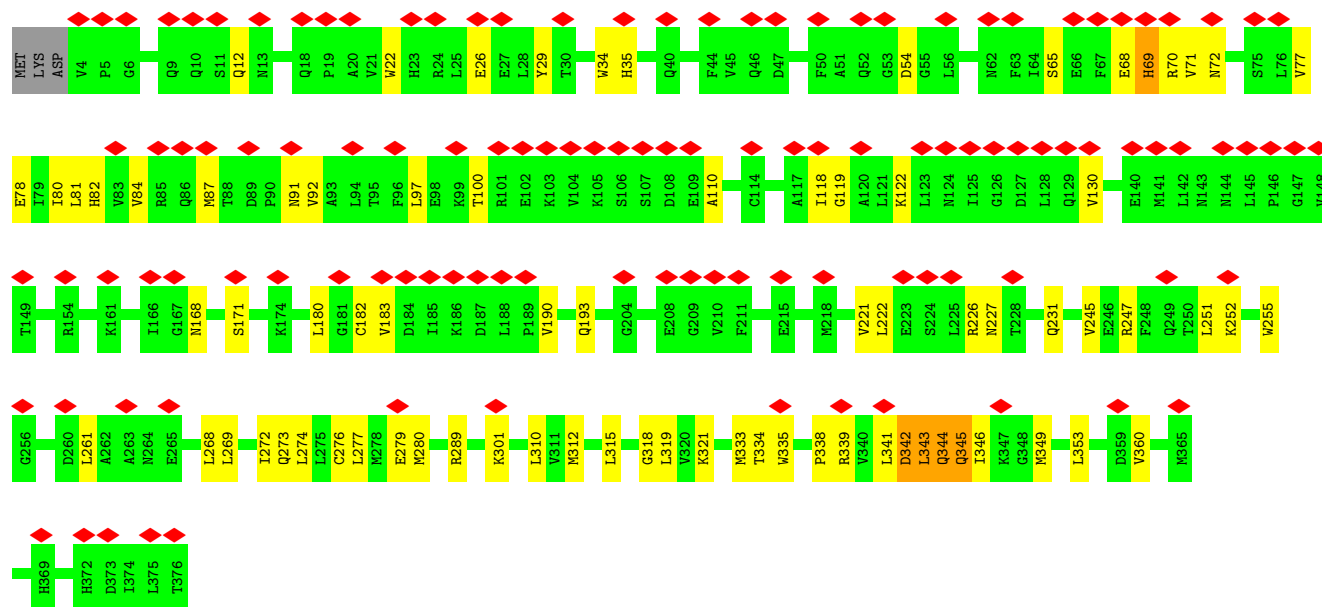
- Molecule 26: 26S proteasome non-ATPase regulatory subunit 7





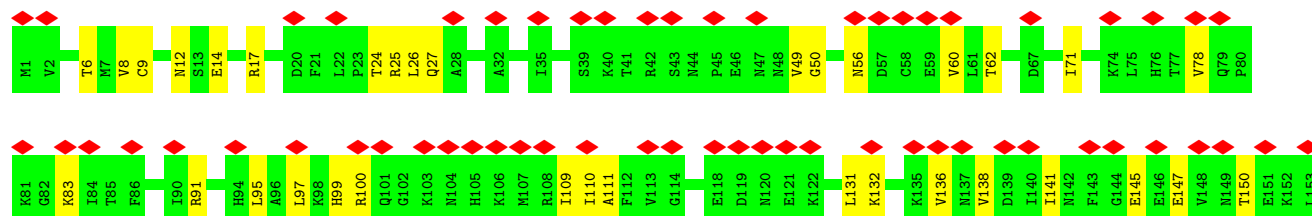
• Molecule 27: 26S proteasome non-ATPase regulatory subunit 13

Chain a: 31% 78% 19% ..

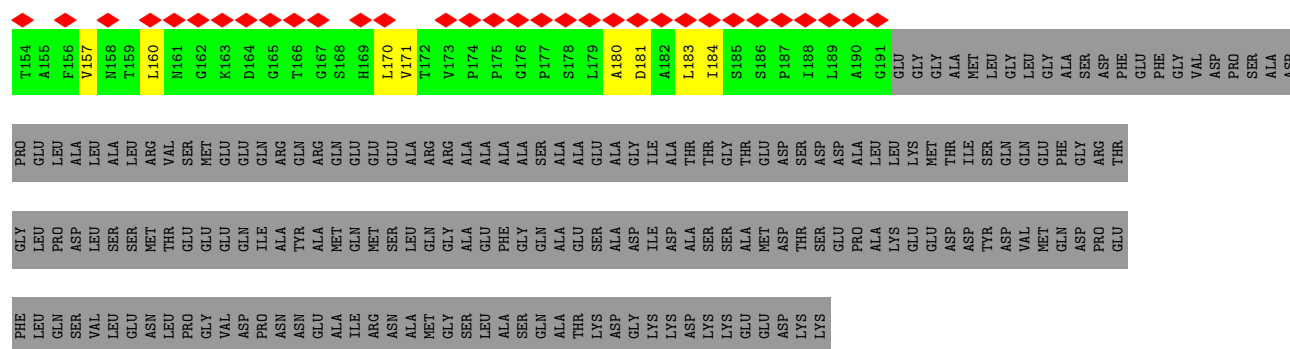


• Molecule 28: 26S proteasome non-ATPase regulatory subunit 4

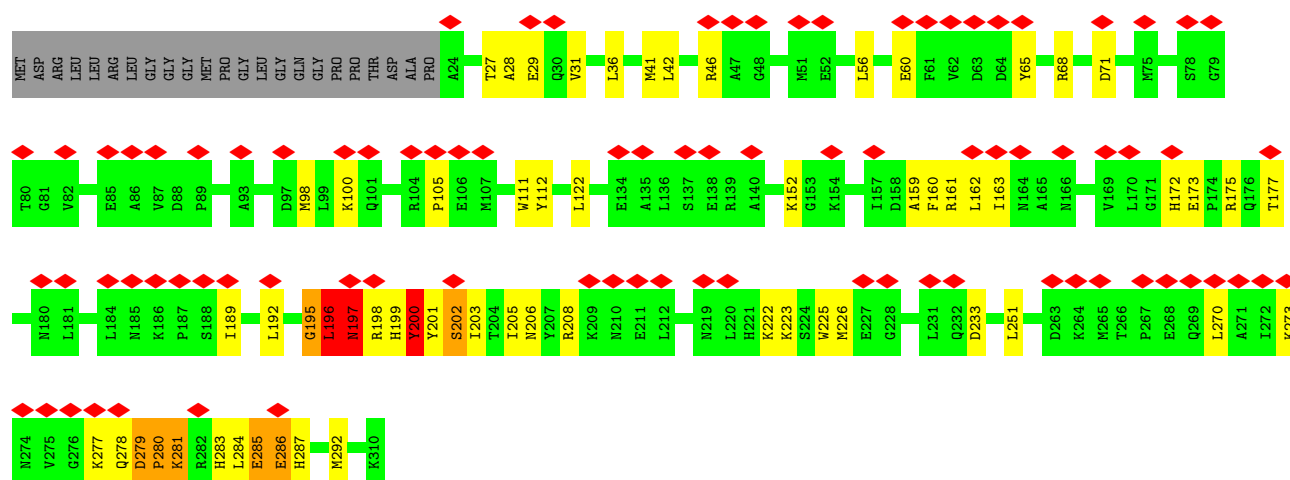
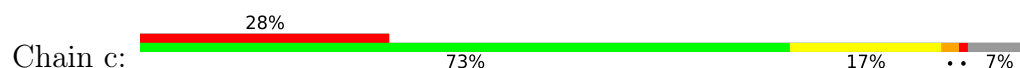
Chain b: 24% 40% 11% 49%



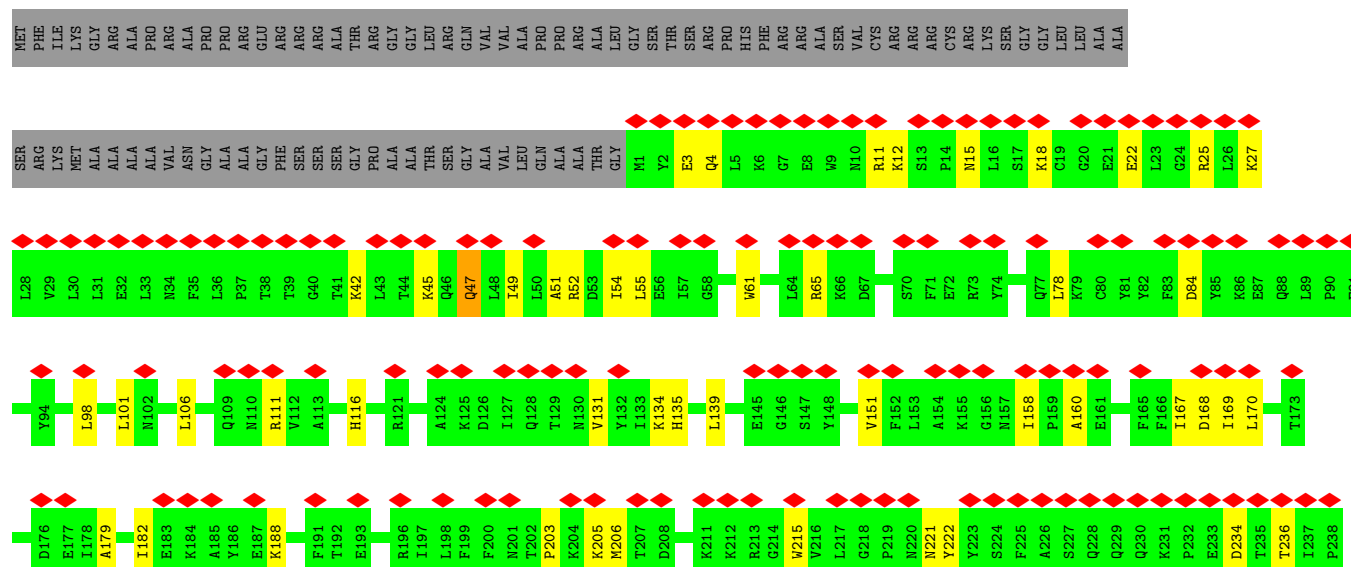
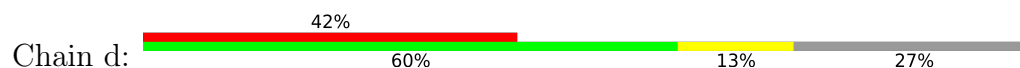




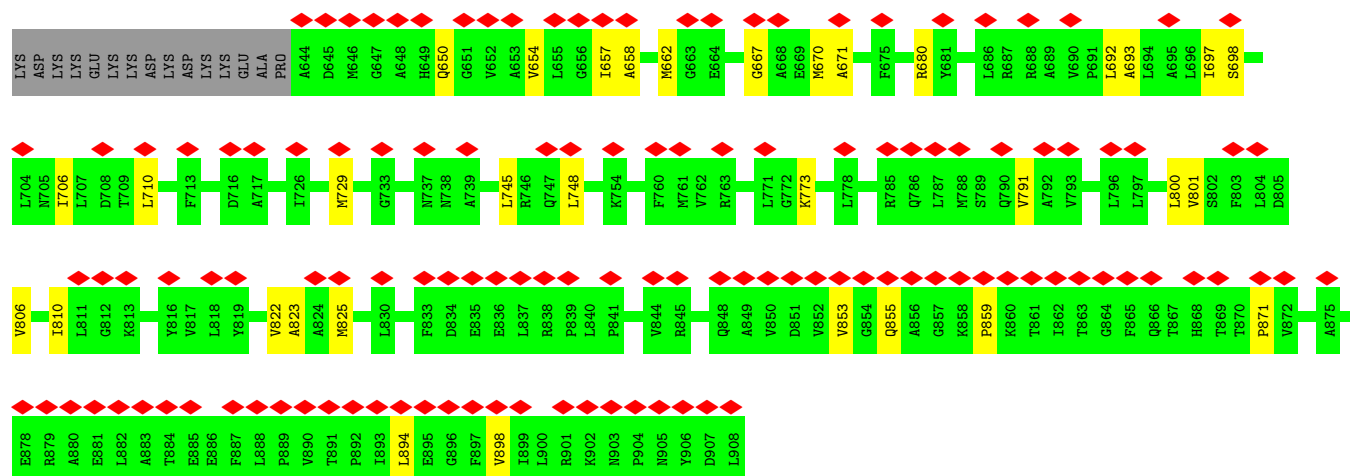
• Molecule 29: 26S proteasome non-ATPase regulatory subunit 14



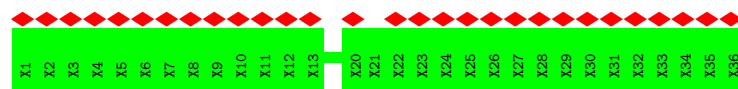
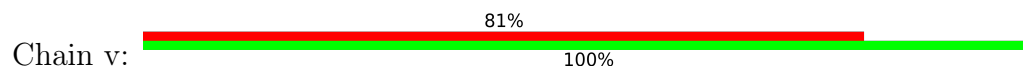
• Molecule 30: 26S proteasome non-ATPase regulatory subunit 8



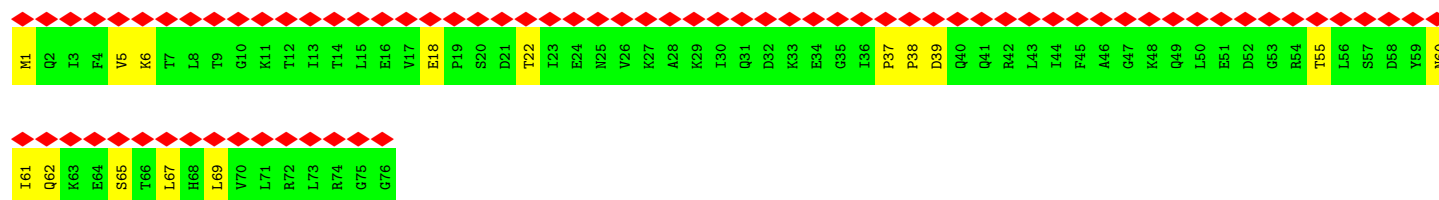
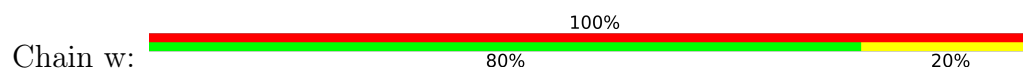




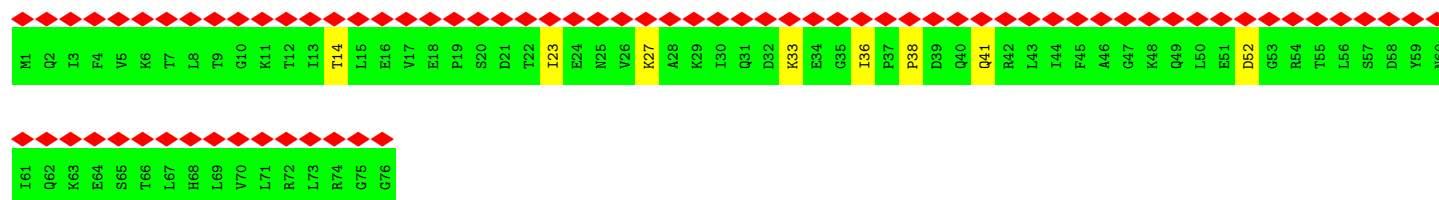
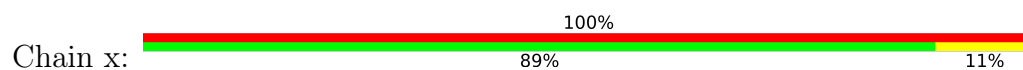
### • Molecule 33: Substrate



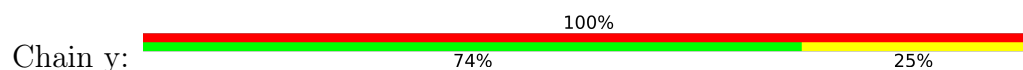
### • Molecule 34: Ubiquitin

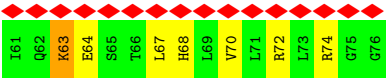


### • Molecule 34: Ubiquitin

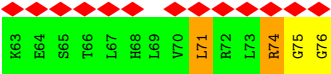
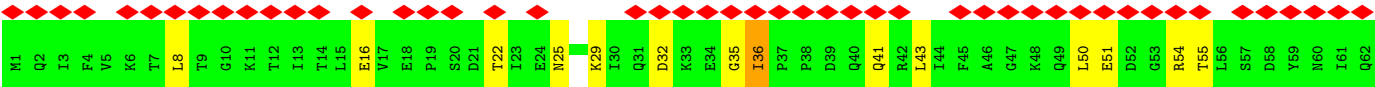


### • Molecule 34: Ubiquitin





● Molecule 34: Ubiquitin



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 24674                                   | 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 ( $e^-/\text{\AA}^2$ ) | 44                                      | Depositor |
| Minimum defocus (nm)                 | 600                                     | Depositor |
| Maximum defocus (nm)                 | 3500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.023                                   | Depositor |
| Minimum map value                    | -0.005                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.001                                   | Depositor |
| Recommended contour level            | 0.00617                                 | Depositor |
| Map size (Å)                         | 411.0, 411.0, 411.0                     | wwPDB     |
| Map dimensions                       | 600, 600, 600                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.685, 0.685, 0.685                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths |             | Bond angles |               |
|-----|-------|--------------|-------------|-------------|---------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$   |
| 1   | A     | 0.18         | 0/3283      | 0.48        | 0/4433        |
| 2   | B     | 0.21         | 0/3254      | 0.51        | 0/4388        |
| 3   | C     | 0.19         | 0/3146      | 0.50        | 0/4226        |
| 4   | D     | 0.23         | 0/3090      | 0.56        | 0/4168        |
| 5   | E     | 0.22         | 0/3145      | 0.54        | 1/4233 (0.0%) |
| 6   | F     | 0.20         | 0/3137      | 0.51        | 0/4223        |
| 7   | G     | 0.19         | 0/1901      | 0.42        | 0/2572        |
| 7   | g     | 0.14         | 0/1913      | 0.40        | 0/2589        |
| 8   | H     | 0.17         | 0/1840      | 0.43        | 0/2495        |
| 8   | h     | 0.16         | 0/1844      | 0.40        | 0/2497        |
| 9   | I     | 0.21         | 0/1963      | 0.42        | 0/2650        |
| 9   | i     | 0.16         | 0/1985      | 0.41        | 0/2677        |
| 10  | J     | 0.15         | 0/1887      | 0.44        | 2/2553 (0.1%) |
| 10  | j     | 0.17         | 0/1887      | 0.43        | 0/2549        |
| 11  | K     | 0.15         | 0/1841      | 0.35        | 0/2486        |
| 11  | k     | 0.14         | 0/1809      | 0.42        | 2/2444 (0.1%) |
| 12  | L     | 0.15         | 0/1911      | 0.37        | 0/2584        |
| 12  | l     | 0.16         | 0/1896      | 0.37        | 0/2565        |
| 13  | M     | 0.18         | 0/1931      | 0.42        | 0/2600        |
| 13  | m     | 0.14         | 0/1916      | 0.38        | 0/2580        |
| 14  | N     | 0.11         | 0/1548      | 0.30        | 0/2097        |
| 14  | n     | 0.13         | 0/1536      | 0.30        | 0/2080        |
| 15  | O     | 0.15         | 0/1672      | 0.40        | 0/2267        |
| 15  | o     | 0.14         | 0/1686      | 0.35        | 0/2282        |
| 16  | P     | 0.14         | 0/1616      | 0.39        | 0/2180        |
| 16  | p     | 0.15         | 0/1620      | 0.38        | 0/2184        |
| 17  | Q     | 0.14         | 0/1627      | 0.37        | 0/2202        |
| 17  | q     | 0.14         | 0/1611      | 0.35        | 0/2182        |
| 18  | R     | 0.13         | 0/1590      | 0.31        | 0/2147        |
| 18  | r     | 0.15         | 0/1580      | 0.37        | 0/2135        |
| 19  | S     | 0.15         | 0/1671      | 0.39        | 0/2252        |
| 19  | s     | 0.17         | 0/1680      | 0.44        | 1/2264 (0.0%) |

| Mol | Chain | Bond lengths |          | Bond angles |                  |
|-----|-------|--------------|----------|-------------|------------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5          |
| 20  | T     | 0.14         | 0/1716   | 0.38        | 0/2323           |
| 20  | t     | 0.14         | 0/1720   | 0.38        | 0/2328           |
| 21  | U     | 0.17         | 0/6984   | 0.46        | 0/9435           |
| 22  | V     | 0.17         | 0/3681   | 0.41        | 0/4969           |
| 23  | W     | 0.17         | 0/3644   | 0.47        | 0/4901           |
| 24  | X     | 0.16         | 0/3381   | 0.42        | 1/4558 (0.0%)    |
| 25  | Y     | 0.15         | 0/3261   | 0.46        | 2/4393 (0.0%)    |
| 26  | Z     | 0.21         | 0/2324   | 0.57        | 1/3150 (0.0%)    |
| 27  | a     | 0.22         | 0/3053   | 0.53        | 0/4133           |
| 28  | b     | 0.19         | 0/1478   | 0.51        | 0/2001           |
| 29  | c     | 0.32         | 0/2302   | 0.68        | 3/3110 (0.1%)    |
| 30  | d     | 0.20         | 0/2162   | 0.50        | 0/2919           |
| 31  | e     | 0.15         | 0/437    | 0.47        | 0/595            |
| 32  | f     | 0.22         | 0/6640   | 0.52        | 2/8988 (0.0%)    |
| 34  | w     | 0.13         | 0/607    | 0.36        | 0/816            |
| 34  | x     | 0.11         | 0/607    | 0.28        | 0/816            |
| 34  | y     | 0.30         | 0/607    | 0.58        | 0/816            |
| 34  | z     | 0.44         | 0/607    | 0.76        | 0/816            |
| All | All   | 0.18         | 0/110227 | 0.45        | 15/148851 (0.0%) |

There are no bond length outliers.

All (15) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 24  | X     | 317 | PRO  | N-CA-C   | -7.93 | 103.18      | 113.57   |
| 29  | c     | 279 | ASP  | CA-C-N   | 7.05  | 128.65      | 119.84   |
| 29  | c     | 279 | ASP  | C-N-CA   | 7.05  | 128.65      | 119.84   |
| 11  | k     | 120 | ALA  | CA-C-N   | 6.88  | 134.68      | 121.54   |
| 11  | k     | 120 | ALA  | C-N-CA   | 6.88  | 134.68      | 121.54   |
| 5   | E     | 166 | PRO  | N-CA-C   | 6.48  | 118.60      | 110.70   |
| 10  | J     | 22  | ALA  | CA-C-N   | -6.14 | 112.00      | 122.56   |
| 10  | J     | 22  | ALA  | C-N-CA   | -6.14 | 112.00      | 122.56   |
| 26  | Z     | 19  | VAL  | N-CA-C   | -5.91 | 107.05      | 112.96   |
| 29  | c     | 195 | GLY  | N-CA-C   | 5.65  | 120.79      | 113.27   |
| 32  | f     | 613 | LEU  | CA-CB-CG | -5.47 | 97.16       | 116.30   |
| 19  | s     | 69  | GLU  | N-CA-CB  | 5.33  | 118.55      | 110.28   |
| 32  | f     | 339 | ILE  | N-CA-C   | -5.15 | 107.70      | 112.43   |
| 25  | Y     | 291 | HIS  | CA-C-N   | 5.05  | 131.19      | 121.54   |
| 25  | Y     | 291 | HIS  | C-N-CA   | 5.05  | 131.19      | 121.54   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3229  | 0        | 3261     | 55      | 0            |
| 2   | B     | 3207  | 0        | 3278     | 60      | 0            |
| 3   | C     | 3105  | 0        | 3219     | 64      | 0            |
| 4   | D     | 3040  | 0        | 3076     | 57      | 0            |
| 5   | E     | 3097  | 0        | 3174     | 52      | 0            |
| 6   | F     | 3098  | 0        | 3187     | 55      | 0            |
| 7   | G     | 1867  | 0        | 1867     | 19      | 0            |
| 7   | g     | 1879  | 0        | 1872     | 13      | 0            |
| 8   | H     | 1801  | 0        | 1773     | 15      | 0            |
| 8   | h     | 1805  | 0        | 1798     | 16      | 0            |
| 9   | I     | 1933  | 0        | 1923     | 22      | 0            |
| 9   | i     | 1955  | 0        | 1955     | 14      | 0            |
| 10  | J     | 1861  | 0        | 1846     | 18      | 0            |
| 10  | j     | 1861  | 0        | 1865     | 17      | 0            |
| 11  | K     | 1813  | 0        | 1796     | 19      | 0            |
| 11  | k     | 1782  | 0        | 1766     | 15      | 0            |
| 12  | L     | 1876  | 0        | 1856     | 20      | 0            |
| 12  | l     | 1861  | 0        | 1839     | 16      | 0            |
| 13  | M     | 1893  | 0        | 1885     | 10      | 0            |
| 13  | m     | 1881  | 0        | 1868     | 23      | 0            |
| 14  | N     | 1521  | 0        | 1494     | 10      | 0            |
| 14  | n     | 1510  | 0        | 1483     | 8       | 0            |
| 15  | O     | 1645  | 0        | 1648     | 11      | 0            |
| 15  | o     | 1659  | 0        | 1681     | 17      | 0            |
| 16  | P     | 1587  | 0        | 1598     | 12      | 0            |
| 16  | p     | 1591  | 0        | 1609     | 22      | 0            |
| 17  | Q     | 1591  | 0        | 1589     | 12      | 0            |
| 17  | q     | 1578  | 0        | 1569     | 18      | 0            |
| 18  | R     | 1559  | 0        | 1523     | 16      | 0            |
| 18  | r     | 1549  | 0        | 1506     | 15      | 0            |
| 19  | S     | 1641  | 0        | 1639     | 15      | 0            |
| 19  | s     | 1650  | 0        | 1645     | 19      | 0            |
| 20  | T     | 1683  | 0        | 1662     | 19      | 0            |
| 20  | t     | 1687  | 0        | 1666     | 19      | 0            |
| 21  | U     | 6867  | 0        | 6929     | 85      | 0            |
| 22  | V     | 3612  | 0        | 3682     | 55      | 0            |
| 23  | W     | 3596  | 0        | 3713     | 54      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 24  | X     | 3335   | 0        | 3435     | 49      | 0            |
| 25  | Y     | 3202   | 0        | 3204     | 36      | 0            |
| 26  | Z     | 2281   | 0        | 2312     | 63      | 0            |
| 27  | a     | 2995   | 0        | 3012     | 58      | 0            |
| 28  | b     | 1458   | 0        | 1505     | 29      | 0            |
| 29  | c     | 2260   | 0        | 2276     | 77      | 0            |
| 30  | d     | 2116   | 0        | 2146     | 29      | 0            |
| 31  | e     | 425    | 0        | 328      | 9       | 0            |
| 32  | f     | 6529   | 0        | 6541     | 72      | 0            |
| 33  | v     | 180    | 0        | 45       | 0       | 0            |
| 34  | w     | 601    | 0        | 629      | 9       | 0            |
| 34  | x     | 601    | 0        | 629      | 5       | 0            |
| 34  | y     | 601    | 0        | 626      | 14      | 0            |
| 34  | z     | 601    | 0        | 629      | 21      | 0            |
| 35  | A     | 31     | 0        | 12       | 0       | 0            |
| 35  | B     | 31     | 0        | 12       | 2       | 0            |
| 35  | C     | 31     | 0        | 12       | 1       | 0            |
| 35  | F     | 31     | 0        | 12       | 2       | 0            |
| 36  | A     | 1      | 0        | 0        | 0       | 0            |
| 36  | B     | 1      | 0        | 0        | 0       | 0            |
| 36  | C     | 1      | 0        | 0        | 0       | 0            |
| 36  | D     | 1      | 0        | 0        | 0       | 0            |
| 36  | F     | 1      | 0        | 0        | 0       | 0            |
| 37  | D     | 27     | 0        | 12       | 0       | 0            |
| 38  | c     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 108712 | 0        | 109117   | 1292    | 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 6.

All (1292) 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) |
|-----------------|------------------|--------------------------|-------------------|
| 34:z:8:LEU:HD13 | 34:z:74:ARG:CG   | 1.74                     | 1.17              |
| 3:C:90:HIS:HB3  | 3:C:91:PRO:HD3   | 1.22                     | 1.09              |
| 34:z:8:LEU:CD1  | 34:z:74:ARG:HG3  | 1.91                     | 1.00              |
| 34:z:8:LEU:HD13 | 34:z:74:ARG:HG3  | 0.99                     | 0.98              |
| 3:C:90:HIS:CB   | 3:C:91:PRO:HD3   | 1.96                     | 0.95              |
| 29:c:278:GLN:C  | 29:c:280:PRO:HD2 | 1.93                     | 0.93              |
| 29:c:279:ASP:N  | 29:c:280:PRO:HD2 | 1.82                     | 0.92              |
| 4:D:159:LYS:HG3 | 4:D:160:PRO:HD3  | 1.52                     | 0.90              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:c:192:LEU:HA   | 29:c:196:LEU:HB2  | 1.56                     | 0.87              |
| 34:z:36:ILE:HB    | 34:z:41:GLN:HE21  | 1.44                     | 0.83              |
| 29:c:278:GLN:HG2  | 29:c:280:PRO:CD   | 2.09                     | 0.82              |
| 29:c:160:PHE:HB3  | 29:c:201:TYR:CD1  | 2.14                     | 0.82              |
| 2:B:68:ILE:HG12   | 32:f:670:MET:HE1  | 1.59                     | 0.81              |
| 29:c:162:LEU:HD12 | 29:c:200:TYR:HB3  | 1.62                     | 0.78              |
| 29:c:278:GLN:HG2  | 29:c:280:PRO:HD2  | 1.64                     | 0.78              |
| 3:C:90:HIS:HB3    | 3:C:91:PRO:CD     | 2.09                     | 0.78              |
| 4:D:157:ASP:H     | 4:D:159:LYS:HZ2   | 1.32                     | 0.77              |
| 21:U:773:PHE:HB2  | 29:c:177:THR:HB   | 1.68                     | 0.76              |
| 29:c:160:PHE:HB3  | 29:c:201:TYR:CG   | 2.22                     | 0.75              |
| 9:I:53:HIS:CG     | 9:I:54:LYS:H      | 2.06                     | 0.74              |
| 24:X:102:ALA:O    | 24:X:106:GLU:HG2  | 1.87                     | 0.74              |
| 1:A:48:VAL:HG13   | 2:B:69:LYS:HE2    | 1.70                     | 0.73              |
| 4:D:335:LEU:HB2   | 4:D:336:PRO:HD3   | 1.68                     | 0.73              |
| 29:c:279:ASP:HA   | 29:c:283:HIS:HB3  | 1.70                     | 0.73              |
| 9:I:53:HIS:NE2    | 9:I:55:LEU:HB2    | 2.04                     | 0.72              |
| 29:c:162:LEU:CD1  | 29:c:200:TYR:HB3  | 2.21                     | 0.71              |
| 24:X:103:THR:HA   | 24:X:106:GLU:HB2  | 1.71                     | 0.71              |
| 4:D:335:LEU:CB    | 4:D:336:PRO:HD3   | 2.22                     | 0.70              |
| 12:L:41:LYS:HZ1   | 12:L:181:GLU:HA   | 1.58                     | 0.69              |
| 19:s:27:THR:HB    | 19:s:40:SER:H     | 1.59                     | 0.68              |
| 26:Z:145:HIS:NE2  | 26:Z:152:SER:HB3  | 2.08                     | 0.68              |
| 11:k:156:MET:HE3  | 11:k:157:ASP:H    | 1.57                     | 0.68              |
| 27:a:180:LEU:HD11 | 27:a:221:VAL:HG11 | 1.75                     | 0.68              |
| 27:a:342:ASP:O    | 27:a:343:LEU:C    | 2.36                     | 0.68              |
| 34:z:8:LEU:CD1    | 34:z:74:ARG:CG    | 2.62                     | 0.68              |
| 34:z:8:LEU:CD1    | 34:z:74:ARG:HB2   | 2.24                     | 0.67              |
| 10:J:52:LYS:HG3   | 10:J:53:LEU:HG    | 1.77                     | 0.67              |
| 7:G:18:PRO:O      | 7:G:19:GLU:HB2    | 1.94                     | 0.67              |
| 3:C:90:HIS:CB     | 3:C:91:PRO:CD     | 2.72                     | 0.67              |
| 6:F:339:ASP:HB3   | 6:F:342:LEU:HD13  | 1.77                     | 0.67              |
| 29:c:42:LEU:HB2   | 29:c:46:ARG:HH21  | 1.58                     | 0.67              |
| 26:Z:167:ALA:HB3  | 29:c:46:ARG:HH12  | 1.60                     | 0.67              |
| 2:B:120:HIS:HA    | 2:B:134:SER:HA    | 1.78                     | 0.66              |
| 1:A:279:ALA:HB1   | 2:B:307:ARG:HG3   | 1.76                     | 0.66              |
| 6:F:86:LEU:HD12   | 6:F:87:PRO:HD3    | 1.78                     | 0.66              |
| 19:s:68:ILE:HD11  | 19:s:92:LEU:HD13  | 1.77                     | 0.66              |
| 32:f:654:VAL:HA   | 32:f:657:ILE:HD12 | 1.78                     | 0.66              |
| 11:k:206:MET:HE1  | 11:k:210:LEU:HB3  | 1.78                     | 0.66              |
| 9:I:143:TYR:HB2   | 9:I:146:GLN:HE21  | 1.61                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:X:368:MET:HB2  | 24:X:373:LYS:HB2  | 1.77                     | 0.65              |
| 27:a:343:LEU:O    | 27:a:346:ILE:HG13 | 1.96                     | 0.65              |
| 31:e:25:GLU:HG3   | 31:e:27:TRP:H     | 1.62                     | 0.65              |
| 24:X:102:ALA:C    | 24:X:106:GLU:HG2  | 2.22                     | 0.65              |
| 32:f:96:LEU:HD13  | 32:f:129:LEU:HD13 | 1.79                     | 0.65              |
| 4:D:45:LYS:HG2    | 21:U:187:LEU:HB2  | 1.78                     | 0.65              |
| 23:W:190:MET:HB3  | 23:W:202:THR:HG23 | 1.77                     | 0.65              |
| 5:E:8:ALA:HB1     | 6:F:40:GLU:HG3    | 1.79                     | 0.64              |
| 10:j:211:MET:HE3  | 10:j:217:LEU:HB2  | 1.79                     | 0.64              |
| 21:U:620:GLU:HG3  | 21:U:651:GLY:HA2  | 1.80                     | 0.64              |
| 29:c:122:LEU:HD23 | 29:c:201:TYR:CZ   | 2.33                     | 0.64              |
| 21:U:819:VAL:HG12 | 21:U:821:LYS:H    | 1.61                     | 0.64              |
| 23:W:401:THR:HG23 | 23:W:402:ILE:HD12 | 1.79                     | 0.64              |
| 34:z:43:LEU:HB3   | 34:z:50:LEU:HD12  | 1.79                     | 0.64              |
| 19:S:27:THR:HB    | 19:S:40:SER:H     | 1.63                     | 0.64              |
| 6:F:251:LEU:HD11  | 6:F:256:LEU:HD21  | 1.79                     | 0.63              |
| 19:s:148:LEU:HD23 | 19:s:178:VAL:HG12 | 1.79                     | 0.63              |
| 29:c:195:GLY:HA3  | 29:c:200:TYR:CE2  | 2.33                     | 0.63              |
| 29:c:281:LYS:HA   | 29:c:281:LYS:NZ   | 2.13                     | 0.63              |
| 34:z:16:GLU:O     | 34:z:29:LYS:NZ    | 2.31                     | 0.63              |
| 22:V:397:ARG:HH21 | 30:d:116:HIS:HB3  | 1.63                     | 0.63              |
| 32:f:573:ILE:HD12 | 32:f:576:ILE:HD13 | 1.79                     | 0.63              |
| 2:B:286:GLU:HB3   | 3:C:274:LEU:HD23  | 1.80                     | 0.63              |
| 21:U:772:TRP:HB3  | 21:U:775:LEU:HD13 | 1.81                     | 0.63              |
| 21:U:799:LYS:HE2  | 21:U:925:VAL:HG21 | 1.81                     | 0.63              |
| 19:S:145:LEU:HD22 | 19:S:178:VAL:HB   | 1.80                     | 0.62              |
| 28:b:157:VAL:HG21 | 28:b:170:LEU:HB2  | 1.81                     | 0.62              |
| 5:E:77:PRO:HG2    | 5:E:79:TYR:HE1    | 1.64                     | 0.62              |
| 28:b:9:CYS:HB2    | 28:b:111:ALA:HA   | 1.80                     | 0.62              |
| 21:U:360:VAL:HG23 | 21:U:365:CYS:HB2  | 1.81                     | 0.62              |
| 22:V:259:LEU:HD11 | 22:V:294:ARG:HD3  | 1.81                     | 0.62              |
| 23:W:436:MET:HE3  | 29:c:226:MET:HG2  | 1.81                     | 0.62              |
| 21:U:619:VAL:HG23 | 21:U:651:GLY:HA3  | 1.81                     | 0.62              |
| 27:a:273:GLN:HB3  | 27:a:310:LEU:HD11 | 1.81                     | 0.62              |
| 3:C:396:GLU:HG3   | 3:C:402:LYS:HZ2   | 1.65                     | 0.61              |
| 6:F:376:SER:HB3   | 6:F:414:GLU:HG3   | 1.81                     | 0.61              |
| 34:z:8:LEU:CD1    | 34:z:74:ARG:CB    | 2.78                     | 0.61              |
| 7:G:165:ALA:HB3   | 8:H:56:LEU:HD22   | 1.82                     | 0.61              |
| 26:Z:145:HIS:HB2  | 26:Z:151:THR:HA   | 1.82                     | 0.61              |
| 30:d:188:LYS:HD2  | 30:d:221:ASN:HD21 | 1.65                     | 0.61              |
| 32:f:566:HIS:HB3  | 32:f:569:LYS:HD2  | 1.82                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:218:PRO:HB2   | 2:B:343:ARG:HD3   | 1.81                     | 0.61              |
| 3:C:11:LEU:HB2    | 3:C:15:LYS:HG2    | 1.81                     | 0.61              |
| 11:k:210:LEU:HA   | 11:k:214:ASN:HD21 | 1.65                     | 0.61              |
| 30:d:78:LEU:HD13  | 30:d:98:LEU:HD21  | 1.83                     | 0.61              |
| 1:A:213:LEU:HA    | 1:A:319:MET:HB3   | 1.83                     | 0.61              |
| 21:U:545:LEU:HB3  | 21:U:577:ILE:HG21 | 1.82                     | 0.60              |
| 26:Z:144:VAL:O    | 26:Z:145:HIS:HB2  | 2.01                     | 0.60              |
| 27:a:34:TRP:HB3   | 27:a:71:VAL:HG22  | 1.83                     | 0.60              |
| 8:h:203:MET:HE3   | 8:h:208:ILE:HG21  | 1.83                     | 0.60              |
| 13:m:23:VAL:HG12  | 13:m:27:MET:HE1   | 1.83                     | 0.60              |
| 19:S:4:PRO:HB2    | 20:T:100:ARG:HH21 | 1.66                     | 0.60              |
| 22:V:349:ARG:HH12 | 31:e:37:HIS:HE1   | 1.50                     | 0.60              |
| 23:W:198:ASP:OD1  | 23:W:201:ARG:HB3  | 2.02                     | 0.60              |
| 24:X:256:LEU:HD22 | 24:X:319:ILE:HG22 | 1.84                     | 0.60              |
| 25:Y:69:LEU:O     | 25:Y:73:MET:HB2   | 2.02                     | 0.60              |
| 30:d:98:LEU:HA    | 30:d:101:LEU:HD12 | 1.84                     | 0.60              |
| 26:Z:212:LEU:HD21 | 27:a:353:LEU:HD13 | 1.82                     | 0.60              |
| 28:b:138:VAL:HB   | 28:b:160:LEU:HD11 | 1.84                     | 0.60              |
| 27:a:343:LEU:O    | 27:a:344:GLN:C    | 2.45                     | 0.60              |
| 2:B:234:LEU:HD11  | 35:B:501:ATP:H2'  | 1.83                     | 0.59              |
| 6:F:141:ASP:H     | 6:F:144:LYS:HE3   | 1.66                     | 0.59              |
| 9:i:143:TYR:HB2   | 9:i:146:GLN:HE21  | 1.66                     | 0.59              |
| 25:Y:239:LYS:HG3  | 25:Y:240:VAL:HG13 | 1.84                     | 0.59              |
| 30:d:3:GLU:O      | 30:d:25:ARG:NH1   | 2.36                     | 0.59              |
| 12:l:42:THR:HA    | 12:l:217:LYS:HE3  | 1.84                     | 0.59              |
| 34:z:75:GLY:O     | 34:z:76:GLY:C     | 2.45                     | 0.59              |
| 3:C:185:GLY:HA3   | 3:C:311:ILE:HA    | 1.84                     | 0.59              |
| 34:z:74:ARG:HA    | 34:z:74:ARG:NE    | 2.17                     | 0.59              |
| 3:C:138:MET:HB2   | 3:C:212:ILE:HG23  | 1.84                     | 0.59              |
| 17:Q:86:ARG:NH1   | 17:Q:90:ASP:OD1   | 2.36                     | 0.59              |
| 25:Y:142:PHE:HE2  | 25:Y:176:ARG:HD2  | 1.67                     | 0.59              |
| 21:U:376:MET:HA   | 21:U:740:GLY:H    | 1.68                     | 0.59              |
| 22:V:192:MET:HE2  | 22:V:230:PHE:HZ   | 1.67                     | 0.59              |
| 34:z:22:THR:HA    | 34:z:55:THR:HA    | 1.83                     | 0.59              |
| 31:e:54:ASN:OD1   | 31:e:57:ARG:NH2   | 2.36                     | 0.59              |
| 13:M:211:LEU:O    | 13:M:232:ARG:NH2  | 2.35                     | 0.59              |
| 32:f:894:LEU:HA   | 32:f:898:VAL:HG21 | 1.83                     | 0.59              |
| 32:f:367:SER:O    | 32:f:371:ASN:ND2  | 2.36                     | 0.59              |
| 21:U:37:GLU:HG3   | 22:V:269:LYS:HE3  | 1.84                     | 0.59              |
| 24:X:249:THR:HA   | 24:X:252:LYS:HD3  | 1.85                     | 0.59              |
| 34:y:63:LYS:HD2   | 34:y:64:GLU:HG3   | 1.85                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:z:75:GLY:O     | 34:z:76:GLY:O     | 2.21                     | 0.59              |
| 3:C:406:LYS:HB2   | 9:I:80:THR:HG22   | 1.85                     | 0.59              |
| 24:X:141:LYS:HE2  | 24:X:179:ALA:HB1  | 1.85                     | 0.59              |
| 23:W:198:ASP:OD1  | 23:W:201:ARG:CB   | 2.51                     | 0.58              |
| 27:a:182:CYS:SG   | 27:a:183:VAL:N    | 2.76                     | 0.58              |
| 10:j:45:VAL:HG21  | 10:j:61:LYS:HD2   | 1.84                     | 0.58              |
| 16:p:65:GLN:OE1   | 17:q:86:ARG:NH2   | 2.36                     | 0.58              |
| 3:C:198:LEU:HD11  | 35:C:501:ATP:H2'  | 1.85                     | 0.58              |
| 25:Y:50:MET:HB3   | 25:Y:53:TYR:HB3   | 1.85                     | 0.58              |
| 13:m:34:SER:OG    | 13:m:65:ARG:NH1   | 2.36                     | 0.58              |
| 34:y:42:ARG:HB3   | 34:y:70:VAL:HB    | 1.85                     | 0.58              |
| 4:D:160:PRO:O     | 4:D:162:VAL:HG12  | 2.03                     | 0.58              |
| 6:F:228:PRO:O     | 6:F:233:LYS:NZ    | 2.37                     | 0.58              |
| 12:l:55:GLU:HG2   | 12:l:56:LEU:HG    | 1.85                     | 0.58              |
| 21:U:345:ASN:O    | 21:U:743:ASN:ND2  | 2.35                     | 0.58              |
| 23:W:174:TYR:O    | 23:W:182:ARG:NH2  | 2.36                     | 0.58              |
| 27:a:69:HIS:ND1   | 27:a:70:ARG:HG2   | 2.18                     | 0.58              |
| 1:A:398:ARG:NH1   | 2:B:195:GLN:OE1   | 2.36                     | 0.58              |
| 13:M:136:MET:HE1  | 13:M:163:CYS:HB3  | 1.85                     | 0.58              |
| 22:V:355:ARG:NH1  | 31:e:27:TRP:O     | 2.36                     | 0.58              |
| 23:W:329:ARG:HE   | 23:W:351:TRP:HE1  | 1.50                     | 0.58              |
| 24:X:1:MET:HE1    | 24:X:36:GLN:HB2   | 1.85                     | 0.58              |
| 21:U:505:ASP:HB3  | 21:U:508:THR:HG22 | 1.86                     | 0.58              |
| 6:F:295:ARG:HB2   | 6:F:304:ARG:HH22  | 1.67                     | 0.58              |
| 27:a:69:HIS:O     | 27:a:70:ARG:HD2   | 2.03                     | 0.58              |
| 27:a:342:ASP:HB2  | 27:a:344:GLN:NE2  | 2.19                     | 0.58              |
| 32:f:531:ASN:O    | 32:f:565:ASN:ND2  | 2.37                     | 0.58              |
| 5:E:254:GLN:HA    | 5:E:257:LEU:HG    | 1.86                     | 0.58              |
| 9:I:22:GLU:HA     | 9:I:25:MET:HG3    | 1.86                     | 0.58              |
| 34:z:36:ILE:HB    | 34:z:41:GLN:NE2   | 2.15                     | 0.58              |
| 3:C:69:GLN:HB3    | 3:C:118:ASN:HD21  | 1.68                     | 0.58              |
| 9:I:180:LYS:HB2   | 9:I:184:MET:HE3   | 1.85                     | 0.58              |
| 20:t:25:ASP:HA    | 20:t:187:PHE:HA   | 1.86                     | 0.57              |
| 5:E:83:CYS:HB2    | 5:E:89:LYS:HE2    | 1.85                     | 0.57              |
| 13:M:187:ARG:O    | 13:M:191:LYS:NZ   | 2.36                     | 0.57              |
| 32:f:386:GLY:HA2  | 32:f:418:LEU:HG   | 1.85                     | 0.57              |
| 15:o:70:THR:HG23  | 15:o:72:ARG:H     | 1.68                     | 0.57              |
| 9:I:53:HIS:CG     | 9:I:54:LYS:N      | 2.72                     | 0.57              |
| 32:f:208:LEU:HD13 | 32:f:217:LEU:HD12 | 1.85                     | 0.57              |
| 19:s:204:ARG:NH1  | 19:s:206:GLU:OE1  | 2.37                     | 0.57              |
| 26:Z:106:ILE:HG23 | 26:Z:153:LYS:HD2  | 1.85                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:q:168:GLN:NE2  | 17:q:175:LEU:O    | 2.38                     | 0.57              |
| 4:D:52:GLU:OE1    | 21:U:596:ASN:ND2  | 2.37                     | 0.57              |
| 8:H:177:ARG:NH1   | 24:X:202:CYS:SG   | 2.78                     | 0.57              |
| 10:j:116:GLN:NE2  | 10:j:120:GLN:OE1  | 2.38                     | 0.57              |
| 17:Q:35:MET:HE1   | 17:Q:181:ARG:HB2  | 1.86                     | 0.57              |
| 7:G:205:VAL:HG13  | 7:G:206:LEU:HD12  | 1.87                     | 0.57              |
| 21:U:899:ARG:NH2  | 21:U:917:THR:OG1  | 2.38                     | 0.57              |
| 32:f:662:MET:HE1  | 32:f:697:ILE:HG13 | 1.85                     | 0.57              |
| 8:H:143:ARG:NH1   | 8:H:144:PRO:O     | 2.38                     | 0.57              |
| 12:L:196:ARG:HG2  | 12:L:239:ARG:HH21 | 1.70                     | 0.57              |
| 2:B:71:TYR:CD2    | 32:f:670:MET:HB3  | 2.40                     | 0.57              |
| 16:p:35:VAL:HG12  | 16:p:36:THR:HG23  | 1.87                     | 0.57              |
| 2:B:125:THR:OG1   | 2:B:126:SER:N     | 2.38                     | 0.56              |
| 3:C:209:CYS:SG    | 3:C:210:THR:N     | 2.77                     | 0.56              |
| 11:K:118:ASN:OD1  | 12:L:82:ARG:NH2   | 2.37                     | 0.56              |
| 3:C:232:ARG:NH1   | 3:C:275:GLU:OE2   | 2.39                     | 0.56              |
| 27:a:312:MET:HA   | 27:a:315:LEU:HD12 | 1.88                     | 0.56              |
| 29:c:161:ARG:H    | 29:c:201:TYR:HB3  | 1.69                     | 0.56              |
| 4:D:325:GLY:N     | 4:D:328:ASP:OD1   | 2.37                     | 0.56              |
| 12:L:72:ILE:HD13  | 12:L:88:MET:HE1   | 1.87                     | 0.56              |
| 20:T:174:ARG:NH1  | 20:T:206:GLU:O    | 2.38                     | 0.56              |
| 25:Y:363:ASN:O    | 25:Y:367:GLN:NE2  | 2.38                     | 0.56              |
| 27:a:318:GLY:O    | 27:a:321:LYS:NZ   | 2.39                     | 0.56              |
| 29:c:28:ALA:HB2   | 29:c:175:ARG:HD3  | 1.86                     | 0.56              |
| 4:D:159:LYS:H     | 4:D:160:PRO:CD    | 2.18                     | 0.56              |
| 21:U:740:GLY:HA3  | 21:U:744:VAL:HG12 | 1.87                     | 0.56              |
| 18:R:64:ARG:NH1   | 18:R:67:GLU:OE2   | 2.39                     | 0.56              |
| 21:U:556:MET:HE2  | 21:U:563:ALA:HB2  | 1.87                     | 0.56              |
| 23:W:357:ARG:NH1  | 23:W:360:GLU:OE2  | 2.39                     | 0.56              |
| 29:c:284:LEU:O    | 29:c:285:GLU:C    | 2.48                     | 0.56              |
| 32:f:388:ASP:OD2  | 32:f:773:LYS:NZ   | 2.38                     | 0.56              |
| 22:V:235:LEU:HD11 | 22:V:251:LEU:HG   | 1.88                     | 0.56              |
| 23:W:316:ARG:NH2  | 23:W:381:LEU:HA   | 2.21                     | 0.56              |
| 29:c:29:GLU:HG3   | 29:c:65:TYR:HB2   | 1.86                     | 0.56              |
| 32:f:415:GLY:HA3  | 32:f:447:ALA:HB1  | 1.87                     | 0.56              |
| 14:N:107:GLU:OE1  | 14:N:110:GLN:NE2  | 2.37                     | 0.56              |
| 25:Y:222:TYR:OH   | 25:Y:285:ASP:OD1  | 2.23                     | 0.56              |
| 26:Z:263:ALA:HB3  | 29:c:292:MET:HE3  | 1.88                     | 0.56              |
| 28:b:56:ASN:HB2   | 28:b:83:LYS:H     | 1.71                     | 0.56              |
| 29:c:251:LEU:HD21 | 29:c:284:LEU:HG   | 1.87                     | 0.56              |
| 30:d:61:TRP:HB3   | 30:d:65:ARG:HH21  | 1.71                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:f:412:ALA:HA   | 32:f:447:ALA:HB2  | 1.88                     | 0.56              |
| 9:i:119:GLN:NE2   | 10:j:79:ASP:OD1   | 2.39                     | 0.56              |
| 25:Y:161:THR:HG22 | 25:Y:165:LYS:HE2  | 1.86                     | 0.56              |
| 7:G:43:ARG:HH21   | 7:G:164:LYS:HG2   | 1.71                     | 0.56              |
| 22:V:289:LEU:HB3  | 22:V:312:ALA:HB2  | 1.87                     | 0.56              |
| 29:c:162:LEU:HA   | 29:c:200:TYR:HB3  | 1.88                     | 0.56              |
| 8:h:89:ARG:HG2    | 8:h:117:VAL:HG11  | 1.88                     | 0.56              |
| 6:F:84:LYS:HG2    | 6:F:161:LEU:HD22  | 1.88                     | 0.56              |
| 16:P:143:ALA:HA   | 16:P:146:MET:HE2  | 1.88                     | 0.56              |
| 21:U:9:ILE:O      | 21:U:44:LYS:NZ    | 2.39                     | 0.56              |
| 21:U:333:MET:HE1  | 21:U:795:LEU:HD13 | 1.86                     | 0.56              |
| 22:V:104:THR:HA   | 22:V:107:ARG:HD3  | 1.88                     | 0.56              |
| 32:f:72:ARG:HH22  | 32:f:117:GLU:HB3  | 1.72                     | 0.56              |
| 11:k:160:GLY:O    | 12:l:82:ARG:NH2   | 2.39                     | 0.56              |
| 1:A:422:LYS:HD3   | 1:A:425:ALA:HB3   | 1.87                     | 0.55              |
| 3:C:217:SER:OG    | 4:D:248:ARG:NH2   | 2.38                     | 0.55              |
| 21:U:58:GLN:HB2   | 21:U:87:LEU:HD12  | 1.88                     | 0.55              |
| 21:U:813:TYR:HE1  | 21:U:883:ARG:HE   | 1.54                     | 0.55              |
| 27:a:222:LEU:HB2  | 27:a:226:ARG:HH21 | 1.71                     | 0.55              |
| 34:y:63:LYS:O     | 34:y:63:LYS:HG3   | 2.03                     | 0.55              |
| 1:A:308:GLY:HA2   | 6:F:234:THR:HG21  | 1.87                     | 0.55              |
| 12:L:80:ASP:OD2   | 12:L:126:ARG:NH1  | 2.39                     | 0.55              |
| 21:U:792:ASN:HB3  | 21:U:914:LEU:HB3  | 1.87                     | 0.55              |
| 22:V:74:ASP:OD2   | 22:V:107:ARG:NH2  | 2.39                     | 0.55              |
| 29:c:189:ILE:HA   | 29:c:192:LEU:HG   | 1.88                     | 0.55              |
| 15:o:1:THR:N      | 15:o:168:GLY:O    | 2.39                     | 0.55              |
| 34:x:36:ILE:HB    | 34:x:41:GLN:HE21  | 1.72                     | 0.55              |
| 6:F:343:LEU:HD13  | 6:F:348:LEU:HB3   | 1.87                     | 0.55              |
| 20:T:25:ASP:OD1   | 20:T:41:ARG:NH2   | 2.39                     | 0.55              |
| 28:b:141:ILE:HA   | 28:b:171:VAL:HB   | 1.88                     | 0.55              |
| 32:f:855:GLN:HG3  | 32:f:859:PRO:HG2  | 1.88                     | 0.55              |
| 20:t:27:LEU:HD11  | 20:t:34:ALA:HB1   | 1.88                     | 0.55              |
| 6:F:31:GLU:OE1    | 6:F:35:LYS:NZ     | 2.40                     | 0.55              |
| 23:W:293:ASP:HB2  | 23:W:296:LEU:HD23 | 1.88                     | 0.55              |
| 23:W:406:VAL:HG23 | 23:W:413:ILE:HG22 | 1.89                     | 0.55              |
| 24:X:401:LEU:HD22 | 25:Y:365:GLN:HE21 | 1.70                     | 0.55              |
| 26:Z:212:LEU:HA   | 26:Z:215:VAL:HG12 | 1.88                     | 0.55              |
| 32:f:151:LEU:HA   | 32:f:154:TRP:HD1  | 1.72                     | 0.55              |
| 34:x:36:ILE:O     | 34:x:41:GLN:NE2   | 2.40                     | 0.55              |
| 1:A:186:LYS:HG2   | 6:F:409:ARG:HH22  | 1.71                     | 0.55              |
| 1:A:312:ARG:HB2   | 1:A:315:ILE:HD13  | 1.86                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:45:LEU:HB3    | 4:D:61:ILE:HG21   | 1.88                     | 0.55              |
| 3:C:99:VAL:HG12   | 3:C:123:LEU:HD12  | 1.87                     | 0.55              |
| 16:P:177:ARG:NH2  | 19:s:150:ASP:OD2  | 2.38                     | 0.55              |
| 26:Z:34:ARG:NH1   | 26:Z:98:GLY:O     | 2.39                     | 0.55              |
| 32:f:618:GLU:O    | 32:f:650:GLN:NE2  | 2.40                     | 0.55              |
| 12:l:146:GLN:NE2  | 12:l:148:CYS:SG   | 2.80                     | 0.55              |
| 5:E:331:ILE:HD11  | 5:E:364:GLN:HG2   | 1.88                     | 0.55              |
| 7:G:137:CYS:SG    | 7:G:138:MET:N     | 2.79                     | 0.55              |
| 9:I:53:HIS:CD2    | 9:I:54:LYS:H      | 2.24                     | 0.55              |
| 22:V:228:ARG:NH2  | 22:V:257:ASN:O    | 2.40                     | 0.55              |
| 22:V:416:ARG:NH2  | 25:Y:351:ASN:OD1  | 2.39                     | 0.55              |
| 23:W:89:LEU:HA    | 23:W:92:LYS:HE3   | 1.89                     | 0.55              |
| 1:A:35:THR:O      | 1:A:39:SER:OG     | 2.25                     | 0.55              |
| 3:C:195:GLY:HA2   | 3:C:198:LEU:HD13  | 1.87                     | 0.55              |
| 5:E:15:LYS:HD3    | 6:F:47:LEU:HD23   | 1.88                     | 0.55              |
| 19:S:43:CYS:O     | 19:S:194:ARG:NH2  | 2.40                     | 0.55              |
| 22:V:256:ARG:NH2  | 31:e:21:GLU:O     | 2.40                     | 0.55              |
| 25:Y:32:ARG:NH2   | 25:Y:61:LEU:O     | 2.40                     | 0.55              |
| 11:k:155:HIS:NE2  | 11:k:157:ASP:OD1  | 2.40                     | 0.55              |
| 1:A:61:GLU:O      | 3:C:106:ASN:ND2   | 2.39                     | 0.55              |
| 5:E:242:ARG:HH21  | 5:E:253:ILE:HG13  | 1.72                     | 0.55              |
| 7:G:141:ILE:HG22  | 7:G:151:VAL:HG22  | 1.89                     | 0.55              |
| 7:G:244:GLU:O     | 23:W:92:LYS:NZ    | 2.38                     | 0.55              |
| 20:T:63:LEU:HD21  | 20:T:106:LEU:HD13 | 1.89                     | 0.55              |
| 26:Z:31:ASN:HA    | 26:Z:33:LYS:NZ    | 2.21                     | 0.55              |
| 29:c:56:LEU:HA    | 29:c:111:TRP:HA   | 1.88                     | 0.55              |
| 3:C:215:SER:HA    | 3:C:249:ASP:HB2   | 1.88                     | 0.54              |
| 5:E:253:ILE:HG22  | 5:E:257:LEU:HD23  | 1.87                     | 0.54              |
| 12:L:196:ARG:NH1  | 12:L:237:GLU:O    | 2.35                     | 0.54              |
| 22:V:269:LYS:O    | 22:V:273:LYS:NZ   | 2.40                     | 0.54              |
| 10:j:183:THR:HG22 | 10:j:185:ASP:H    | 1.72                     | 0.54              |
| 1:A:103:ASN:ND2   | 6:F:167:GLU:OE1   | 2.40                     | 0.54              |
| 1:A:292:ASP:HB2   | 1:A:295:VAL:HB    | 1.89                     | 0.54              |
| 8:H:148:GLN:OE1   | 8:H:158:TRP:NE1   | 2.40                     | 0.54              |
| 10:J:65:LEU:HD13  | 10:J:88:ARG:HG3   | 1.89                     | 0.54              |
| 15:O:24:MET:HE3   | 19:s:187:VAL:HG21 | 1.88                     | 0.54              |
| 26:Z:26:ILE:HD11  | 26:Z:35:VAL:HG22  | 1.87                     | 0.54              |
| 29:c:285:GLU:O    | 29:c:286:GLU:C    | 2.50                     | 0.54              |
| 9:i:119:GLN:HG3   | 10:j:78:ALA:HB1   | 1.89                     | 0.54              |
| 19:s:4:PRO:O      | 20:t:100:ARG:NH2  | 2.40                     | 0.54              |
| 8:H:51:LYS:NZ     | 8:H:200:GLU:O     | 2.40                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:L:164:ARG:NH1  | 12:L:198:THR:O    | 2.40                     | 0.54              |
| 23:W:371:THR:HG22 | 23:W:372:ARG:HG3  | 1.89                     | 0.54              |
| 27:a:77:VAL:HA    | 27:a:80:ILE:HG22  | 1.89                     | 0.54              |
| 20:t:92:LEU:HD12  | 20:t:112:ILE:HD11 | 1.89                     | 0.54              |
| 21:U:336:GLU:OE2  | 21:U:417:LYS:NZ   | 2.41                     | 0.54              |
| 1:A:89:SER:HA     | 1:A:93:LEU:HD23   | 1.89                     | 0.54              |
| 1:A:347:ASP:O     | 1:A:351:ARG:NH2   | 2.41                     | 0.54              |
| 3:C:320:PRO:O     | 3:C:325:ARG:NH1   | 2.41                     | 0.54              |
| 4:D:156:SER:N     | 4:D:159:LYS:HG2   | 2.22                     | 0.54              |
| 29:c:122:LEU:HD23 | 29:c:201:TYR:OH   | 2.08                     | 0.54              |
| 32:f:791:VAL:HG12 | 32:f:823:ALA:HB1  | 1.89                     | 0.54              |
| 4:D:349:THR:HA    | 4:D:352:MET:HB2   | 1.88                     | 0.54              |
| 24:X:258:LYS:NZ   | 24:X:263:THR:O    | 2.39                     | 0.54              |
| 18:r:7:LYS:HD2    | 18:r:109:PRO:HB2  | 1.89                     | 0.54              |
| 18:R:7:LYS:HG2    | 18:R:12:VAL:HG22  | 1.90                     | 0.54              |
| 29:c:285:GLU:O    | 29:c:287:HIS:N    | 2.41                     | 0.54              |
| 2:B:296:ASP:OD1   | 2:B:303:ARG:NH2   | 2.41                     | 0.54              |
| 19:S:125:ASP:OD1  | 19:S:129:SER:N    | 2.41                     | 0.54              |
| 32:f:557:TRP:HZ3  | 32:f:801:VAL:HG12 | 1.73                     | 0.54              |
| 20:t:44:ARG:NH2   | 20:t:47:ASN:OD1   | 2.41                     | 0.54              |
| 34:z:8:LEU:HD13   | 34:z:74:ARG:CB    | 2.32                     | 0.54              |
| 5:E:135:ILE:HG22  | 5:E:182:LEU:HD23  | 1.90                     | 0.54              |
| 21:U:649:ARG:HD2  | 21:U:675:MET:HE1  | 1.89                     | 0.54              |
| 27:a:261:LEU:HD11 | 27:a:268:LEU:HD11 | 1.89                     | 0.54              |
| 8:h:208:ILE:HD11  | 8:h:230:LEU:HD11  | 1.88                     | 0.54              |
| 5:E:247:THR:HG22  | 5:E:248:SER:H     | 1.73                     | 0.54              |
| 8:H:205:GLU:HB3   | 8:H:227:LYS:HE2   | 1.89                     | 0.54              |
| 23:W:316:ARG:HH21 | 23:W:381:LEU:HD12 | 1.73                     | 0.53              |
| 8:h:93:LEU:HD13   | 8:h:113:ARG:HB3   | 1.90                     | 0.53              |
| 4:D:60:TYR:HB2    | 21:U:603:LEU:HD11 | 1.89                     | 0.53              |
| 11:K:121:LEU:HD23 | 11:K:160:GLY:HA3  | 1.90                     | 0.53              |
| 32:f:745:LEU:HD23 | 32:f:748:LEU:HD12 | 1.90                     | 0.53              |
| 4:D:341:LYS:HB2   | 4:D:364:VAL:HG13  | 1.89                     | 0.53              |
| 12:L:45:VAL:HG12  | 12:L:214:ILE:HG12 | 1.91                     | 0.53              |
| 22:V:321:ALA:HB1  | 22:V:324:PHE:HB3  | 1.90                     | 0.53              |
| 24:X:256:LEU:HG   | 24:X:260:MET:HE1  | 1.90                     | 0.53              |
| 24:X:318:ILE:O    | 24:X:318:ILE:HG13 | 2.08                     | 0.53              |
| 27:a:342:ASP:HB2  | 27:a:344:GLN:HE22 | 1.72                     | 0.53              |
| 2:B:281:ILE:HG22  | 2:B:326:LYS:HB2   | 1.90                     | 0.53              |
| 4:D:119:ILE:O     | 4:D:121:ARG:NH1   | 2.39                     | 0.53              |
| 24:X:421:LEU:HD12 | 26:Z:283:ARG:HH21 | 1.74                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:383:LEU:HD22  | 2:B:423:LYS:HD2   | 1.90                     | 0.53              |
| 6:F:97:LEU:O      | 6:F:120:LYS:N     | 2.41                     | 0.53              |
| 23:W:422:ASN:O    | 23:W:426:ASN:ND2  | 2.42                     | 0.53              |
| 21:U:509:GLY:HA3  | 21:U:544:ILE:HG12 | 1.90                     | 0.53              |
| 22:V:339:LEU:O    | 22:V:404:LYS:NZ   | 2.41                     | 0.53              |
| 24:X:332:GLU:HA   | 24:X:335:LEU:HB2  | 1.90                     | 0.53              |
| 29:c:161:ARG:O    | 29:c:201:TYR:HB3  | 2.07                     | 0.53              |
| 2:B:196:GLU:OE1   | 2:B:349:ARG:NH1   | 2.42                     | 0.53              |
| 32:f:333:LEU:HD11 | 32:f:871:PRO:HG3  | 1.91                     | 0.53              |
| 7:g:11:ARG:O      | 7:g:24:GLN:NE2    | 2.40                     | 0.53              |
| 6:F:180:ARG:NH1   | 6:F:241:ALA:O     | 2.42                     | 0.53              |
| 21:U:568:GLU:OE2  | 21:U:572:ARG:NE   | 2.35                     | 0.53              |
| 29:c:270:LEU:HA   | 29:c:273:LYS:HG2  | 1.90                     | 0.53              |
| 29:c:281:LYS:HA   | 29:c:281:LYS:HZ2  | 1.73                     | 0.53              |
| 34:w:1:MET:HE3    | 34:w:18:GLU:HA    | 1.91                     | 0.53              |
| 9:I:136:TYR:HB2   | 9:I:148:TYR:HB2   | 1.91                     | 0.53              |
| 24:X:203:PRO:HB2  | 24:X:207:GLN:HB2  | 1.90                     | 0.53              |
| 29:c:60:GLU:OE2   | 34:y:74:ARG:NH2   | 2.42                     | 0.53              |
| 10:j:90:GLU:HG3   | 10:j:110:TYR:CZ   | 2.43                     | 0.53              |
| 2:B:90:GLU:OE1    | 2:B:93:GLU:N      | 2.42                     | 0.52              |
| 5:E:234:GLU:HB2   | 5:E:237:ALA:HB3   | 1.91                     | 0.52              |
| 6:F:295:ARG:HH12  | 6:F:342:LEU:HD21  | 1.74                     | 0.52              |
| 23:W:451:MET:HE2  | 26:Z:101:LEU:HD23 | 1.90                     | 0.52              |
| 24:X:317:PRO:HD2  | 24:X:319:ILE:HG13 | 1.90                     | 0.52              |
| 32:f:345:PRO:HA   | 32:f:348:ILE:HD12 | 1.90                     | 0.52              |
| 3:C:57:ARG:HH21   | 21:U:644:TYR:HA   | 1.74                     | 0.52              |
| 20:T:44:ARG:NH2   | 20:T:47:ASN:OD1   | 2.42                     | 0.52              |
| 27:a:247:ARG:HE   | 27:a:251:LEU:HB2  | 1.73                     | 0.52              |
| 7:G:10:ASP:O      | 7:G:24:GLN:NE2    | 2.42                     | 0.52              |
| 8:H:119:GLN:HG3   | 9:I:81:SER:HB2    | 1.91                     | 0.52              |
| 13:M:68:ASN:OD1   | 13:M:224:HIS:ND1  | 2.41                     | 0.52              |
| 17:Q:4:LEU:HD22   | 17:Q:45:LEU:HD23  | 1.90                     | 0.52              |
| 18:r:141:ARG:O    | 18:r:141:ARG:NH1  | 2.42                     | 0.52              |
| 7:G:93:ARG:HE     | 7:G:121:ILE:HD13  | 1.73                     | 0.52              |
| 32:f:335:ARG:NH2  | 32:f:340:MET:SD   | 2.82                     | 0.52              |
| 13:m:37:ILE:HD11  | 13:m:193:VAL:HG13 | 1.92                     | 0.52              |
| 10:J:211:MET:HB2  | 10:J:217:LEU:HD13 | 1.91                     | 0.52              |
| 15:O:140:ASP:OD2  | 20:t:171:ARG:NH2  | 2.40                     | 0.52              |
| 21:U:55:ARG:NH1   | 21:U:56:SER:OG    | 2.43                     | 0.52              |
| 23:W:68:VAL:HG12  | 23:W:72:LYS:NZ    | 2.25                     | 0.52              |
| 7:g:158:GLY:O     | 8:h:84:ARG:NH2    | 2.43                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:s:195:ILE:HB   | 19:s:206:GLU:HB3  | 1.91                     | 0.52              |
| 7:G:80:MET:HE2    | 7:G:91:VAL:HG23   | 1.91                     | 0.52              |
| 11:K:146:VAL:HG11 | 11:K:222:PRO:HA   | 1.92                     | 0.52              |
| 12:L:165:SER:OG   | 12:L:169:ARG:NH1  | 2.42                     | 0.52              |
| 23:W:121:LYS:O    | 23:W:125:ILE:HG12 | 2.10                     | 0.52              |
| 24:X:379:ASP:HB2  | 24:X:384:VAL:HB   | 1.91                     | 0.52              |
| 25:Y:301:ILE:HD11 | 25:Y:343:LEU:HB2  | 1.92                     | 0.52              |
| 28:b:24:THR:HG22  | 28:b:26:LEU:H     | 1.75                     | 0.52              |
| 9:i:46:ALA:HB1    | 9:i:197:LEU:HD11  | 1.91                     | 0.52              |
| 10:j:188:ILE:HD12 | 10:j:208:LEU:HD21 | 1.92                     | 0.52              |
| 6:F:304:ARG:O     | 6:F:308:ARG:NH1   | 2.43                     | 0.52              |
| 9:I:86:LEU:HD12   | 9:I:114:LEU:HD21  | 1.90                     | 0.52              |
| 32:f:231:LEU:HB3  | 32:f:853:VAL:HG22 | 1.90                     | 0.52              |
| 14:n:192:ASP:OD1  | 14:n:192:ASP:N    | 2.43                     | 0.52              |
| 5:E:286:ASP:HB3   | 5:E:289:LEU:HG    | 1.92                     | 0.52              |
| 19:S:150:ASP:OD2  | 16:p:177:ARG:NH2  | 2.43                     | 0.52              |
| 24:X:397:TYR:O    | 25:Y:365:GLN:NE2  | 2.43                     | 0.52              |
| 25:Y:104:MET:HE1  | 25:Y:130:LYS:HB2  | 1.92                     | 0.52              |
| 27:a:279:GLU:OE2  | 27:a:339:ARG:NH1  | 2.39                     | 0.52              |
| 34:w:22:THR:HA    | 34:w:55:THR:HA    | 1.91                     | 0.52              |
| 5:E:126:ASP:HB3   | 5:E:195:PHE:HB2   | 1.92                     | 0.52              |
| 5:E:196:LEU:HD21  | 5:E:221:TYR:CD2   | 2.45                     | 0.52              |
| 23:W:154:GLU:HG2  | 23:W:159:VAL:HG12 | 1.92                     | 0.52              |
| 29:c:100:LYS:HG2  | 29:c:105:PRO:HB3  | 1.92                     | 0.52              |
| 22:V:337:LEU:HD21 | 22:V:364:THR:HG23 | 1.92                     | 0.51              |
| 32:f:171:GLN:NE2  | 32:f:210:GLU:OE1  | 2.43                     | 0.51              |
| 17:q:53:THR:HG22  | 17:q:100:VAL:HG12 | 1.91                     | 0.51              |
| 19:s:125:ASP:OD1  | 19:s:129:SER:N    | 2.43                     | 0.51              |
| 4:D:249:ASP:OD1   | 4:D:252:ARG:NH2   | 2.43                     | 0.51              |
| 22:V:192:MET:HE1  | 22:V:211:TYR:HE1  | 1.75                     | 0.51              |
| 22:V:469:THR:O    | 22:V:470:ARG:NE   | 2.43                     | 0.51              |
| 30:d:203:PRO:HD2  | 30:d:206:MET:HG2  | 1.92                     | 0.51              |
| 5:E:52:SER:HB3    | 6:F:136:VAL:HB    | 1.91                     | 0.51              |
| 5:E:97:ARG:NH2    | 5:E:112:PRO:O     | 2.44                     | 0.51              |
| 20:T:25:ASP:HA    | 20:T:187:PHE:HA   | 1.93                     | 0.51              |
| 26:Z:166:GLU:O    | 29:c:46:ARG:NH1   | 2.43                     | 0.51              |
| 29:c:279:ASP:N    | 29:c:280:PRO:CD   | 2.66                     | 0.51              |
| 10:j:158:ALA:HB3  | 11:k:58:LEU:HD21  | 1.92                     | 0.51              |
| 13:M:108:LEU:HD11 | 13:M:137:LEU:HB3  | 1.91                     | 0.51              |
| 27:a:343:LEU:O    | 27:a:345:GLN:N    | 2.44                     | 0.51              |
| 29:c:196:LEU:O    | 29:c:198:ARG:N    | 2.44                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:n:1:THR:N      | 14:n:130:SER:OG   | 2.43                     | 0.51              |
| 3:C:11:LEU:HD12   | 3:C:15:LYS:HE3    | 1.92                     | 0.51              |
| 5:E:219:PHE:HA    | 5:E:222:ALA:HB3   | 1.92                     | 0.51              |
| 11:K:51:GLU:HB3   | 11:K:53:ARG:HH11  | 1.76                     | 0.51              |
| 12:L:41:LYS:NZ    | 12:L:181:GLU:HA   | 2.25                     | 0.51              |
| 21:U:198:LEU:HD13 | 21:U:219:CYS:HA   | 1.92                     | 0.51              |
| 26:Z:125:ASP:HB3  | 26:Z:128:PRO:HD2  | 1.93                     | 0.51              |
| 27:a:70:ARG:HH21  | 28:b:17:ARG:HA    | 1.74                     | 0.51              |
| 32:f:384:ALA:HB2  | 32:f:419:LEU:HD23 | 1.93                     | 0.51              |
| 8:h:175:GLU:OE2   | 9:i:53:HIS:NE2    | 2.43                     | 0.51              |
| 34:z:36:ILE:HG21  | 34:z:71:LEU:HD22  | 1.93                     | 0.51              |
| 1:A:70:THR:HB     | 2:B:164:MET:HE2   | 1.93                     | 0.51              |
| 2:B:224:LEU:HD21  | 2:B:235:LEU:HD22  | 1.91                     | 0.51              |
| 4:D:299:PHE:HB2   | 4:D:301:GLN:HE22  | 1.75                     | 0.51              |
| 16:P:138:VAL:HG11 | 16:P:146:MET:HB3  | 1.93                     | 0.51              |
| 23:W:256:ILE:HG23 | 23:W:262:LYS:HB3  | 1.93                     | 0.51              |
| 25:Y:247:LEU:HD12 | 25:Y:250:LEU:HD11 | 1.92                     | 0.51              |
| 34:z:74:ARG:NE    | 34:z:74:ARG:CA    | 2.73                     | 0.51              |
| 4:D:157:ASP:H     | 4:D:159:LYS:NZ    | 2.07                     | 0.51              |
| 30:d:167:ILE:HA   | 30:d:170:LEU:HB3  | 1.92                     | 0.51              |
| 4:D:99:ASN:HA     | 4:D:115:ILE:HG12  | 1.93                     | 0.51              |
| 32:f:76:GLU:HB3   | 32:f:80:ARG:HH12  | 1.75                     | 0.51              |
| 13:m:184:MET:HE2  | 13:m:188:ASP:HB2  | 1.92                     | 0.51              |
| 19:s:16:ALA:HB2   | 19:s:121:VAL:HG23 | 1.93                     | 0.51              |
| 5:E:188:ALA:HB2   | 5:E:195:PHE:HZ    | 1.75                     | 0.51              |
| 12:L:44:ALA:HB2   | 12:L:142:PRO:HB3  | 1.92                     | 0.51              |
| 23:W:358:VAL:O    | 23:W:362:ASN:ND2  | 2.44                     | 0.51              |
| 25:Y:25:LEU:HD21  | 25:Y:284:LYS:HZ1  | 1.76                     | 0.51              |
| 29:c:162:LEU:HA   | 29:c:200:TYR:CB   | 2.41                     | 0.51              |
| 18:r:6:PHE:HB3    | 18:r:139:MET:HE2  | 1.91                     | 0.51              |
| 4:D:169:GLY:O     | 4:D:340:GLN:NE2   | 2.41                     | 0.50              |
| 14:N:144:ARG:NH2  | 14:N:151:GLU:OE1  | 2.44                     | 0.50              |
| 32:f:93:PRO:HG2   | 32:f:96:LEU:HB2   | 1.93                     | 0.50              |
| 4:D:264:ILE:HB    | 4:D:309:MET:HG2   | 1.92                     | 0.50              |
| 5:E:101:ASP:HB3   | 5:E:105:LEU:H     | 1.76                     | 0.50              |
| 21:U:82:LEU:O     | 21:U:129:ARG:NH2  | 2.44                     | 0.50              |
| 27:a:343:LEU:O    | 27:a:346:ILE:N    | 2.41                     | 0.50              |
| 16:P:35:VAL:HG12  | 16:P:36:THR:HG23  | 1.93                     | 0.50              |
| 23:W:455:LEU:HD13 | 26:Z:101:LEU:HD12 | 1.92                     | 0.50              |
| 25:Y:316:LEU:HB3  | 25:Y:354:VAL:HG23 | 1.93                     | 0.50              |
| 26:Z:236:LEU:HD21 | 27:a:335:TRP:HB2  | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:103:VAL:HG21  | 4:D:132:LEU:HD21  | 1.93                     | 0.50              |
| 23:W:198:ASP:CG   | 23:W:201:ARG:HB3  | 2.37                     | 0.50              |
| 25:Y:127:THR:O    | 25:Y:131:THR:OG1  | 2.26                     | 0.50              |
| 27:a:54:ASP:N     | 27:a:54:ASP:OD1   | 2.44                     | 0.50              |
| 29:c:200:TYR:N    | 29:c:200:TYR:CD2  | 2.78                     | 0.50              |
| 1:A:364:VAL:HG12  | 1:A:404:ALA:HB3   | 1.94                     | 0.50              |
| 1:A:398:ARG:NH2   | 2:B:196:GLU:OE2   | 2.44                     | 0.50              |
| 2:B:121:ALA:N     | 2:B:133:VAL:O     | 2.44                     | 0.50              |
| 3:C:281:ASP:OD2   | 3:C:307:ARG:NH2   | 2.45                     | 0.50              |
| 21:U:16:GLU:HG2   | 30:d:27:LYS:HE3   | 1.93                     | 0.50              |
| 22:V:85:ALA:HB2   | 22:V:93:PHE:HB2   | 1.93                     | 0.50              |
| 22:V:177:ASN:O    | 22:V:179:LYS:NZ   | 2.44                     | 0.50              |
| 32:f:487:LEU:HA   | 32:f:524:MET:HE1  | 1.93                     | 0.50              |
| 14:N:192:ASP:OD1  | 14:N:192:ASP:N    | 2.44                     | 0.50              |
| 22:V:192:MET:HE2  | 22:V:230:PHE:CZ   | 2.45                     | 0.50              |
| 29:c:162:LEU:HD13 | 29:c:200:TYR:HD1  | 1.76                     | 0.50              |
| 14:n:1:THR:OG1    | 14:n:33:LYS:NZ    | 2.41                     | 0.50              |
| 20:t:27:LEU:HD22  | 20:t:184:TYR:HB2  | 1.94                     | 0.50              |
| 20:t:122:LEU:HG   | 20:t:137:LEU:HD12 | 1.94                     | 0.50              |
| 2:B:181:GLN:O     | 2:B:241:ASN:ND2   | 2.45                     | 0.50              |
| 3:C:299:ASP:OD1   | 3:C:299:ASP:N     | 2.45                     | 0.50              |
| 3:C:307:ARG:HG3   | 3:C:309:GLY:H     | 1.77                     | 0.50              |
| 4:D:210:CYS:SG    | 4:D:335:LEU:HG    | 2.52                     | 0.50              |
| 14:N:174:ILE:HB   | 14:N:189:LEU:HB2  | 1.93                     | 0.50              |
| 22:V:191:LEU:HA   | 22:V:194:LYS:HD2  | 1.93                     | 0.50              |
| 24:X:58:ALA:HA    | 24:X:99:MET:HE3   | 1.93                     | 0.50              |
| 1:A:384:GLU:HB3   | 2:B:344:PRO:HG3   | 1.94                     | 0.50              |
| 16:P:34:MET:O     | 18:r:166:ARG:NH1  | 2.42                     | 0.50              |
| 19:S:198:VAL:HG22 | 19:S:203:ILE:HG12 | 1.93                     | 0.50              |
| 25:Y:220:VAL:HA   | 25:Y:223:THR:HG22 | 1.93                     | 0.50              |
| 8:h:64:LYS:NZ     | 8:h:76:TYR:OH     | 2.42                     | 0.50              |
| 2:B:388:ASP:N     | 2:B:388:ASP:OD1   | 2.45                     | 0.50              |
| 5:E:98:VAL:HA     | 5:E:110:TYR:HA    | 1.94                     | 0.50              |
| 5:E:144:GLU:O     | 5:E:297:ARG:NH2   | 2.44                     | 0.50              |
| 9:I:155:ASN:OD1   | 10:J:77:THR:OG1   | 2.30                     | 0.50              |
| 18:R:39:PRO:HA    | 18:R:184:TRP:HE1  | 1.77                     | 0.50              |
| 21:U:580:ARG:HA   | 21:U:583:MET:HE2  | 1.93                     | 0.50              |
| 23:W:68:VAL:HG12  | 23:W:72:LYS:HZ2   | 1.76                     | 0.50              |
| 24:X:122:ARG:HD2  | 24:X:125:LEU:HB2  | 1.93                     | 0.50              |
| 26:Z:229:GLN:HG3  | 27:a:338:PRO:HG2  | 1.93                     | 0.50              |
| 27:a:252:LYS:HA   | 27:a:255:TRP:HE3  | 1.77                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:g:128:ASN:HB2   | 7:g:131:MET:HE1   | 1.94                     | 0.50              |
| 13:m:68:ASN:OD1   | 13:m:224:HIS:ND1  | 2.39                     | 0.50              |
| 16:p:107:PRO:HG2  | 16:p:124:LEU:HD12 | 1.93                     | 0.50              |
| 21:U:889:LEU:HD13 | 21:U:909:GLY:H    | 1.77                     | 0.49              |
| 25:Y:41:LEU:HD21  | 25:Y:57:LEU:HD11  | 1.94                     | 0.49              |
| 26:Z:235:ASN:ND2  | 27:a:349:MET:SD   | 2.85                     | 0.49              |
| 29:c:192:LEU:HA   | 29:c:196:LEU:CB   | 2.38                     | 0.49              |
| 20:t:43:MET:HE1   | 20:t:67:LEU:HD23  | 1.93                     | 0.49              |
| 3:C:218:GLU:O     | 3:C:221:GLN:NE2   | 2.46                     | 0.49              |
| 3:C:331:ILE:HA    | 3:C:334:ARG:HE    | 1.78                     | 0.49              |
| 5:E:196:LEU:HD21  | 5:E:221:TYR:HD2   | 1.75                     | 0.49              |
| 27:a:227:ASN:O    | 27:a:231:GLN:NE2  | 2.37                     | 0.49              |
| 1:A:252:GLU:HA    | 6:F:259:MET:HE1   | 1.94                     | 0.49              |
| 12:L:166:GLN:OE1  | 12:L:169:ARG:NH2  | 2.41                     | 0.49              |
| 13:m:8:ASP:O      | 13:m:22:GLN:NE2   | 2.38                     | 0.49              |
| 19:s:184:GLU:OE2  | 19:s:211:ARG:NH1  | 2.46                     | 0.49              |
| 2:B:109:VAL:HG11  | 3:C:94:LYS:HE2    | 1.94                     | 0.49              |
| 20:T:27:LEU:HD22  | 20:T:184:TYR:HB2  | 1.94                     | 0.49              |
| 21:U:906:LEU:HD13 | 21:U:912:ILE:HD13 | 1.95                     | 0.49              |
| 28:b:12:ASN:HD22  | 28:b:78:VAL:HG22  | 1.77                     | 0.49              |
| 28:b:50:GLY:HA2   | 28:b:71:ILE:HD11  | 1.93                     | 0.49              |
| 29:c:195:GLY:O    | 29:c:196:LEU:C    | 2.55                     | 0.49              |
| 32:f:213:GLN:HB3  | 32:f:216:MET:HE1  | 1.94                     | 0.49              |
| 4:D:185:LEU:HD21  | 4:D:224:THR:HG22  | 1.94                     | 0.49              |
| 11:K:53:ARG:NH1   | 11:K:206:MET:SD   | 2.86                     | 0.49              |
| 15:O:1:THR:N      | 15:O:168:GLY:O    | 2.46                     | 0.49              |
| 25:Y:238:GLU:HA   | 25:Y:242:LYS:HB2  | 1.93                     | 0.49              |
| 32:f:459:CYS:O    | 34:w:6:LYS:NZ     | 2.35                     | 0.49              |
| 11:k:129:ASP:N    | 11:k:129:ASP:OD1  | 2.46                     | 0.49              |
| 19:s:45:LYS:HE3   | 19:s:203:ILE:HD12 | 1.95                     | 0.49              |
| 34:y:42:ARG:HE    | 34:y:72:ARG:HE    | 1.60                     | 0.49              |
| 5:E:188:ALA:HB2   | 5:E:195:PHE:CZ    | 2.48                     | 0.49              |
| 18:R:3:THR:HG23   | 18:R:16:ALA:HB2   | 1.93                     | 0.49              |
| 21:U:543:LYS:HE3  | 21:U:546:ARG:HH22 | 1.78                     | 0.49              |
| 21:U:903:PHE:HB2  | 21:U:915:LYS:HB2  | 1.94                     | 0.49              |
| 26:Z:34:ARG:NH1   | 26:Z:97:THR:O     | 2.40                     | 0.49              |
| 32:f:822:VAL:HA   | 32:f:825:MET:HE2  | 1.94                     | 0.49              |
| 2:B:74:MET:HB2    | 32:f:610:GLN:HE22 | 1.77                     | 0.49              |
| 2:B:313:LEU:O     | 2:B:346:ARG:NH1   | 2.45                     | 0.49              |
| 22:V:98:LEU:HD11  | 22:V:206:VAL:HG22 | 1.95                     | 0.49              |
| 27:a:343:LEU:HG   | 27:a:346:ILE:HD12 | 1.93                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:h:124:SER:OG    | 8:h:125:GLY:N     | 2.46                     | 0.49              |
| 3:C:20:LEU:HD12   | 3:C:21:ARG:HG3    | 1.94                     | 0.49              |
| 6:F:169:ASP:OD1   | 6:F:169:ASP:N     | 2.45                     | 0.49              |
| 10:J:4:ASP:OD1    | 10:J:4:ASP:N      | 2.45                     | 0.49              |
| 12:L:107:ARG:NH2  | 20:T:74:GLU:OE2   | 2.39                     | 0.49              |
| 12:L:226:ASP:OD1  | 12:L:226:ASP:N    | 2.46                     | 0.49              |
| 17:Q:21:ALA:HB3   | 17:Q:29:LYS:HB3   | 1.94                     | 0.49              |
| 26:Z:74:TYR:O     | 26:Z:78:MET:HG2   | 2.13                     | 0.49              |
| 9:i:62:SER:OG     | 9:i:65:ILE:O      | 2.29                     | 0.49              |
| 17:q:153:ARG:NH1  | 17:q:184:ASP:OD2  | 2.43                     | 0.49              |
| 2:B:233:THR:OG1   | 35:B:501:ATP:O2B  | 2.30                     | 0.49              |
| 5:E:60:VAL:HA     | 5:E:71:VAL:HG12   | 1.95                     | 0.49              |
| 19:S:157:ASN:ND2  | 16:p:176:ASP:OD2  | 2.46                     | 0.49              |
| 20:T:91:TRP:HE3   | 20:T:92:LEU:HD12  | 1.77                     | 0.49              |
| 29:c:198:ARG:HG3  | 29:c:199:HIS:ND1  | 2.28                     | 0.49              |
| 10:j:160:ALA:O    | 10:j:169:ARG:NH2  | 2.46                     | 0.49              |
| 2:B:429:LYS:NZ    | 3:C:306:LEU:O     | 2.40                     | 0.49              |
| 3:C:161:ILE:HA    | 3:C:164:VAL:HG12  | 1.94                     | 0.49              |
| 32:f:83:ARG:O     | 32:f:87:THR:OG1   | 2.23                     | 0.49              |
| 14:n:144:ARG:NH2  | 14:n:151:GLU:OE1  | 2.46                     | 0.49              |
| 34:y:43:LEU:HB3   | 34:y:50:LEU:HD12  | 1.95                     | 0.49              |
| 1:A:372:LEU:HD11  | 11:K:207:GLU:HA   | 1.94                     | 0.48              |
| 2:B:342:ILE:HA    | 2:B:347:ILE:HD11  | 1.95                     | 0.48              |
| 6:F:122:ALA:HB3   | 6:F:134:LEU:HD21  | 1.95                     | 0.48              |
| 20:T:26:MET:HE3   | 20:T:186:ARG:HG2  | 1.94                     | 0.48              |
| 1:A:140:VAL:HA    | 1:A:152:PRO:HA    | 1.94                     | 0.48              |
| 6:F:180:ARG:NH1   | 6:F:244:THR:O     | 2.46                     | 0.48              |
| 9:I:70:GLU:O      | 9:I:223:THR:OG1   | 2.29                     | 0.48              |
| 23:W:443:THR:HA   | 23:W:446:ILE:HG12 | 1.95                     | 0.48              |
| 5:E:309:ARG:NH1   | 5:E:335:SER:O     | 2.47                     | 0.48              |
| 21:U:381:THR:HG22 | 21:U:412:HIS:HA   | 1.94                     | 0.48              |
| 23:W:455:LEU:HD21 | 26:Z:103:LYS:HG2  | 1.95                     | 0.48              |
| 24:X:106:GLU:OE1  | 24:X:106:GLU:HA   | 2.13                     | 0.48              |
| 10:j:140:GLY:O    | 10:j:213:ARG:NH1  | 2.43                     | 0.48              |
| 13:m:228:PRO:HD2  | 13:m:231:ILE:HD12 | 1.95                     | 0.48              |
| 18:r:63:CYS:HA    | 18:r:74:ILE:HD12  | 1.94                     | 0.48              |
| 6:F:362:ARG:NH2   | 6:F:388:THR:O     | 2.46                     | 0.48              |
| 24:X:334:ASN:OD1  | 24:X:337:ARG:NH2  | 2.44                     | 0.48              |
| 34:x:14:THR:O     | 34:x:33:LYS:NZ    | 2.46                     | 0.48              |
| 2:B:375:ALA:HB2   | 2:B:413:LYS:HB3   | 1.94                     | 0.48              |
| 3:C:187:LEU:HB3   | 3:C:314:LYS:HA    | 1.94                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:159:LYS:N     | 4:D:160:PRO:CD    | 2.77                     | 0.48              |
| 5:E:238:ILE:HD13  | 5:E:253:ILE:HD11  | 1.96                     | 0.48              |
| 34:x:23:ILE:HB    | 34:x:52:ASP:HA    | 1.95                     | 0.48              |
| 1:A:306:LEU:O     | 1:A:312:ARG:NH1   | 2.47                     | 0.48              |
| 2:B:383:LEU:HD11  | 2:B:419:PHE:HB3   | 1.95                     | 0.48              |
| 21:U:886:PRO:HA   | 21:U:889:LEU:HG   | 1.96                     | 0.48              |
| 22:V:113:LEU:HB3  | 22:V:135:LEU:HD13 | 1.96                     | 0.48              |
| 34:w:60:ASN:OD1   | 34:w:62:GLN:NE2   | 2.42                     | 0.48              |
| 2:B:389:ASP:OD1   | 2:B:389:ASP:N     | 2.47                     | 0.48              |
| 4:D:173:GLN:NE2   | 4:D:332:GLU:O     | 2.47                     | 0.48              |
| 26:Z:102:HIS:HD2  | 26:Z:104:ASN:HB3  | 1.79                     | 0.48              |
| 9:i:140:ASP:OD1   | 9:i:140:ASP:N     | 2.47                     | 0.48              |
| 11:k:13:ASN:HB2   | 12:l:126:ARG:HD3  | 1.96                     | 0.48              |
| 29:c:195:GLY:HA3  | 29:c:200:TYR:CZ   | 2.48                     | 0.48              |
| 11:K:5:ARG:NH2    | 11:K:26:TYR:OH    | 2.46                     | 0.48              |
| 11:K:221:GLN:HB2  | 11:K:224:GLN:HG2  | 1.95                     | 0.48              |
| 28:b:132:LYS:HD3  | 34:z:32:ASP:OD1   | 2.14                     | 0.48              |
| 7:g:132:ARG:HB3   | 13:m:124:LEU:HD23 | 1.96                     | 0.48              |
| 1:A:297:ARG:HH22  | 6:F:306:VAL:HG21  | 1.79                     | 0.48              |
| 15:O:97:ALA:HB1   | 15:O:127:MET:HE3  | 1.94                     | 0.48              |
| 20:T:56:ASP:O     | 20:T:108:ASN:ND2  | 2.45                     | 0.48              |
| 24:X:103:THR:HA   | 24:X:106:GLU:HG2  | 1.96                     | 0.48              |
| 24:X:309:TYR:HB3  | 24:X:312:GLU:HB2  | 1.95                     | 0.48              |
| 4:D:153:MET:HE1   | 4:D:226:ALA:HB1   | 1.96                     | 0.47              |
| 21:U:789:ILE:HB   | 21:U:911:ILE:HA   | 1.95                     | 0.47              |
| 23:W:344:THR:HG23 | 23:W:347:GLY:H    | 1.78                     | 0.47              |
| 25:Y:210:SER:HB3  | 25:Y:213:LEU:HD23 | 1.96                     | 0.47              |
| 5:E:173:TYR:HE1   | 5:E:298:LYS:HB3   | 1.79                     | 0.47              |
| 7:G:32:ILE:HD13   | 7:G:137:CYS:HB2   | 1.96                     | 0.47              |
| 22:V:120:PHE:HE1  | 22:V:149:PRO:HG2  | 1.79                     | 0.47              |
| 23:W:360:GLU:HB3  | 23:W:392:PHE:HZ   | 1.80                     | 0.47              |
| 32:f:398:TRP:HA   | 32:f:401:LYS:HD3  | 1.95                     | 0.47              |
| 4:D:45:LYS:NZ     | 21:U:156:GLU:OE2  | 2.39                     | 0.47              |
| 6:F:246:ALA:HB1   | 6:F:280:PRO:HB2   | 1.96                     | 0.47              |
| 21:U:483:LEU:HD11 | 21:U:781:LEU:HD11 | 1.97                     | 0.47              |
| 21:U:613:ASP:OD1  | 21:U:616:ARG:NH2  | 2.44                     | 0.47              |
| 23:W:205:ILE:HA   | 23:W:208:LYS:HE2  | 1.96                     | 0.47              |
| 26:Z:67:VAL:HG11  | 28:b:91:ARG:HG2   | 1.96                     | 0.47              |
| 11:k:76:CYS:SG    | 11:k:77:ALA:N     | 2.87                     | 0.47              |
| 13:m:198:TYR:OH   | 13:m:236:GLU:OE1  | 2.32                     | 0.47              |
| 17:q:39:SER:OG    | 17:q:40:GLU:N     | 2.48                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:84:LYS:O      | 6:F:85:THR:C      | 2.56                     | 0.47              |
| 7:G:112:ASP:N     | 7:G:112:ASP:OD1   | 2.47                     | 0.47              |
| 9:I:216:LEU:HD12  | 9:I:225:ILE:HG12  | 1.96                     | 0.47              |
| 10:J:40:ILE:HD11  | 10:J:210:VAL:HB   | 1.96                     | 0.47              |
| 27:a:65:SER:HA    | 27:a:68:GLU:HB2   | 1.95                     | 0.47              |
| 27:a:80:ILE:HG12  | 27:a:100:THR:HG21 | 1.96                     | 0.47              |
| 15:o:113:ILE:HG12 | 15:o:119:THR:HG22 | 1.97                     | 0.47              |
| 19:s:95:ILE:O     | 19:s:98:SER:OG    | 2.31                     | 0.47              |
| 2:B:80:ARG:O      | 2:B:84:GLN:HB2    | 2.14                     | 0.47              |
| 5:E:121:ASN:HA    | 5:E:197:LYS:HD2   | 1.96                     | 0.47              |
| 24:X:421:LEU:HD11 | 26:Z:280:ILE:HG12 | 1.96                     | 0.47              |
| 24:X:422:THR:HB   | 26:Z:283:ARG:HH12 | 1.80                     | 0.47              |
| 29:c:198:ARG:HG3  | 29:c:199:HIS:HD1  | 1.79                     | 0.47              |
| 3:C:339:THR:HG23  | 25:Y:174:TRP:HZ3  | 1.80                     | 0.47              |
| 22:V:100:MET:O    | 22:V:103:SER:OG   | 2.30                     | 0.47              |
| 23:W:409:LEU:HD11 | 24:X:344:ARG:HH21 | 1.80                     | 0.47              |
| 12:l:196:ARG:NH1  | 12:l:237:GLU:O    | 2.48                     | 0.47              |
| 34:x:27:LYS:HB3   | 34:x:38:PRO:HB3   | 1.96                     | 0.47              |
| 2:B:230:THR:HG21  | 2:B:353:PHE:HB3   | 1.97                     | 0.47              |
| 3:C:215:SER:OG    | 3:C:218:GLU:OE1   | 2.27                     | 0.47              |
| 6:F:188:ILE:HD11  | 6:F:191:LEU:HD12  | 1.97                     | 0.47              |
| 8:H:109:GLN:HB3   | 8:H:113:ARG:HH12  | 1.78                     | 0.47              |
| 12:L:139:ASP:N    | 12:L:139:ASP:OD1  | 2.46                     | 0.47              |
| 14:N:9:ASP:N      | 14:N:9:ASP:OD1    | 2.45                     | 0.47              |
| 19:S:92:LEU:HD23  | 19:S:124:PHE:HE2  | 1.80                     | 0.47              |
| 32:f:446:LEU:HD12 | 32:f:480:GLY:HA2  | 1.96                     | 0.47              |
| 32:f:613:LEU:HD23 | 32:f:613:LEU:HA   | 1.65                     | 0.47              |
| 8:h:143:ARG:NH1   | 8:h:145:TYR:OH    | 2.48                     | 0.47              |
| 16:p:138:VAL:HG11 | 16:p:146:MET:HB3  | 1.97                     | 0.47              |
| 2:B:197:ILE:HG12  | 2:B:235:LEU:HD21  | 1.96                     | 0.47              |
| 3:C:191:PRO:O     | 3:C:196:LYS:NZ    | 2.48                     | 0.47              |
| 17:Q:35:MET:HG2   | 17:Q:45:LEU:HG    | 1.97                     | 0.47              |
| 20:T:43:MET:HG2   | 20:T:64:LYS:HG3   | 1.97                     | 0.47              |
| 22:V:121:PHE:HB3  | 22:V:128:ARG:HD2  | 1.96                     | 0.47              |
| 23:W:51:GLU:CD    | 23:W:55:ARG:HH12  | 2.23                     | 0.47              |
| 29:c:279:ASP:HA   | 29:c:283:HIS:CB   | 2.39                     | 0.47              |
| 30:d:168:ASP:OD1  | 30:d:169:ILE:N    | 2.47                     | 0.47              |
| 23:W:171:VAL:HG12 | 23:W:182:ARG:HG3  | 1.97                     | 0.47              |
| 32:f:146:GLY:O    | 32:f:148:GLN:NE2  | 2.48                     | 0.47              |
| 24:X:143:TYR:OH   | 25:Y:248:GLU:O    | 2.33                     | 0.47              |
| 27:a:77:VAL:HG21  | 27:a:110:ALA:HB1  | 1.97                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 29:c:27:THR:HG22 | 29:c:28:ALA:H     | 1.79                     | 0.47              |
| 30:d:131:VAL:HA  | 30:d:134:LYS:HB3  | 1.97                     | 0.47              |
| 8:h:3:GLU:CD     | 13:m:127:ALA:HB3  | 2.39                     | 0.47              |
| 20:t:12:LEU:HD21 | 20:t:176:LEU:HD11 | 1.96                     | 0.47              |
| 3:C:228:ALA:HA   | 3:C:272:THR:HG23  | 1.97                     | 0.46              |
| 4:D:86:PRO:HB2   | 5:E:105:LEU:HD22  | 1.98                     | 0.46              |
| 8:H:111:VAL:HG21 | 8:H:147:PHE:HD2   | 1.79                     | 0.46              |
| 18:R:182:ASP:OD1 | 18:R:182:ASP:N    | 2.44                     | 0.46              |
| 27:a:35:HIS:NE2  | 28:b:14:GLU:O     | 2.48                     | 0.46              |
| 29:c:281:LYS:HZ2 | 29:c:284:LEU:HD13 | 1.81                     | 0.46              |
| 11:k:120:ALA:O   | 11:k:121:LEU:HG   | 2.14                     | 0.46              |
| 12:l:189:LYS:NZ  | 12:l:234:GLU:O    | 2.43                     | 0.46              |
| 2:B:180:PRO:HG3  | 3:C:283:PHE:HE2   | 1.80                     | 0.46              |
| 4:D:336:PRO:HG3  | 4:D:369:LYS:HB3   | 1.97                     | 0.46              |
| 5:E:56:ILE:O     | 5:E:100:LEU:N     | 2.42                     | 0.46              |
| 11:K:95:GLU:HG3  | 11:K:107:MET:HE1  | 1.96                     | 0.46              |
| 19:S:22:ILE:HG12 | 19:S:197:ILE:HG13 | 1.97                     | 0.46              |
| 24:X:380:GLN:HB2 | 25:Y:314:LEU:HA   | 1.96                     | 0.46              |
| 27:a:119:GLY:HA2 | 27:a:122:LYS:HB3  | 1.97                     | 0.46              |
| 8:h:34:PRO:HA    | 8:h:164:GLY:HA3   | 1.97                     | 0.46              |
| 13:m:136:MET:HE3 | 13:m:163:CYS:HB3  | 1.96                     | 0.46              |
| 16:p:10:ALA:HB1  | 16:p:146:MET:HE1  | 1.97                     | 0.46              |
| 17:q:52:ASP:OD1  | 18:r:88:TYR:OH    | 2.32                     | 0.46              |
| 34:y:5:VAL:HG22  | 34:y:67:LEU:HB2   | 1.96                     | 0.46              |
| 6:F:320:PHE:CE2  | 6:F:326:VAL:HB    | 2.50                     | 0.46              |
| 14:N:84:LYS:HG3  | 14:N:120:MET:HB2  | 1.97                     | 0.46              |
| 23:W:235:GLN:HG2 | 23:W:350:ARG:HH22 | 1.80                     | 0.46              |
| 32:f:115:PRO:HA  | 32:f:119:LYS:HD3  | 1.98                     | 0.46              |
| 32:f:323:ASN:HB3 | 32:f:326:LEU:HB2  | 1.97                     | 0.46              |
| 10:j:66:ASP:OD2  | 10:j:95:ARG:NH2   | 2.41                     | 0.46              |
| 10:j:137:ASP:OD2 | 10:j:143:ARG:NH1  | 2.43                     | 0.46              |
| 14:n:104:ASP:OD1 | 14:n:104:ASP:N    | 2.48                     | 0.46              |
| 17:q:31:ASP:OD1  | 17:q:31:ASP:N     | 2.48                     | 0.46              |
| 17:q:47:VAL:HG13 | 17:q:101:ASN:HB2  | 1.97                     | 0.46              |
| 2:B:195:GLN:NE2  | 2:B:199:GLU:OE2   | 2.46                     | 0.46              |
| 24:X:316:ASP:OD2 | 24:X:321:THR:OG1  | 2.33                     | 0.46              |
| 15:o:209:THR:OG1 | 16:p:169:GLN:NE2  | 2.41                     | 0.46              |
| 19:s:211:ARG:NH2 | 19:s:213:ASP:OD2  | 2.48                     | 0.46              |
| 20:t:97:TYR:HA   | 20:t:100:ARG:HG2  | 1.98                     | 0.46              |
| 1:A:279:ALA:HB2  | 2:B:310:LEU:HD23  | 1.98                     | 0.46              |
| 2:B:106:PRO:HB3  | 3:C:121:TYR:HB2   | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:85:ILE:HD11   | 29:c:152:LYS:HE2  | 1.96                     | 0.46              |
| 4:D:156:SER:O     | 4:D:157:ASP:HB2   | 2.15                     | 0.46              |
| 5:E:265:ASP:HA    | 5:E:269:THR:HA    | 1.97                     | 0.46              |
| 6:F:258:GLN:HB2   | 6:F:263:ASP:HB2   | 1.97                     | 0.46              |
| 10:J:79:ASP:HB3   | 10:J:127:PHE:HD1  | 1.81                     | 0.46              |
| 21:U:202:VAL:HA   | 21:U:205:TYR:HB2  | 1.97                     | 0.46              |
| 29:c:31:VAL:HB    | 29:c:205:ILE:HG13 | 1.98                     | 0.46              |
| 29:c:197:ASN:C    | 29:c:199:HIS:N    | 2.73                     | 0.46              |
| 32:f:534:VAL:HA   | 32:f:537:THR:HG22 | 1.97                     | 0.46              |
| 1:A:55:LEU:HA     | 1:A:58:LYS:HG2    | 1.97                     | 0.46              |
| 5:E:23:ASP:OD1    | 5:E:27:LYS:NZ     | 2.49                     | 0.46              |
| 6:F:49:ASP:O      | 28:b:27:GLN:NE2   | 2.49                     | 0.46              |
| 14:N:115:PRO:HD2  | 14:N:119:MET:HB3  | 1.97                     | 0.46              |
| 21:U:803:LYS:O    | 21:U:893:THR:N    | 2.40                     | 0.46              |
| 26:Z:43:TRP:HB3   | 26:Z:90:ARG:HH21  | 1.80                     | 0.46              |
| 26:Z:193:ASN:HA   | 26:Z:196:HIS:CE1  | 2.51                     | 0.46              |
| 28:b:181:ASP:HA   | 28:b:184:ILE:HG12 | 1.97                     | 0.46              |
| 17:q:4:LEU:HD22   | 17:q:45:LEU:HD23  | 1.98                     | 0.46              |
| 34:z:51:GLU:HB2   | 34:z:54:ARG:HD3   | 1.97                     | 0.46              |
| 2:B:227:PRO:O     | 2:B:230:THR:OG1   | 2.31                     | 0.46              |
| 20:T:20:VAL:HG23  | 20:T:120:SER:HB3  | 1.97                     | 0.46              |
| 21:U:580:ARG:HH12 | 21:U:768:GLN:HE22 | 1.61                     | 0.46              |
| 21:U:796:LYS:HE3  | 21:U:796:LYS:HB3  | 1.83                     | 0.46              |
| 22:V:322:VAL:HG11 | 31:e:27:TRP:HZ3   | 1.81                     | 0.46              |
| 23:W:108:CYS:O    | 23:W:112:VAL:HG23 | 2.16                     | 0.46              |
| 24:X:27:LEU:HD23  | 24:X:30:ILE:HD12  | 1.98                     | 0.46              |
| 24:X:170:GLN:OE1  | 24:X:192:SER:OG   | 2.33                     | 0.46              |
| 25:Y:2:PRO:HD2    | 25:Y:5:ASN:HB2    | 1.97                     | 0.46              |
| 10:j:183:THR:HB   | 10:j:186:LEU:HB2  | 1.98                     | 0.46              |
| 11:k:107:MET:HG2  | 11:k:112:VAL:HG23 | 1.97                     | 0.46              |
| 18:r:141:ARG:HA   | 18:r:141:ARG:HD2  | 1.71                     | 0.46              |
| 20:t:1:THR:N      | 20:t:104:ASN:OD1  | 2.48                     | 0.46              |
| 1:A:213:LEU:HD13  | 1:A:340:LYS:HE2   | 1.98                     | 0.46              |
| 6:F:289:ASP:OD1   | 6:F:289:ASP:N     | 2.48                     | 0.46              |
| 14:N:119:MET:HE2  | 20:T:57:TYR:HD2   | 1.80                     | 0.46              |
| 18:R:166:ARG:NH2  | 17:q:144:ASP:OD2  | 2.49                     | 0.46              |
| 21:U:353:LEU:HD22 | 21:U:385:PHE:HE2  | 1.80                     | 0.46              |
| 27:a:276:CYS:SG   | 27:a:277:LEU:N    | 2.88                     | 0.46              |
| 32:f:317:LEU:HG   | 32:f:321:MET:HE1  | 1.98                     | 0.46              |
| 16:p:62:THR:OG1   | 17:q:85:ARG:NH2   | 2.48                     | 0.46              |
| 6:F:278:LYS:HG3   | 6:F:280:PRO:HD2   | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:413:THR:OG1   | 6:F:414:GLU:OE1   | 2.32                     | 0.46              |
| 9:I:119:GLN:NE2   | 10:J:79:ASP:OD1   | 2.41                     | 0.46              |
| 11:K:9:ASP:OD1    | 11:K:9:ASP:N      | 2.47                     | 0.46              |
| 15:O:54:MET:HG2   | 16:P:96:TYR:CZ    | 2.50                     | 0.46              |
| 25:Y:345:CYS:HA   | 25:Y:356:THR:HA   | 1.98                     | 0.46              |
| 27:a:321:LYS:O    | 27:a:334:THR:OG1  | 2.34                     | 0.46              |
| 7:g:6:SER:HA      | 7:g:11:ARG:HH22   | 1.81                     | 0.46              |
| 12:l:140:MET:HE3  | 12:l:140:MET:HB3  | 1.87                     | 0.46              |
| 20:t:15:LYS:HG2   | 20:t:20:VAL:HG22  | 1.97                     | 0.46              |
| 2:B:71:TYR:CE2    | 32:f:670:MET:HB3  | 2.50                     | 0.46              |
| 2:B:115:ILE:HD11  | 2:B:146:PRO:HD3   | 1.97                     | 0.46              |
| 2:B:150:VAL:HA    | 2:B:162:VAL:HA    | 1.97                     | 0.46              |
| 4:D:61:ILE:HD12   | 21:U:639:LEU:HD23 | 1.98                     | 0.46              |
| 4:D:200:ARG:HH12  | 4:D:302:ASN:HA    | 1.80                     | 0.46              |
| 30:d:234:ASP:OD2  | 30:d:236:THR:OG1  | 2.30                     | 0.46              |
| 32:f:318:THR:HA   | 32:f:321:MET:HE2  | 1.98                     | 0.46              |
| 32:f:547:GLU:HA   | 32:f:550:LEU:HB2  | 1.97                     | 0.46              |
| 8:h:118:MET:HE3   | 8:h:118:MET:HB2   | 1.84                     | 0.46              |
| 12:l:80:ASP:OD2   | 12:l:126:ARG:NH1  | 2.45                     | 0.46              |
| 16:p:53:LEU:HG    | 16:p:107:PRO:HB3  | 1.98                     | 0.46              |
| 3:C:48:GLN:HB3    | 4:D:65:GLN:HE22   | 1.81                     | 0.45              |
| 3:C:375:ARG:HG2   | 3:C:377:HIS:H     | 1.81                     | 0.45              |
| 11:K:51:GLU:HB3   | 11:K:53:ARG:NH1   | 2.31                     | 0.45              |
| 19:S:158:MET:HE2  | 19:S:161:VAL:HG21 | 1.98                     | 0.45              |
| 21:U:103:LYS:HB2  | 21:U:103:LYS:HE3  | 1.79                     | 0.45              |
| 21:U:118:LEU:HD13 | 21:U:122:GLU:HG3  | 1.98                     | 0.45              |
| 21:U:245:ALA:HA   | 21:U:248:ILE:HG12 | 1.98                     | 0.45              |
| 21:U:895:PRO:HG2  | 21:U:902:PRO:HD3  | 1.97                     | 0.45              |
| 22:V:75:ILE:HG22  | 22:V:120:PHE:HE2  | 1.80                     | 0.45              |
| 29:c:172:HIS:CD2  | 29:c:198:ARG:HA   | 2.51                     | 0.45              |
| 30:d:47:GLN:H     | 30:d:47:GLN:HE21  | 1.62                     | 0.45              |
| 30:d:84:ASP:OD1   | 30:d:84:ASP:N     | 2.47                     | 0.45              |
| 1:A:158:ASP:OD2   | 1:A:160:THR:OG1   | 2.24                     | 0.45              |
| 17:Q:44:LEU:HD11  | 17:Q:102:LEU:HD22 | 1.98                     | 0.45              |
| 21:U:387:ARG:NH1  | 21:U:426:TYR:OH   | 2.49                     | 0.45              |
| 21:U:764:LEU:O    | 21:U:767:THR:OG1  | 2.34                     | 0.45              |
| 25:Y:74:LYS:HB3   | 25:Y:74:LYS:HE3   | 1.81                     | 0.45              |
| 26:Z:7:GLN:NE2    | 26:Z:8:LYS:HG2    | 2.31                     | 0.45              |
| 26:Z:130:ASP:OD1  | 26:Z:130:ASP:N    | 2.48                     | 0.45              |
| 32:f:806:VAL:HG23 | 32:f:810:ILE:HB   | 1.99                     | 0.45              |
| 7:g:89:SER:HA     | 13:m:117:MET:HE1  | 1.97                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:o:100:LEU:HB3  | 15:o:111:TYR:HB2  | 1.98                     | 0.45              |
| 1:A:336:ARG:NH2   | 35:F:501:ATP:O3G  | 2.47                     | 0.45              |
| 2:B:65:LEU:HD23   | 2:B:68:ILE:HD12   | 1.98                     | 0.45              |
| 4:D:154:LEU:C     | 4:D:159:LYS:HB3   | 2.41                     | 0.45              |
| 5:E:71:VAL:HG21   | 5:E:100:LEU:HD11  | 1.98                     | 0.45              |
| 16:P:12:MET:HE3   | 16:P:171:MET:HG2  | 1.97                     | 0.45              |
| 24:X:1:MET:O      | 24:X:33:ARG:NH2   | 2.49                     | 0.45              |
| 27:a:168:ASN:OD1  | 27:a:171:SER:OG   | 2.33                     | 0.45              |
| 30:d:139:LEU:HD11 | 30:d:151:VAL:HG13 | 1.96                     | 0.45              |
| 9:i:82:ASP:HB3    | 9:i:130:PHE:HD1   | 1.80                     | 0.45              |
| 2:B:289:ALA:HB2   | 3:C:274:LEU:HD22  | 1.97                     | 0.45              |
| 12:L:204:ASP:N    | 12:L:204:ASP:OD1  | 2.49                     | 0.45              |
| 22:V:92:ARG:HG2   | 22:V:96:ARG:HH21  | 1.82                     | 0.45              |
| 29:c:278:GLN:HG2  | 29:c:280:PRO:CG   | 2.47                     | 0.45              |
| 32:f:240:VAL:O    | 32:f:245:ASN:ND2  | 2.47                     | 0.45              |
| 32:f:348:ILE:HD13 | 32:f:381:VAL:HG21 | 1.97                     | 0.45              |
| 17:q:182:ILE:HD11 | 17:q:191:LEU:HD11 | 1.98                     | 0.45              |
| 1:A:325:ASP:OD1   | 1:A:325:ASP:N     | 2.44                     | 0.45              |
| 3:C:90:HIS:CG     | 3:C:91:PRO:HD3    | 2.51                     | 0.45              |
| 5:E:81:VAL:HG12   | 5:E:105:LEU:HD23  | 1.98                     | 0.45              |
| 6:F:332:THR:HG21  | 6:F:338:LEU:HD21  | 1.99                     | 0.45              |
| 15:O:21:THR:HG22  | 15:O:26:VAL:HA    | 1.99                     | 0.45              |
| 21:U:510:GLU:HA   | 21:U:547:GLY:HA3  | 1.98                     | 0.45              |
| 23:W:357:ARG:HA   | 23:W:357:ARG:HD3  | 1.80                     | 0.45              |
| 26:Z:72:HIS:CE1   | 28:b:60:VAL:HB    | 2.52                     | 0.45              |
| 3:C:307:ARG:HG2   | 3:C:310:ARG:HG2   | 1.99                     | 0.45              |
| 5:E:257:LEU:HA    | 5:E:260:LEU:HB2   | 1.99                     | 0.45              |
| 6:F:306:VAL:O     | 6:F:309:THR:OG1   | 2.31                     | 0.45              |
| 21:U:216:VAL:HA   | 21:U:220:LEU:HD23 | 1.99                     | 0.45              |
| 29:c:200:TYR:CE2  | 29:c:201:TYR:CZ   | 3.05                     | 0.45              |
| 29:c:201:TYR:O    | 29:c:202:SER:HB2  | 2.16                     | 0.45              |
| 32:f:131:MET:HE2  | 32:f:131:MET:HB2  | 1.79                     | 0.45              |
| 12:l:120:THR:O    | 13:m:129:ARG:NH1  | 2.49                     | 0.45              |
| 6:F:97:LEU:HB2    | 6:F:121:CYS:HB2   | 1.98                     | 0.45              |
| 15:O:81:ARG:HA    | 15:O:84:LYS:HG2   | 1.99                     | 0.45              |
| 21:U:131:GLU:HB2  | 21:U:159:ARG:HH12 | 1.81                     | 0.45              |
| 24:X:282:ARG:NH1  | 24:X:312:GLU:OE2  | 2.49                     | 0.45              |
| 26:Z:131:LEU:O    | 29:c:223:LYS:NZ   | 2.36                     | 0.45              |
| 27:a:72:ASN:HB2   | 28:b:17:ARG:HH22  | 1.82                     | 0.45              |
| 27:a:341:LEU:O    | 27:a:342:ASP:C    | 2.59                     | 0.45              |
| 7:g:112:ASP:OD1   | 7:g:112:ASP:N     | 2.50                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:m:108:LEU:HD13 | 13:m:147:GLN:HB2  | 1.99                     | 0.45              |
| 5:E:257:LEU:HA    | 5:E:260:LEU:HD12  | 1.99                     | 0.45              |
| 7:G:20:GLY:HA3    | 8:H:28:ALA:HA     | 1.99                     | 0.45              |
| 9:I:134:LEU:N     | 9:I:150:SER:OG    | 2.46                     | 0.45              |
| 16:P:205:ASP:HB3  | 18:r:192:VAL:HG11 | 1.98                     | 0.45              |
| 21:U:36:ALA:HB1   | 22:V:269:LYS:HB3  | 1.99                     | 0.45              |
| 23:W:69:ALA:HA    | 23:W:72:LYS:HE2   | 1.99                     | 0.45              |
| 25:Y:66:ASP:HB3   | 25:Y:69:LEU:HB3   | 1.99                     | 0.45              |
| 27:a:344:GLN:O    | 27:a:346:ILE:N    | 2.50                     | 0.45              |
| 29:c:41:MET:HE1   | 29:c:112:TYR:CG   | 2.50                     | 0.45              |
| 15:o:63:LEU:HD11  | 15:o:79:ALA:HB2   | 1.99                     | 0.45              |
| 1:A:123:VAL:HG11  | 1:A:147:TYR:HB2   | 1.97                     | 0.45              |
| 7:G:167:ALA:HB3   | 7:G:176:THR:HG23  | 1.98                     | 0.45              |
| 8:H:204:THR:OG1   | 8:H:206:ASP:OD1   | 2.31                     | 0.45              |
| 21:U:196:LYS:HA   | 21:U:199:ARG:HG2  | 1.98                     | 0.45              |
| 27:a:269:LEU:HD23 | 27:a:272:ILE:HD11 | 1.99                     | 0.45              |
| 1:A:351:ARG:NH1   | 1:A:378:PRO:O     | 2.46                     | 0.45              |
| 20:T:166:ARG:NH2  | 20:T:200:GLU:OE1  | 2.44                     | 0.45              |
| 21:U:376:MET:HA   | 21:U:740:GLY:N    | 2.32                     | 0.45              |
| 22:V:278:GLU:HA   | 22:V:285:TRP:HZ2  | 1.82                     | 0.45              |
| 26:Z:72:HIS:HE1   | 28:b:60:VAL:HB    | 1.81                     | 0.45              |
| 34:y:44:ILE:HB    | 34:y:68:HIS:HB2   | 1.99                     | 0.45              |
| 19:S:145:LEU:HD21 | 19:S:182:ALA:HB2  | 1.99                     | 0.44              |
| 22:V:212:TYR:HA   | 22:V:253:LEU:HD11 | 1.98                     | 0.44              |
| 26:Z:15:VAL:HG11  | 26:Z:50:VAL:HG12  | 1.99                     | 0.44              |
| 26:Z:197:GLY:O    | 29:c:225:TRP:NE1  | 2.50                     | 0.44              |
| 27:a:84:VAL:HG11  | 27:a:97:LEU:HD12  | 1.99                     | 0.44              |
| 31:e:33:ASP:HB3   | 31:e:36:ALA:HB2   | 1.99                     | 0.44              |
| 11:k:146:VAL:HG11 | 11:k:222:PRO:HA   | 1.98                     | 0.44              |
| 6:F:358:ASN:O     | 6:F:362:ARG:NH1   | 2.49                     | 0.44              |
| 19:S:187:VAL:HG21 | 15:o:24:MET:HE3   | 2.00                     | 0.44              |
| 21:U:583:MET:HE2  | 21:U:583:MET:HB3  | 1.65                     | 0.44              |
| 23:W:198:ASP:OD1  | 23:W:201:ARG:HB2  | 2.17                     | 0.44              |
| 26:Z:59:ASP:OD2   | 28:b:99:HIS:NE2   | 2.50                     | 0.44              |
| 27:a:84:VAL:HA    | 27:a:87:MET:HG3   | 1.98                     | 0.44              |
| 29:c:159:ALA:H    | 29:c:205:ILE:HD11 | 1.83                     | 0.44              |
| 29:c:195:GLY:HA3  | 29:c:200:TYR:OH   | 2.17                     | 0.44              |
| 32:f:425:GLY:HA3  | 32:f:451:VAL:HG11 | 2.00                     | 0.44              |
| 7:g:132:ARG:HA    | 7:g:133:PRO:HD3   | 1.87                     | 0.44              |
| 12:l:7:ASP:OD1    | 12:l:7:ASP:N      | 2.49                     | 0.44              |
| 2:B:181:GLN:HG2   | 2:B:237:LYS:HE2   | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:223:ILE:HD11  | 2:B:347:ILE:HG21  | 2.00                     | 0.44              |
| 3:C:68:GLU:OE2    | 3:C:117:ARG:NH2   | 2.48                     | 0.44              |
| 3:C:277:LEU:HG    | 3:C:310:ARG:HH22  | 1.81                     | 0.44              |
| 7:G:147:GLN:HE22  | 15:O:72:ARG:HH21  | 1.66                     | 0.44              |
| 21:U:448:LEU:HA   | 21:U:483:LEU:HD23 | 1.99                     | 0.44              |
| 21:U:759:SER:HA   | 21:U:782:ALA:HA   | 2.00                     | 0.44              |
| 26:Z:177:ARG:HA   | 26:Z:180:LYS:HD3  | 1.99                     | 0.44              |
| 29:c:278:GLN:C    | 29:c:280:PRO:CD   | 2.80                     | 0.44              |
| 30:d:15:ASN:HD22  | 30:d:18:LYS:HB3   | 1.83                     | 0.44              |
| 32:f:522:CYS:HB3  | 32:f:534:VAL:HG21 | 1.99                     | 0.44              |
| 32:f:692:LEU:HB3  | 32:f:800:LEU:HD12 | 2.00                     | 0.44              |
| 13:m:136:MET:HE2  | 13:m:148:LEU:HD11 | 1.99                     | 0.44              |
| 2:B:58:CYS:SG     | 2:B:59:ARG:N      | 2.91                     | 0.44              |
| 3:C:277:LEU:O     | 3:C:310:ARG:NH1   | 2.50                     | 0.44              |
| 6:F:321:GLN:HE21  | 6:F:323:ASN:HD21  | 1.66                     | 0.44              |
| 10:J:11:SER:OG    | 10:J:15:HIS:N     | 2.50                     | 0.44              |
| 27:a:97:LEU:HD22  | 27:a:118:ILE:HG13 | 1.99                     | 0.44              |
| 32:f:428:GLN:HA   | 32:f:431:LYS:HE2  | 2.00                     | 0.44              |
| 7:g:231:THR:OG1   | 7:g:234:GLU:OE1   | 2.28                     | 0.44              |
| 14:n:4:MET:HE1    | 14:n:159:ALA:HB3  | 2.00                     | 0.44              |
| 15:o:30:ASN:HD22  | 15:o:30:ASN:C     | 2.25                     | 0.44              |
| 17:q:18:ASP:OD1   | 17:q:18:ASP:N     | 2.48                     | 0.44              |
| 1:A:34:LYS:NZ     | 3:C:173:GLU:OE2   | 2.42                     | 0.44              |
| 1:A:428:ARG:NH2   | 10:J:24:GLU:OE2   | 2.36                     | 0.44              |
| 1:A:430:MET:HE1   | 10:J:156:TRP:HZ2  | 1.81                     | 0.44              |
| 15:O:163:ILE:HG12 | 15:O:170:GLY:HA2  | 1.99                     | 0.44              |
| 26:Z:21:ASP:OD1   | 26:Z:22:HIS:N     | 2.50                     | 0.44              |
| 12:l:72:ILE:HG22  | 12:l:134:ILE:HG12 | 2.00                     | 0.44              |
| 19:s:64:LEU:O     | 19:s:68:ILE:HG12  | 2.17                     | 0.44              |
| 8:H:59:GLU:HG3    | 8:H:206:ASP:HB2   | 1.99                     | 0.44              |
| 8:H:111:VAL:HG22  | 8:H:136:ILE:HD12  | 2.00                     | 0.44              |
| 16:P:190:ILE:HG12 | 16:P:195:ILE:HD12 | 1.99                     | 0.44              |
| 18:R:7:LYS:HD2    | 18:R:109:PRO:HB2  | 2.00                     | 0.44              |
| 23:W:329:ARG:HE   | 23:W:351:TRP:NE1  | 2.16                     | 0.44              |
| 26:Z:82:PHE:HA    | 26:Z:85:VAL:HG12  | 2.00                     | 0.44              |
| 29:c:122:LEU:HD23 | 29:c:201:TYR:CE1  | 2.52                     | 0.44              |
| 30:d:55:LEU:HD23  | 30:d:55:LEU:HA    | 1.85                     | 0.44              |
| 34:y:37:PRO:HA    | 34:y:38:PRO:HD3   | 1.92                     | 0.44              |
| 3:C:168:PRO:HG3   | 3:C:175:PHE:HE2   | 1.83                     | 0.44              |
| 11:K:71:ASP:OD1   | 11:K:71:ASP:N     | 2.51                     | 0.44              |
| 24:X:35:ILE:HD12  | 24:X:46:LYS:HD2   | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:Z:70:LEU:HD11  | 26:Z:108:ILE:HG23 | 2.00                     | 0.44              |
| 1:A:141:GLY:N     | 1:A:151:ILE:O     | 2.40                     | 0.44              |
| 3:C:187:LEU:HB2   | 3:C:311:ILE:HG21  | 2.00                     | 0.44              |
| 3:C:343:ASN:HB3   | 3:C:346:LYS:HD3   | 2.00                     | 0.44              |
| 4:D:385:LEU:HD23  | 4:D:398:ASP:HB2   | 2.00                     | 0.44              |
| 6:F:380:ASN:HB3   | 6:F:383:GLU:HB2   | 1.99                     | 0.44              |
| 8:H:10:LEU:HD13   | 8:H:21:GLN:HB2    | 2.00                     | 0.44              |
| 10:J:185:ASP:OD1  | 10:J:185:ASP:N    | 2.49                     | 0.44              |
| 11:K:41:GLN:HE21  | 11:K:166:ASP:HA   | 1.83                     | 0.44              |
| 21:U:190:ASN:HB3  | 21:U:193:PHE:HE1  | 1.82                     | 0.44              |
| 24:X:255:LEU:HD22 | 24:X:267:VAL:HG13 | 2.00                     | 0.44              |
| 26:Z:260:VAL:O    | 26:Z:264:SER:OG   | 2.30                     | 0.44              |
| 27:a:274:LEU:HD13 | 27:a:319:LEU:HD21 | 1.99                     | 0.44              |
| 27:a:344:GLN:C    | 27:a:346:ILE:N    | 2.76                     | 0.44              |
| 29:c:163:ILE:HG22 | 29:c:200:TYR:HA   | 1.98                     | 0.44              |
| 30:d:22:GLU:HA    | 30:d:25:ARG:HD2   | 1.99                     | 0.44              |
| 17:q:38:MET:O     | 17:q:65:GLN:NE2   | 2.47                     | 0.44              |
| 6:F:438:TYR:OH    | 11:K:19:GLY:O     | 2.34                     | 0.44              |
| 10:J:42:VAL:HG22  | 10:J:210:VAL:HG12 | 1.99                     | 0.44              |
| 20:T:63:LEU:HG    | 20:T:110:MET:HE1  | 1.99                     | 0.44              |
| 9:i:66:TYR:HD2    | 9:i:87:THR:HG21   | 1.81                     | 0.44              |
| 1:A:263:MET:O     | 1:A:266:THR:OG1   | 2.33                     | 0.43              |
| 5:E:124:HIS:O     | 5:E:196:LEU:HG    | 2.18                     | 0.43              |
| 7:G:18:PRO:O      | 7:G:19:GLU:CB     | 2.65                     | 0.43              |
| 7:G:130:GLU:HG2   | 7:G:131:MET:HG2   | 2.00                     | 0.43              |
| 10:J:39:ASP:OD1   | 10:J:39:ASP:N     | 2.50                     | 0.43              |
| 18:R:191:ASN:HD21 | 16:p:203:ARG:HH12 | 1.65                     | 0.43              |
| 21:U:447:GLY:HA3  | 21:U:480:GLY:HA2  | 1.99                     | 0.43              |
| 21:U:794:ASP:OD1  | 21:U:794:ASP:N    | 2.51                     | 0.43              |
| 22:V:416:ARG:NH2  | 25:Y:348:ASP:OD2  | 2.51                     | 0.43              |
| 30:d:215:TRP:HE3  | 30:d:222:TYR:HB3  | 1.83                     | 0.43              |
| 32:f:698:SER:HB2  | 32:f:706:ILE:HD13 | 1.99                     | 0.43              |
| 1:A:347:ASP:N     | 1:A:347:ASP:OD1   | 2.45                     | 0.43              |
| 3:C:207:THR:HG23  | 3:C:209:CYS:H     | 1.83                     | 0.43              |
| 5:E:312:ILE:HD13  | 5:E:340:GLY:HA3   | 1.99                     | 0.43              |
| 9:I:239:LYS:O     | 9:I:242:GLU:N     | 2.51                     | 0.43              |
| 21:U:554:LEU:HA   | 21:U:588:MET:HE1  | 2.00                     | 0.43              |
| 22:V:135:LEU:HD21 | 22:V:171:VAL:HG13 | 1.99                     | 0.43              |
| 23:W:419:LYS:HE3  | 23:W:424:LEU:HD22 | 1.99                     | 0.43              |
| 30:d:51:ALA:HA    | 30:d:54:ILE:HG12  | 1.99                     | 0.43              |
| 12:l:117:GLN:CG   | 13:m:82:ALA:HB1   | 2.48                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:222:GLY:HA3   | 6:F:348:LEU:HA    | 2.01                     | 0.43              |
| 6:F:333:ASN:ND2   | 35:F:501:ATP:O2G  | 2.39                     | 0.43              |
| 9:I:73:ALA:HB3    | 9:I:137:ILE:HD11  | 2.00                     | 0.43              |
| 17:Q:58:GLU:OE1   | 17:Q:62:LYS:NZ    | 2.50                     | 0.43              |
| 22:V:224:LEU:HA   | 22:V:227:VAL:HB   | 2.01                     | 0.43              |
| 23:W:375:MET:HE1  | 23:W:411:GLY:HA2  | 2.00                     | 0.43              |
| 30:d:42:LYS:HA    | 30:d:45:LYS:HB2   | 2.00                     | 0.43              |
| 8:h:3:GLU:N       | 13:m:125:TYR:HB3  | 2.33                     | 0.43              |
| 2:B:291:GLY:HA3   | 2:B:309:MET:HG3   | 2.00                     | 0.43              |
| 3:C:99:VAL:HA     | 3:C:123:LEU:HB2   | 2.01                     | 0.43              |
| 11:K:4:THR:OG1    | 11:K:5:ARG:N      | 2.50                     | 0.43              |
| 18:R:21:THR:HG22  | 18:R:26:ILE:HG12  | 2.01                     | 0.43              |
| 23:W:361:HIS:HA   | 23:W:364:ARG:HH21 | 1.83                     | 0.43              |
| 24:X:182:ASN:ND2  | 25:Y:248:GLU:OE2  | 2.51                     | 0.43              |
| 13:m:43:ASP:OD1   | 13:m:43:ASP:N     | 2.49                     | 0.43              |
| 1:A:65:ILE:HG21   | 32:f:680:ARG:NH1  | 2.33                     | 0.43              |
| 3:C:83:LYS:HB3    | 3:C:99:VAL:HG22   | 2.01                     | 0.43              |
| 5:E:75:ASN:ND2    | 6:F:129:ARG:O     | 2.51                     | 0.43              |
| 13:M:36:ALA:HB2   | 13:M:65:ARG:NH2   | 2.33                     | 0.43              |
| 21:U:191:LYS:HD3  | 21:U:194:ARG:HD3  | 2.01                     | 0.43              |
| 21:U:611:ASN:HB3  | 21:U:614:VAL:HG12 | 2.00                     | 0.43              |
| 26:Z:54:PHE:O     | 26:Z:95:TYR:OH    | 2.36                     | 0.43              |
| 27:a:344:GLN:C    | 27:a:346:ILE:H    | 2.26                     | 0.43              |
| 32:f:658:ALA:O    | 32:f:662:MET:HG2  | 2.17                     | 0.43              |
| 12:l:139:ASP:OD1  | 12:l:139:ASP:N    | 2.52                     | 0.43              |
| 20:t:50:MET:HE2   | 20:t:197:VAL:HG13 | 1.99                     | 0.43              |
| 3:C:86:LEU:HD21   | 3:C:94:LYS:HD2    | 2.00                     | 0.43              |
| 4:D:313:ARG:NH2   | 4:D:316:THR:OG1   | 2.52                     | 0.43              |
| 6:F:92:ASN:N      | 6:F:125:LYS:O     | 2.49                     | 0.43              |
| 9:I:54:LYS:C      | 9:I:55:LEU:HD12   | 2.43                     | 0.43              |
| 22:V:90:GLU:HG2   | 22:V:92:ARG:H     | 1.84                     | 0.43              |
| 22:V:128:ARG:HA   | 22:V:131:LEU:HG   | 1.99                     | 0.43              |
| 23:W:316:ARG:HD3  | 23:W:316:ARG:HA   | 1.43                     | 0.43              |
| 26:Z:190:ARG:HA   | 26:Z:193:ASN:HD22 | 1.83                     | 0.43              |
| 30:d:158:ILE:HG22 | 30:d:160:ALA:H    | 1.83                     | 0.43              |
| 32:f:667:GLY:O    | 32:f:671:ALA:HB2  | 2.19                     | 0.43              |
| 32:f:710:LEU:HB3  | 32:f:729:MET:HG2  | 2.01                     | 0.43              |
| 15:o:163:ILE:HG12 | 15:o:170:GLY:HA2  | 2.00                     | 0.43              |
| 18:r:51:ASP:OD2   | 19:s:100:ARG:NH2  | 2.47                     | 0.43              |
| 6:F:188:ILE:HD13  | 6:F:235:LEU:HD22  | 2.00                     | 0.43              |
| 8:H:49:GLU:O      | 8:H:64:LYS:NZ     | 2.47                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:O:214:GLU:HG3  | 16:P:198:ARG:HG2  | 2.01                     | 0.43              |
| 21:U:688:LEU:HD22 | 21:U:713:TYR:HE1  | 1.83                     | 0.43              |
| 21:U:788:VAL:HG12 | 21:U:909:GLY:HA2  | 2.00                     | 0.43              |
| 23:W:240:TYR:HA   | 23:W:243:ILE:HD12 | 1.99                     | 0.43              |
| 25:Y:212:GLU:HG2  | 25:Y:213:LEU:HD22 | 2.00                     | 0.43              |
| 26:Z:11:VAL:O     | 26:Z:163:GLY:N    | 2.49                     | 0.43              |
| 27:a:26:GLU:HA    | 27:a:29:TYR:CE1   | 2.54                     | 0.43              |
| 10:j:168:VAL:HG23 | 10:j:194:ALA:HB1  | 2.00                     | 0.43              |
| 18:r:32:LYS:HA    | 18:r:32:LYS:HD3   | 1.79                     | 0.43              |
| 2:B:387:LYS:HA    | 2:B:387:LYS:HD3   | 1.88                     | 0.43              |
| 5:E:272:ARG:O     | 5:E:274:LYS:NZ    | 2.52                     | 0.43              |
| 21:U:436:ALA:HB3  | 21:U:472:ILE:HD11 | 2.00                     | 0.43              |
| 32:f:45:LEU:HB3   | 32:f:50:LYS:HD3   | 2.00                     | 0.43              |
| 32:f:505:MET:SD   | 32:f:506:GLY:N    | 2.91                     | 0.43              |
| 16:p:11:VAL:HG23  | 16:p:54:ALA:HB2   | 2.00                     | 0.43              |
| 1:A:220:THR:HG21  | 1:A:343:PHE:HB3   | 2.01                     | 0.43              |
| 3:C:164:VAL:HG13  | 3:C:165:ILE:HG13  | 2.00                     | 0.43              |
| 3:C:251:ILE:H     | 3:C:295:THR:HB    | 1.84                     | 0.43              |
| 5:E:166:PRO:O     | 5:E:293:GLY:HA2   | 2.19                     | 0.43              |
| 5:E:385:ASP:OD1   | 5:E:385:ASP:N     | 2.51                     | 0.43              |
| 6:F:129:ARG:HH22  | 6:F:260:PHE:HB3   | 1.83                     | 0.43              |
| 18:R:41:LEU:HD23  | 18:R:103:GLY:HA3  | 2.01                     | 0.43              |
| 22:V:253:LEU:O    | 22:V:257:ASN:ND2  | 2.52                     | 0.43              |
| 10:j:39:ASP:OD1   | 10:j:39:ASP:N     | 2.52                     | 0.43              |
| 12:l:47:VAL:HG22  | 12:l:212:ILE:HG12 | 1.99                     | 0.43              |
| 34:w:39:ASP:OD1   | 34:w:39:ASP:N     | 2.51                     | 0.43              |
| 34:w:61:ILE:HG23  | 34:w:65:SER:HB2   | 2.00                     | 0.43              |
| 1:A:49:GLU:HA     | 1:A:52:ILE:HG22   | 2.01                     | 0.43              |
| 4:D:207:PRO:HG2   | 4:D:335:LEU:HD11  | 2.01                     | 0.43              |
| 21:U:524:LYS:NZ   | 21:U:562:GLU:O    | 2.39                     | 0.43              |
| 23:W:452:ILE:O    | 23:W:456:GLN:N    | 2.52                     | 0.43              |
| 28:b:62:THR:HG21  | 28:b:71:ILE:HD13  | 2.01                     | 0.43              |
| 29:c:281:LYS:HA   | 29:c:281:LYS:HD3  | 1.66                     | 0.43              |
| 8:h:19:LEU:HD23   | 8:h:19:LEU:HA     | 1.91                     | 0.43              |
| 12:L:192:LEU:HD12 | 12:L:205:LEU:HD13 | 2.01                     | 0.42              |
| 12:L:214:ILE:HD12 | 12:L:224:TYR:HE2  | 1.84                     | 0.42              |
| 22:V:495:ARG:HD3  | 26:Z:282:ASN:HD21 | 1.84                     | 0.42              |
| 28:b:147:GLU:HG2  | 28:b:150:THR:HG22 | 2.01                     | 0.42              |
| 32:f:62:ARG:HH21  | 32:f:74:ALA:HA    | 1.84                     | 0.42              |
| 1:A:59:ILE:HA     | 1:A:62:LEU:HG     | 2.01                     | 0.42              |
| 2:B:188:GLY:HA3   | 2:B:364:ILE:HD13  | 2.00                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:75:ASN:OD1    | 5:E:75:ASN:N      | 2.52                     | 0.42              |
| 10:J:67:ASP:OD1   | 10:J:67:ASP:N     | 2.49                     | 0.42              |
| 22:V:287:ARG:NH2  | 31:e:17:ASP:OD2   | 2.52                     | 0.42              |
| 24:X:70:LEU:HD22  | 24:X:92:LEU:HD13  | 2.01                     | 0.42              |
| 25:Y:231:LEU:HD12 | 25:Y:234:PRO:HG2  | 2.01                     | 0.42              |
| 28:b:97:LEU:HG    | 28:b:100:ARG:HH21 | 1.84                     | 0.42              |
| 31:e:16:ASP:OD1   | 31:e:16:ASP:N     | 2.51                     | 0.42              |
| 15:o:190:THR:HG22 | 15:o:192:PRO:HD3  | 2.01                     | 0.42              |
| 17:q:44:LEU:HD13  | 17:q:104:LEU:HD12 | 2.00                     | 0.42              |
| 2:B:113:GLU:HG2   | 2:B:114:GLU:HG2   | 2.01                     | 0.42              |
| 2:B:360:THR:O     | 2:B:364:ILE:HG12  | 2.19                     | 0.42              |
| 3:C:135:VAL:HA    | 3:C:138:MET:SD    | 2.59                     | 0.42              |
| 19:S:16:ALA:HB2   | 19:S:121:VAL:HG23 | 2.00                     | 0.42              |
| 20:T:79:ASP:OD1   | 20:T:79:ASP:N     | 2.53                     | 0.42              |
| 21:U:185:MET:SD   | 21:U:194:ARG:NH2  | 2.92                     | 0.42              |
| 27:a:81:LEU:HA    | 27:a:84:VAL:HG12  | 2.00                     | 0.42              |
| 15:o:112:SER:HB3  | 15:o:125:VAL:HG11 | 2.01                     | 0.42              |
| 1:A:213:LEU:HD12  | 1:A:337:LEU:HD13  | 2.00                     | 0.42              |
| 5:E:237:ALA:N     | 5:E:242:ARG:HH22  | 2.17                     | 0.42              |
| 13:M:34:SER:OG    | 13:M:35:THR:N     | 2.51                     | 0.42              |
| 14:N:32:ASP:O     | 14:N:45:ARG:NH2   | 2.52                     | 0.42              |
| 17:Q:77:PRO:HD2   | 17:Q:108:ASP:HB2  | 2.02                     | 0.42              |
| 21:U:623:GLY:HA3  | 21:U:658:ILE:HG13 | 2.00                     | 0.42              |
| 22:V:224:LEU:HD12 | 22:V:261:TYR:HE1  | 1.85                     | 0.42              |
| 22:V:228:ARG:HH22 | 22:V:261:TYR:HB2  | 1.84                     | 0.42              |
| 23:W:85:GLU:HA    | 23:W:88:MET:HG3   | 2.00                     | 0.42              |
| 27:a:276:CYS:HB2  | 27:a:280:MET:HE2  | 2.00                     | 0.42              |
| 20:t:53:ALA:HB2   | 20:t:110:MET:HG3  | 2.02                     | 0.42              |
| 34:w:37:PRO:HA    | 34:w:38:PRO:HD3   | 1.90                     | 0.42              |
| 5:E:33:LEU:HA     | 5:E:36:LEU:HG     | 2.01                     | 0.42              |
| 5:E:331:ILE:HD13  | 5:E:367:PHE:HD2   | 1.85                     | 0.42              |
| 13:M:37:ILE:HD11  | 13:M:193:VAL:HG13 | 2.01                     | 0.42              |
| 17:Q:26:VAL:HG21  | 18:R:136:TYR:HE2  | 1.85                     | 0.42              |
| 24:X:422:THR:OXT  | 26:Z:283:ARG:NH2  | 2.52                     | 0.42              |
| 27:a:122:LYS:HD3  | 27:a:130:VAL:HG13 | 2.00                     | 0.42              |
| 30:d:203:PRO:HG2  | 30:d:205:LYS:HB3  | 2.00                     | 0.42              |
| 32:f:99:LEU:HA    | 32:f:102:HIS:HB2  | 2.01                     | 0.42              |
| 9:i:151:ASP:OD1   | 9:i:155:ASN:N     | 2.53                     | 0.42              |
| 34:z:74:ARG:CA    | 34:z:74:ARG:HE    | 2.33                     | 0.42              |
| 5:E:173:TYR:HB2   | 5:E:388:PRO:HB2   | 2.01                     | 0.42              |
| 10:J:31:THR:OG1   | 10:J:163:ARG:O    | 2.38                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:W:203:GLN:HE21 | 23:W:203:GLN:HB3  | 1.72                     | 0.42              |
| 25:Y:32:ARG:HH12  | 25:Y:61:LEU:HD22  | 1.84                     | 0.42              |
| 26:Z:187:LEU:HD23 | 26:Z:187:LEU:HA   | 1.94                     | 0.42              |
| 27:a:245:VAL:HG21 | 27:a:301:LYS:HG2  | 2.00                     | 0.42              |
| 28:b:131:LEU:HD22 | 28:b:136:VAL:HB   | 2.00                     | 0.42              |
| 30:d:49:ILE:HD12  | 30:d:52:ARG:HH21  | 1.85                     | 0.42              |
| 7:g:138:MET:HB2   | 7:g:154:CYS:HB2   | 2.01                     | 0.42              |
| 9:i:197:LEU:HA    | 9:i:200:THR:HG22  | 2.02                     | 0.42              |
| 11:k:90:ASP:OD1   | 18:r:69:ARG:NH2   | 2.45                     | 0.42              |
| 16:p:2:SER:OG     | 16:p:3:ILE:N      | 2.52                     | 0.42              |
| 2:B:293:LYS:HA    | 2:B:338:ASP:HA    | 2.02                     | 0.42              |
| 4:D:200:ARG:HH22  | 4:D:302:ASN:HA    | 1.85                     | 0.42              |
| 4:D:212:LYS:NZ    | 4:D:311:THR:O     | 2.52                     | 0.42              |
| 4:D:300:ASP:OD1   | 4:D:300:ASP:N     | 2.51                     | 0.42              |
| 7:G:138:MET:SD    | 7:G:140:LEU:HG    | 2.60                     | 0.42              |
| 18:R:192:VAL:HG11 | 16:p:205:ASP:HB3  | 2.00                     | 0.42              |
| 19:S:10:GLY:HA3   | 19:S:42:LYS:HE2   | 2.00                     | 0.42              |
| 22:V:337:LEU:HD22 | 22:V:367:VAL:HG11 | 2.02                     | 0.42              |
| 24:X:103:THR:HA   | 24:X:106:GLU:CB   | 2.44                     | 0.42              |
| 26:Z:102:HIS:CD2  | 26:Z:104:ASN:HB3  | 2.55                     | 0.42              |
| 29:c:36:LEU:HD11  | 29:c:71:ASP:HA    | 2.01                     | 0.42              |
| 29:c:197:ASN:O    | 29:c:200:TYR:N    | 2.52                     | 0.42              |
| 1:A:301:GLU:HB2   | 6:F:254:PRO:HG2   | 2.02                     | 0.42              |
| 1:A:429:TYR:OH    | 11:K:33:LEU:O     | 2.38                     | 0.42              |
| 2:B:232:LYS:HG2   | 2:B:353:PHE:HD2   | 1.84                     | 0.42              |
| 4:D:60:TYR:HB2    | 21:U:603:LEU:HD21 | 2.01                     | 0.42              |
| 4:D:335:LEU:CB    | 4:D:336:PRO:CD    | 2.95                     | 0.42              |
| 14:N:120:MET:HE3  | 14:N:120:MET:HB3  | 1.93                     | 0.42              |
| 24:X:254:MET:HE1  | 24:X:270:LEU:HD13 | 2.01                     | 0.42              |
| 26:Z:9:VAL:HG23   | 26:Z:48:LEU:HD22  | 2.00                     | 0.42              |
| 26:Z:275:LEU:HD22 | 26:Z:279:LYS:HE2  | 2.01                     | 0.42              |
| 29:c:206:ASN:OD1  | 29:c:206:ASN:N    | 2.51                     | 0.42              |
| 30:d:106:LEU:HG   | 30:d:111:ARG:HB2  | 2.01                     | 0.42              |
| 7:g:58:ASP:OD1    | 7:g:58:ASP:N      | 2.49                     | 0.42              |
| 7:g:86:ASP:OD1    | 13:m:120:HIS:NE2  | 2.37                     | 0.42              |
| 13:m:230:ASP:OD1  | 13:m:230:ASP:N    | 2.52                     | 0.42              |
| 18:r:135:ALA:O    | 18:r:139:MET:HB2  | 2.20                     | 0.42              |
| 34:z:25:ASN:O     | 34:z:29:LYS:HG3   | 2.19                     | 0.42              |
| 10:J:146:GLN:NE2  | 10:J:147:THR:O    | 2.52                     | 0.42              |
| 12:L:115:LYS:NZ   | 12:L:128:TYR:OH   | 2.53                     | 0.42              |
| 15:O:164:PHE:O    | 19:s:38:ARG:NH2   | 2.46                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:P:14:MET:HG2   | 16:P:136:PHE:HB3  | 2.02                     | 0.42              |
| 17:Q:18:ASP:N     | 17:Q:18:ASP:OD1   | 2.50                     | 0.42              |
| 20:T:27:LEU:HD11  | 20:T:34:ALA:HB1   | 2.02                     | 0.42              |
| 22:V:410:ILE:HG21 | 22:V:422:ILE:HG13 | 2.02                     | 0.42              |
| 22:V:494:MET:HE1  | 26:Z:274:ASN:HB3  | 2.02                     | 0.42              |
| 26:Z:97:THR:OG1   | 26:Z:98:GLY:N     | 2.53                     | 0.42              |
| 27:a:91:ASN:OD1   | 27:a:92:VAL:N     | 2.53                     | 0.42              |
| 28:b:6:THR:HB     | 28:b:49:VAL:HG22  | 2.02                     | 0.42              |
| 34:w:5:VAL:HG22   | 34:w:67:LEU:HB2   | 2.02                     | 0.42              |
| 2:B:122:ILE:HD11  | 2:B:130:GLU:HB3   | 2.02                     | 0.42              |
| 4:D:336:PRO:O     | 4:D:337:ASP:C     | 2.62                     | 0.42              |
| 6:F:332:THR:HG21  | 6:F:338:LEU:HD11  | 2.02                     | 0.42              |
| 23:W:79:GLU:HG3   | 23:W:82:LEU:HB2   | 2.01                     | 0.42              |
| 15:o:187:ARG:HB3  | 15:o:188:PRO:HD3  | 2.02                     | 0.42              |
| 16:p:204:MET:HE2  | 16:p:204:MET:HB2  | 1.96                     | 0.42              |
| 18:r:74:ILE:HG23  | 18:r:78:ALA:HB3   | 2.02                     | 0.42              |
| 19:s:145:LEU:HD22 | 19:s:178:VAL:HB   | 2.02                     | 0.42              |
| 20:t:124:TYR:HE1  | 20:t:139:THR:HG22 | 1.85                     | 0.42              |
| 34:y:44:ILE:HD13  | 34:y:49:GLN:HA    | 2.02                     | 0.42              |
| 4:D:118:THR:O     | 29:c:277:LYS:NZ   | 2.53                     | 0.41              |
| 22:V:313:LEU:HD13 | 22:V:328:VAL:HG11 | 2.02                     | 0.41              |
| 28:b:180:ALA:HB1  | 28:b:183:LEU:HB2  | 2.02                     | 0.41              |
| 30:d:4:GLN:HB2    | 30:d:25:ARG:HH22  | 1.85                     | 0.41              |
| 32:f:478:ARG:HH12 | 32:f:509:LYS:HD2  | 1.85                     | 0.41              |
| 7:g:60:LEU:HD21   | 13:m:177:GLU:HG3  | 2.02                     | 0.41              |
| 10:j:229:VAL:O    | 10:j:233:GLU:HG2  | 2.20                     | 0.41              |
| 11:k:41:GLN:NE2   | 11:k:151:PRO:O    | 2.53                     | 0.41              |
| 15:o:63:LEU:HD23  | 15:o:63:LEU:HA    | 1.90                     | 0.41              |
| 16:p:47:ASP:OD1   | 16:p:47:ASP:N     | 2.53                     | 0.41              |
| 18:r:71:LYS:HE3   | 18:r:71:LYS:HA    | 2.02                     | 0.41              |
| 1:A:377:CYS:HB2   | 1:A:380:SER:HB3   | 2.02                     | 0.41              |
| 6:F:247:THR:HG21  | 6:F:278:LYS:HG2   | 2.02                     | 0.41              |
| 7:G:175:SER:OG    | 7:G:201:CYS:SG    | 2.75                     | 0.41              |
| 10:J:189:LYS:HA   | 10:J:232:ILE:HD11 | 2.02                     | 0.41              |
| 22:V:476:PHE:HB3  | 26:Z:260:VAL:HG21 | 2.03                     | 0.41              |
| 29:c:68:ARG:HE    | 29:c:208:ARG:HH12 | 1.66                     | 0.41              |
| 32:f:258:LYS:HA   | 32:f:258:LYS:HD3  | 1.86                     | 0.41              |
| 16:p:30:ILE:HG22  | 16:p:31:GLN:HG2   | 2.01                     | 0.41              |
| 3:C:155:ASP:OD1   | 3:C:156:LYS:N     | 2.54                     | 0.41              |
| 4:D:156:SER:O     | 4:D:157:ASP:CB    | 2.69                     | 0.41              |
| 6:F:226:TYR:CZ    | 6:F:353:GLU:HB3   | 2.55                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:I:90:LEU:HD21   | 9:I:114:LEU:HD22  | 2.02                     | 0.41              |
| 11:K:12:VAL:HG12  | 11:K:23:GLN:HG2   | 2.03                     | 0.41              |
| 21:U:862:LYS:HB3  | 21:U:862:LYS:HE2  | 1.93                     | 0.41              |
| 22:V:201:ARG:NH2  | 22:V:241:ARG:O    | 2.52                     | 0.41              |
| 26:Z:67:VAL:HG12  | 28:b:95:LEU:HD22  | 2.03                     | 0.41              |
| 28:b:56:ASN:N     | 28:b:83:LYS:O     | 2.54                     | 0.41              |
| 32:f:658:ALA:HB2  | 32:f:693:ALA:HB1  | 2.03                     | 0.41              |
| 9:i:201:MET:HE3   | 9:i:201:MET:HB2   | 1.93                     | 0.41              |
| 20:t:92:LEU:HD23  | 20:t:92:LEU:HA    | 1.92                     | 0.41              |
| 2:B:264:PRO:HB3   | 2:B:311:GLU:HG2   | 2.03                     | 0.41              |
| 21:U:632:GLN:HE21 | 21:U:636:VAL:HG11 | 1.84                     | 0.41              |
| 22:V:419:LEU:HD12 | 22:V:456:GLY:HA2  | 2.02                     | 0.41              |
| 23:W:235:GLN:HG2  | 23:W:350:ARG:NH2  | 2.36                     | 0.41              |
| 26:Z:45:LYS:HB3   | 26:Z:47:VAL:HG12  | 2.02                     | 0.41              |
| 27:a:289:ARG:HB2  | 27:a:333:MET:HB3  | 2.02                     | 0.41              |
| 28:b:109:ILE:HB   | 28:b:138:VAL:HG22 | 2.01                     | 0.41              |
| 8:h:9:SER:HA      | 8:h:125:GLY:HA2   | 2.02                     | 0.41              |
| 34:w:6:LYS:O      | 34:w:69:LEU:N     | 2.48                     | 0.41              |
| 4:D:107:THR:HG22  | 5:E:77:PRO:HG3    | 2.01                     | 0.41              |
| 23:W:397:VAL:HG11 | 24:X:341:PRO:HA   | 2.02                     | 0.41              |
| 23:W:408:ARG:HD3  | 24:X:345:VAL:HG23 | 2.01                     | 0.41              |
| 25:Y:262:SER:HA   | 25:Y:267:ARG:HB2  | 2.01                     | 0.41              |
| 26:Z:196:HIS:HA   | 26:Z:199:LYS:HB2  | 2.02                     | 0.41              |
| 30:d:47:GLN:H     | 30:d:47:GLN:NE2   | 2.18                     | 0.41              |
| 32:f:269:ALA:HB1  | 32:f:278:VAL:HG22 | 2.03                     | 0.41              |
| 14:n:178:ALA:HB3  | 14:n:185:GLU:HG2  | 2.01                     | 0.41              |
| 15:o:124:TYR:HE2  | 15:o:135:MET:HE1  | 1.85                     | 0.41              |
| 15:o:203:ARG:NH1  | 15:o:205:GLU:OE1  | 2.42                     | 0.41              |
| 34:y:27:LYS:HB3   | 34:y:38:PRO:HB3   | 2.02                     | 0.41              |
| 1:A:213:LEU:HB3   | 1:A:340:LYS:HD3   | 2.03                     | 0.41              |
| 2:B:31:THR:HG23   | 2:B:32:ARG:HG2    | 2.03                     | 0.41              |
| 4:D:57:GLN:O      | 4:D:61:ILE:HG12   | 2.20                     | 0.41              |
| 5:E:247:THR:O     | 5:E:249:ALA:N     | 2.49                     | 0.41              |
| 9:I:46:ALA:HB1    | 9:I:197:LEU:HD11  | 2.02                     | 0.41              |
| 22:V:127:THR:HG22 | 22:V:194:LYS:HE2  | 2.01                     | 0.41              |
| 11:k:20:ARG:HD3   | 11:k:20:ARG:HA    | 1.93                     | 0.41              |
| 13:m:35:THR:HA    | 13:m:166:GLY:HA3  | 2.02                     | 0.41              |
| 13:m:179:LEU:HD21 | 13:m:192:GLU:HB3  | 2.02                     | 0.41              |
| 17:q:19:ARG:HD3   | 17:q:177:THR:HG22 | 2.01                     | 0.41              |
| 1:A:206:ILE:HG22  | 6:F:373:MET:HE3   | 2.03                     | 0.41              |
| 4:D:309:MET:HE3   | 4:D:327:LEU:HD11  | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:R:93:MET:HE2   | 18:R:93:MET:HB3   | 1.85                     | 0.41              |
| 22:V:221:LEU:HB3  | 22:V:223:LYS:HE3  | 2.03                     | 0.41              |
| 26:Z:259:VAL:HG13 | 29:c:292:MET:HE1  | 2.03                     | 0.41              |
| 29:c:173:GLU:HG3  | 29:c:175:ARG:HB2  | 2.01                     | 0.41              |
| 16:p:4:MET:HE3    | 16:p:4:MET:HB3    | 1.80                     | 0.41              |
| 34:y:17:VAL:HG12  | 34:y:29:LYS:HE3   | 2.02                     | 0.41              |
| 3:C:49:ARG:HD2    | 21:U:639:LEU:HD21 | 2.03                     | 0.41              |
| 4:D:159:LYS:HZ3   | 4:D:160:PRO:HD3   | 1.86                     | 0.41              |
| 5:E:195:PHE:O     | 5:E:196:LEU:O     | 2.39                     | 0.41              |
| 11:K:32:LYS:NZ    | 11:K:175:GLU:OE1  | 2.54                     | 0.41              |
| 17:Q:155:ARG:HA   | 17:Q:158:GLU:HG2  | 2.01                     | 0.41              |
| 26:Z:74:TYR:HE1   | 29:c:98:MET:HB2   | 1.85                     | 0.41              |
| 8:h:14:SER:HB3    | 8:h:18:LYS:H      | 1.85                     | 0.41              |
| 12:l:81:ALA:HB2   | 12:l:130:VAL:HG21 | 2.02                     | 0.41              |
| 17:q:22:ALA:HA    | 17:q:27:GLN:HA    | 2.03                     | 0.41              |
| 1:A:254:ALA:O     | 1:A:258:ARG:HG3   | 2.21                     | 0.41              |
| 4:D:163:MET:HE1   | 4:D:165:ALA:HB3   | 2.02                     | 0.41              |
| 4:D:344:ILE:HG22  | 4:D:375:ILE:HG21  | 2.02                     | 0.41              |
| 5:E:252:GLU:HA    | 5:E:255:ARG:HH21  | 1.85                     | 0.41              |
| 6:F:343:LEU:O     | 6:F:345:SER:N     | 2.54                     | 0.41              |
| 13:M:169:ARG:HE   | 13:M:169:ARG:HB2  | 1.75                     | 0.41              |
| 13:M:230:ASP:OD1  | 13:M:231:ILE:N    | 2.54                     | 0.41              |
| 18:R:122:SER:OG   | 18:R:123:GLY:N    | 2.54                     | 0.41              |
| 20:T:179:ARG:NH1  | 14:n:27:ALA:O     | 2.53                     | 0.41              |
| 25:Y:91:ALA:HB1   | 25:Y:100:ILE:HG22 | 2.03                     | 0.41              |
| 26:Z:198:LEU:HD21 | 27:a:360:VAL:HG13 | 2.03                     | 0.41              |
| 29:c:196:LEU:HD22 | 29:c:196:LEU:HA   | 1.73                     | 0.41              |
| 29:c:222:LYS:HD3  | 29:c:222:LYS:HA   | 1.88                     | 0.41              |
| 16:p:159:ASP:OD1  | 16:p:159:ASP:N    | 2.54                     | 0.41              |
| 19:s:19:ASP:OD1   | 19:s:19:ASP:N     | 2.54                     | 0.41              |
| 20:t:20:VAL:HG23  | 20:t:120:SER:HB3  | 2.03                     | 0.41              |
| 20:t:126:ASP:OD1  | 20:t:130:VAL:N    | 2.53                     | 0.41              |
| 34:y:15:LEU:HD22  | 34:y:29:LYS:HB3   | 2.01                     | 0.41              |
| 1:A:393:GLY:O     | 1:A:397:ILE:HG13  | 2.21                     | 0.41              |
| 1:A:394:MET:HE2   | 2:B:199:GLU:HB3   | 2.03                     | 0.41              |
| 2:B:248:LEU:HD12  | 2:B:282:VAL:HG22  | 2.03                     | 0.41              |
| 3:C:100:ASP:H     | 3:C:103:ILE:HD11  | 1.86                     | 0.41              |
| 21:U:530:GLU:HA   | 21:U:533:VAL:HG22 | 2.03                     | 0.41              |
| 26:Z:39:LEU:H     | 26:Z:94:TRP:HA    | 1.86                     | 0.41              |
| 27:a:12:GLN:HG3   | 27:a:22:TRP:CD1   | 2.56                     | 0.41              |
| 27:a:190:VAL:HA   | 27:a:193:GLN:HB2  | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:b:25:ARG:HH22  | 28:b:145:GLU:HB3  | 1.86                     | 0.41              |
| 30:d:11:ARG:HG3   | 30:d:12:LYS:H     | 1.86                     | 0.41              |
| 9:i:49:ARG:NH1    | 9:i:209:GLU:O     | 2.54                     | 0.41              |
| 15:o:41:ILE:HG12  | 15:o:76:VAL:HG22  | 2.02                     | 0.41              |
| 16:p:87:LEU:HA    | 16:p:90:MET:HG2   | 2.03                     | 0.41              |
| 17:q:19:ARG:HD2   | 17:q:179:SER:HB3  | 2.03                     | 0.41              |
| 18:r:11:GLY:HA2   | 18:r:104:TRP:HZ3  | 1.86                     | 0.41              |
| 3:C:18:SER:HA     | 3:C:22:GLN:HB2    | 2.03                     | 0.40              |
| 4:D:81:ARG:HH12   | 29:c:152:LYS:C    | 2.28                     | 0.40              |
| 16:P:58:THR:O     | 17:Q:85:ARG:NH2   | 2.54                     | 0.40              |
| 21:U:836:THR:HG22 | 32:f:607:LEU:HD21 | 2.04                     | 0.40              |
| 21:U:919:GLU:HG3  | 21:U:920:ASP:H    | 1.86                     | 0.40              |
| 24:X:157:LEU:HD23 | 24:X:157:LEU:HA   | 1.91                     | 0.40              |
| 30:d:179:ALA:HA   | 30:d:182:ILE:HG22 | 2.03                     | 0.40              |
| 1:A:68:SER:HB3    | 3:C:80:MET:HE1    | 2.03                     | 0.40              |
| 1:A:103:ASN:HA    | 1:A:136:GLU:HG2   | 2.02                     | 0.40              |
| 5:E:198:VAL:HB    | 5:E:232:MET:HA    | 2.03                     | 0.40              |
| 6:F:224:LEU:HB3   | 6:F:348:LEU:HG    | 2.02                     | 0.40              |
| 18:R:46:ALA:HB3   | 18:R:98:GLY:HA3   | 2.04                     | 0.40              |
| 21:U:363:SER:OG   | 21:U:365:CYS:SG   | 2.70                     | 0.40              |
| 21:U:835:ILE:HB   | 21:U:838:LYS:HE3  | 2.03                     | 0.40              |
| 24:X:55:SER:HA    | 24:X:95:LEU:HD23  | 2.04                     | 0.40              |
| 24:X:368:MET:HG3  | 24:X:374:PHE:HB3  | 2.03                     | 0.40              |
| 28:b:8:VAL:HA     | 28:b:110:ILE:HG13 | 2.03                     | 0.40              |
| 32:f:384:ALA:HA   | 32:f:419:LEU:HB3  | 2.03                     | 0.40              |
| 1:A:346:PRO:HB3   | 1:A:350:GLY:HA3   | 2.03                     | 0.40              |
| 4:D:414:HIS:O     | 4:D:416:PHE:N     | 2.53                     | 0.40              |
| 9:I:8:ARG:H       | 9:I:8:ARG:HG3     | 1.69                     | 0.40              |
| 11:K:50:VAL:HB    | 11:K:66:LYS:HD3   | 2.04                     | 0.40              |
| 12:L:72:ILE:HG22  | 12:L:134:ILE:HG12 | 2.03                     | 0.40              |
| 22:V:465:ASP:OD1  | 22:V:466:ILE:N    | 2.50                     | 0.40              |
| 24:X:356:LEU:HD12 | 24:X:356:LEU:HA   | 1.89                     | 0.40              |
| 25:Y:283:LYS:HD2  | 25:Y:288:PHE:CE1  | 2.57                     | 0.40              |
| 26:Z:72:HIS:NE2   | 26:Z:111:LEU:HD21 | 2.37                     | 0.40              |
| 29:c:162:LEU:HD13 | 29:c:200:TYR:CD1  | 2.55                     | 0.40              |
| 9:i:218:ARG:NH1   | 9:i:223:THR:OG1   | 2.50                     | 0.40              |
| 15:o:216:ILE:HD11 | 16:p:194:LYS:HD2  | 2.03                     | 0.40              |
| 3:C:394:ASP:OD1   | 3:C:394:ASP:N     | 2.54                     | 0.40              |
| 18:R:37:ILE:HG23  | 18:R:60:ALA:HB2   | 2.04                     | 0.40              |
| 23:W:194:LEU:HG   | 23:W:202:THR:HG21 | 2.04                     | 0.40              |
| 23:W:349:LYS:HE3  | 23:W:349:LYS:HB3  | 1.96                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 26:Z:74:TYR:CE1   | 29:c:98:MET:HB2  | 2.56                     | 0.40              |
| 27:a:78:GLU:O     | 27:a:82:HIS:ND1  | 2.48                     | 0.40              |
| 32:f:378:ASN:OD1  | 32:f:382:ASN:ND2 | 2.54                     | 0.40              |
| 16:p:159:ASP:OD1  | 16:p:162:HIS:ND1 | 2.55                     | 0.40              |
| 1:A:113:ILE:HD11  | 1:A:149:ILE:HD11 | 2.03                     | 0.40              |
| 2:B:217:LYS:HE3   | 2:B:217:LYS:HB2  | 1.85                     | 0.40              |
| 4:D:133:HIS:HB3   | 4:D:137:ASN:H    | 1.86                     | 0.40              |
| 22:V:228:ARG:HH21 | 22:V:258:TYR:HA  | 1.87                     | 0.40              |
| 23:W:361:HIS:HA   | 23:W:364:ARG:HE  | 1.87                     | 0.40              |
| 24:X:400:ALA:O    | 24:X:403:THR:OG1 | 2.37                     | 0.40              |
| 26:Z:31:ASN:HA    | 26:Z:33:LYS:HZ2  | 1.85                     | 0.40              |
| 32:f:333:LEU:HD12 | 32:f:333:LEU:HA  | 1.94                     | 0.40              |
| 34:y:45:PHE:HB3   | 34:y:50:LEU:HD21 | 2.03                     | 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   | A     | 411/433 (95%) | 377 (92%) | 34 (8%)  | 0        | 100         | 100 |
| 2   | B     | 409/440 (93%) | 367 (90%) | 42 (10%) | 0        | 100         | 100 |
| 3   | C     | 394/398 (99%) | 357 (91%) | 35 (9%)  | 2 (0%)   | 24          | 56  |
| 4   | D     | 378/418 (90%) | 322 (85%) | 51 (14%) | 5 (1%)   | 9           | 38  |
| 5   | E     | 387/403 (96%) | 329 (85%) | 57 (15%) | 1 (0%)   | 36          | 65  |
| 6   | F     | 391/439 (89%) | 352 (90%) | 37 (10%) | 2 (0%)   | 24          | 56  |
| 7   | G     | 238/246 (97%) | 222 (93%) | 14 (6%)  | 2 (1%)   | 16          | 48  |
| 7   | g     | 242/246 (98%) | 229 (95%) | 13 (5%)  | 0        | 100         | 100 |
| 8   | H     | 230/234 (98%) | 218 (95%) | 12 (5%)  | 0        | 100         | 100 |
| 8   | h     | 230/234 (98%) | 219 (95%) | 11 (5%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 9   | I     | 246/261 (94%)  | 234 (95%) | 12 (5%)  | 0        | 100         | 100 |
| 9   | i     | 248/261 (95%)  | 242 (98%) | 6 (2%)   | 0        | 100         | 100 |
| 10  | J     | 237/248 (96%)  | 227 (96%) | 10 (4%)  | 0        | 100         | 100 |
| 10  | j     | 237/248 (96%)  | 226 (95%) | 10 (4%)  | 1 (0%)   | 30          | 60  |
| 11  | K     | 236/241 (98%)  | 229 (97%) | 7 (3%)   | 0        | 100         | 100 |
| 11  | k     | 232/241 (96%)  | 224 (97%) | 8 (3%)   | 0        | 100         | 100 |
| 12  | L     | 238/263 (90%)  | 228 (96%) | 10 (4%)  | 0        | 100         | 100 |
| 12  | l     | 236/263 (90%)  | 228 (97%) | 8 (3%)   | 0        | 100         | 100 |
| 13  | M     | 241/255 (94%)  | 230 (95%) | 10 (4%)  | 1 (0%)   | 30          | 60  |
| 13  | m     | 238/255 (93%)  | 231 (97%) | 7 (3%)   | 0        | 100         | 100 |
| 14  | N     | 201/239 (84%)  | 195 (97%) | 6 (3%)   | 0        | 100         | 100 |
| 14  | n     | 200/239 (84%)  | 195 (98%) | 5 (2%)   | 0        | 100         | 100 |
| 15  | O     | 218/277 (79%)  | 211 (97%) | 7 (3%)   | 0        | 100         | 100 |
| 15  | o     | 218/277 (79%)  | 211 (97%) | 7 (3%)   | 0        | 100         | 100 |
| 16  | P     | 202/205 (98%)  | 195 (96%) | 7 (4%)   | 0        | 100         | 100 |
| 16  | p     | 202/205 (98%)  | 194 (96%) | 8 (4%)   | 0        | 100         | 100 |
| 17  | Q     | 198/201 (98%)  | 193 (98%) | 5 (2%)   | 0        | 100         | 100 |
| 17  | q     | 197/201 (98%)  | 191 (97%) | 6 (3%)   | 0        | 100         | 100 |
| 18  | R     | 199/263 (76%)  | 192 (96%) | 7 (4%)   | 0        | 100         | 100 |
| 18  | r     | 199/263 (76%)  | 193 (97%) | 6 (3%)   | 0        | 100         | 100 |
| 19  | S     | 211/241 (88%)  | 203 (96%) | 8 (4%)   | 0        | 100         | 100 |
| 19  | s     | 211/241 (88%)  | 202 (96%) | 9 (4%)   | 0        | 100         | 100 |
| 20  | T     | 214/264 (81%)  | 209 (98%) | 5 (2%)   | 0        | 100         | 100 |
| 20  | t     | 214/264 (81%)  | 207 (97%) | 7 (3%)   | 0        | 100         | 100 |
| 21  | U     | 874/953 (92%)  | 822 (94%) | 52 (6%)  | 0        | 100         | 100 |
| 22  | V     | 442/534 (83%)  | 427 (97%) | 15 (3%)  | 0        | 100         | 100 |
| 23  | W     | 439/456 (96%)  | 431 (98%) | 8 (2%)   | 0        | 100         | 100 |
| 24  | X     | 420/422 (100%) | 403 (96%) | 14 (3%)  | 3 (1%)   | 18          | 50  |
| 25  | Y     | 387/389 (100%) | 368 (95%) | 19 (5%)  | 0        | 100         | 100 |
| 26  | Z     | 284/324 (88%)  | 253 (89%) | 29 (10%) | 2 (1%)   | 18          | 50  |
| 27  | a     | 371/376 (99%)  | 337 (91%) | 29 (8%)  | 5 (1%)   | 9           | 38  |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 28  | b     | 189/377 (50%)     | 170 (90%)   | 19 (10%) | 0        | 100         | 100 |
| 29  | c     | 285/310 (92%)     | 242 (85%)   | 35 (12%) | 8 (3%)   | 4           | 27  |
| 30  | d     | 255/350 (73%)     | 217 (85%)   | 38 (15%) | 0        | 100         | 100 |
| 31  | e     | 48/70 (69%)       | 39 (81%)    | 9 (19%)  | 0        | 100         | 100 |
| 32  | f     | 840/908 (92%)     | 819 (98%)   | 21 (2%)  | 0        | 100         | 100 |
| 34  | w     | 74/76 (97%)       | 72 (97%)    | 2 (3%)   | 0        | 100         | 100 |
| 34  | x     | 74/76 (97%)       | 73 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 34  | y     | 74/76 (97%)       | 73 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 34  | z     | 74/76 (97%)       | 64 (86%)    | 9 (12%)  | 1 (1%)   | 9           | 37  |
| All | All   | 13713/15180 (90%) | 12892 (94%) | 788 (6%) | 33 (0%)  | 44          | 72  |

All (33) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 159 | LYS  |
| 4   | D     | 335 | LEU  |
| 5   | E     | 196 | LEU  |
| 7   | G     | 19  | GLU  |
| 24  | X     | 318 | ILE  |
| 26  | Z     | 145 | HIS  |
| 27  | a     | 343 | LEU  |
| 27  | a     | 344 | GLN  |
| 29  | c     | 196 | LEU  |
| 29  | c     | 197 | ASN  |
| 29  | c     | 202 | SER  |
| 29  | c     | 280 | PRO  |
| 29  | c     | 286 | GLU  |
| 4   | D     | 160 | PRO  |
| 6   | F     | 326 | VAL  |
| 27  | a     | 345 | GLN  |
| 10  | j     | 50  | VAL  |
| 3   | C     | 90  | HIS  |
| 4   | D     | 157 | ASP  |
| 4   | D     | 336 | PRO  |
| 27  | a     | 69  | HIS  |
| 27  | a     | 342 | ASP  |
| 29  | c     | 200 | TYR  |
| 34  | z     | 35  | GLY  |
| 13  | M     | 34  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | Z     | 146 | ASP  |
| 29  | c     | 285 | GLU  |
| 24  | X     | 106 | GLU  |
| 3   | C     | 91  | PRO  |
| 6   | F     | 87  | PRO  |
| 29  | c     | 233 | ASP  |
| 7   | G     | 20  | GLY  |
| 24  | X     | 107 | 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   | A     | 348/372 (94%) | 346 (99%)  | 2 (1%)   | 78          | 79  |
| 2   | B     | 357/385 (93%) | 356 (100%) | 1 (0%)   | 86          | 83  |
| 3   | C     | 340/346 (98%) | 337 (99%)  | 3 (1%)   | 70          | 75  |
| 4   | D     | 333/366 (91%) | 332 (100%) | 1 (0%)   | 86          | 83  |
| 5   | E     | 341/353 (97%) | 341 (100%) | 0        | 100         | 100 |
| 6   | F     | 340/379 (90%) | 336 (99%)  | 4 (1%)   | 63          | 72  |
| 7   | G     | 202/210 (96%) | 201 (100%) | 1 (0%)   | 81          | 80  |
| 7   | g     | 201/210 (96%) | 201 (100%) | 0        | 100         | 100 |
| 8   | H     | 187/191 (98%) | 187 (100%) | 0        | 100         | 100 |
| 8   | h     | 188/191 (98%) | 186 (99%)  | 2 (1%)   | 65          | 73  |
| 9   | I     | 202/221 (91%) | 200 (99%)  | 2 (1%)   | 68          | 74  |
| 9   | i     | 206/221 (93%) | 206 (100%) | 0        | 100         | 100 |
| 10  | J     | 197/211 (93%) | 197 (100%) | 0        | 100         | 100 |
| 10  | j     | 196/211 (93%) | 196 (100%) | 0        | 100         | 100 |
| 11  | K     | 197/203 (97%) | 197 (100%) | 0        | 100         | 100 |
| 11  | k     | 195/203 (96%) | 195 (100%) | 0        | 100         | 100 |
| 12  | L     | 202/224 (90%) | 202 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 12  | l     | 201/224 (90%)  | 199 (99%)  | 2 (1%)   | 68          | 74  |
| 13  | M     | 199/212 (94%)  | 198 (100%) | 1 (0%)   | 81          | 80  |
| 13  | m     | 198/212 (93%)  | 198 (100%) | 0        | 100         | 100 |
| 14  | N     | 158/181 (87%)  | 158 (100%) | 0        | 100         | 100 |
| 14  | n     | 156/181 (86%)  | 156 (100%) | 0        | 100         | 100 |
| 15  | O     | 178/228 (78%)  | 178 (100%) | 0        | 100         | 100 |
| 15  | o     | 181/228 (79%)  | 180 (99%)  | 1 (1%)   | 78          | 79  |
| 16  | P     | 172/174 (99%)  | 172 (100%) | 0        | 100         | 100 |
| 16  | p     | 173/174 (99%)  | 173 (100%) | 0        | 100         | 100 |
| 17  | Q     | 169/171 (99%)  | 167 (99%)  | 2 (1%)   | 63          | 72  |
| 17  | q     | 166/171 (97%)  | 166 (100%) | 0        | 100         | 100 |
| 18  | R     | 156/202 (77%)  | 156 (100%) | 0        | 100         | 100 |
| 18  | r     | 154/202 (76%)  | 154 (100%) | 0        | 100         | 100 |
| 19  | S     | 175/199 (88%)  | 175 (100%) | 0        | 100         | 100 |
| 19  | s     | 177/199 (89%)  | 177 (100%) | 0        | 100         | 100 |
| 20  | T     | 178/215 (83%)  | 178 (100%) | 0        | 100         | 100 |
| 20  | t     | 179/215 (83%)  | 179 (100%) | 0        | 100         | 100 |
| 21  | U     | 752/816 (92%)  | 752 (100%) | 0        | 100         | 100 |
| 22  | V     | 390/460 (85%)  | 390 (100%) | 0        | 100         | 100 |
| 23  | W     | 406/416 (98%)  | 405 (100%) | 1 (0%)   | 87          | 86  |
| 24  | X     | 362/362 (100%) | 361 (100%) | 1 (0%)   | 86          | 83  |
| 25  | Y     | 344/344 (100%) | 344 (100%) | 0        | 100         | 100 |
| 26  | Z     | 257/295 (87%)  | 257 (100%) | 0        | 100         | 100 |
| 27  | a     | 333/336 (99%)  | 333 (100%) | 0        | 100         | 100 |
| 28  | b     | 167/312 (54%)  | 167 (100%) | 0        | 100         | 100 |
| 29  | c     | 252/268 (94%)  | 247 (98%)  | 5 (2%)   | 48          | 64  |
| 30  | d     | 231/294 (79%)  | 229 (99%)  | 2 (1%)   | 70          | 75  |
| 31  | e     | 44/63 (70%)    | 44 (100%)  | 0        | 100         | 100 |
| 32  | f     | 711/763 (93%)  | 711 (100%) | 0        | 100         | 100 |
| 34  | w     | 68/68 (100%)   | 68 (100%)  | 0        | 100         | 100 |
| 34  | x     | 68/68 (100%)   | 68 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |
|-----|-------|-------------------|--------------|----------|-------------|
| 34  | y     | 68/68 (100%)      | 67 (98%)     | 1 (2%)   | 57 68       |
| 34  | z     | 68/68 (100%)      | 65 (96%)     | 3 (4%)   | 25 50       |
| All | All   | 11723/12886 (91%) | 11688 (100%) | 35 (0%)  | 84 83       |

All (35) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | A     | 51    | ASP  |
| 1   | A     | 403   | ILE  |
| 2   | B     | 125   | THR  |
| 3   | C     | 89    | VAL  |
| 3   | C     | 109   | THR  |
| 3   | C     | 210   | THR  |
| 4   | D     | 159   | LYS  |
| 6   | F     | 85    | THR  |
| 6   | F     | 86    | LEU  |
| 6   | F     | 326   | VAL  |
| 6   | F     | 416   | THR  |
| 7   | G     | 21    | ARG  |
| 9   | I     | 52    | ILE  |
| 9   | I     | 54    | LYS  |
| 13  | M     | 34    | SER  |
| 17  | Q     | 46[A] | CYS  |
| 17  | Q     | 46[B] | CYS  |
| 23  | W     | 316   | ARG  |
| 24  | X     | 319   | ILE  |
| 29  | c     | 196   | LEU  |
| 29  | c     | 197   | ASN  |
| 29  | c     | 200   | TYR  |
| 29  | c     | 203   | ILE  |
| 29  | c     | 281   | LYS  |
| 30  | d     | 47    | GLN  |
| 30  | d     | 135   | HIS  |
| 8   | h     | 3     | GLU  |
| 8   | h     | 4     | ARG  |
| 12  | l     | 117   | GLN  |
| 12  | l     | 148   | CYS  |
| 15  | o     | 30    | ASN  |
| 34  | y     | 63    | LYS  |
| 34  | z     | 36    | ILE  |
| 34  | z     | 71    | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | z     | 74  | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (127) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 54  | GLN  |
| 1   | A     | 94  | GLN  |
| 1   | A     | 203 | ASN  |
| 1   | A     | 247 | GLN  |
| 1   | A     | 305 | GLN  |
| 2   | B     | 81  | ASN  |
| 2   | B     | 277 | HIS  |
| 3   | C     | 50  | ASN  |
| 3   | C     | 67  | GLN  |
| 3   | C     | 90  | HIS  |
| 3   | C     | 118 | ASN  |
| 4   | D     | 65  | GLN  |
| 4   | D     | 257 | ASN  |
| 4   | D     | 301 | GLN  |
| 4   | D     | 412 | GLN  |
| 5   | E     | 271 | HIS  |
| 6   | F     | 76  | ASN  |
| 6   | F     | 243 | GLN  |
| 6   | F     | 316 | GLN  |
| 6   | F     | 358 | ASN  |
| 7   | G     | 24  | GLN  |
| 7   | G     | 68  | HIS  |
| 7   | G     | 75  | ASN  |
| 7   | G     | 92  | GLN  |
| 8   | H     | 88  | HIS  |
| 8   | H     | 95  | GLN  |
| 8   | H     | 102 | GLN  |
| 9   | I     | 53  | HIS  |
| 9   | I     | 102 | GLN  |
| 9   | I     | 123 | GLN  |
| 10  | J     | 15  | HIS  |
| 10  | J     | 92  | GLN  |
| 10  | J     | 175 | ASN  |
| 10  | J     | 239 | ASN  |
| 11  | K     | 98  | ASN  |
| 12  | L     | 31  | GLN  |
| 14  | N     | 158 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | O     | 66  | HIS  |
| 15  | O     | 91  | GLN  |
| 16  | P     | 169 | GLN  |
| 17  | Q     | 8   | GLN  |
| 17  | Q     | 55  | GLN  |
| 17  | Q     | 168 | GLN  |
| 18  | R     | 62  | GLN  |
| 21  | U     | 149 | GLN  |
| 21  | U     | 171 | ASN  |
| 21  | U     | 525 | ASN  |
| 21  | U     | 596 | ASN  |
| 21  | U     | 718 | ASN  |
| 21  | U     | 734 | GLN  |
| 21  | U     | 768 | GLN  |
| 22  | V     | 81  | GLN  |
| 22  | V     | 487 | HIS  |
| 22  | V     | 488 | ASN  |
| 23  | W     | 107 | GLN  |
| 23  | W     | 203 | GLN  |
| 23  | W     | 362 | ASN  |
| 23  | W     | 426 | ASN  |
| 23  | W     | 454 | ASN  |
| 24  | X     | 44  | GLN  |
| 24  | X     | 207 | GLN  |
| 24  | X     | 213 | GLN  |
| 24  | X     | 292 | GLN  |
| 24  | X     | 380 | GLN  |
| 24  | X     | 405 | GLN  |
| 24  | X     | 416 | ASN  |
| 25  | Y     | 160 | ASN  |
| 25  | Y     | 365 | GLN  |
| 25  | Y     | 378 | ASN  |
| 26  | Z     | 7   | GLN  |
| 26  | Z     | 12  | HIS  |
| 26  | Z     | 109 | ASN  |
| 26  | Z     | 189 | GLN  |
| 26  | Z     | 193 | ASN  |
| 26  | Z     | 243 | GLN  |
| 26  | Z     | 278 | ASN  |
| 27  | a     | 129 | GLN  |
| 27  | a     | 249 | GLN  |
| 28  | b     | 169 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | c     | 149 | GLN  |
| 29  | c     | 183 | HIS  |
| 29  | c     | 240 | HIS  |
| 30  | d     | 46  | GLN  |
| 30  | d     | 221 | ASN  |
| 31  | e     | 37  | HIS  |
| 32  | f     | 156 | HIS  |
| 32  | f     | 245 | ASN  |
| 32  | f     | 371 | ASN  |
| 32  | f     | 387 | GLN  |
| 32  | f     | 405 | HIS  |
| 32  | f     | 650 | GLN  |
| 32  | f     | 752 | HIS  |
| 32  | f     | 876 | HIS  |
| 7   | g     | 68  | HIS  |
| 7   | g     | 75  | ASN  |
| 7   | g     | 128 | ASN  |
| 8   | h     | 21  | GLN  |
| 8   | h     | 71  | HIS  |
| 9   | i     | 155 | ASN  |
| 9   | i     | 230 | GLN  |
| 10  | j     | 18  | GLN  |
| 10  | j     | 175 | ASN  |
| 10  | j     | 205 | ASN  |
| 11  | k     | 23  | GLN  |
| 11  | k     | 204 | GLN  |
| 12  | l     | 59  | HIS  |
| 12  | l     | 146 | GLN  |
| 14  | n     | 66  | HIS  |
| 14  | n     | 77  | HIS  |
| 14  | n     | 106 | GLN  |
| 15  | o     | 35  | HIS  |
| 16  | p     | 81  | GLN  |
| 16  | p     | 169 | GLN  |
| 16  | p     | 173 | ASN  |
| 17  | q     | 32  | HIS  |
| 17  | q     | 82  | ASN  |
| 18  | r     | 62  | GLN  |
| 18  | r     | 162 | GLN  |
| 19  | s     | 108 | ASN  |
| 19  | s     | 151 | ASN  |
| 19  | s     | 159 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | t     | 2   | GLN  |
| 34  | x     | 41  | GLN  |
| 34  | y     | 41  | GLN  |
| 34  | y     | 60  | ASN  |
| 34  | z     | 41  | GLN  |
| 34  | z     | 60  | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 35  | ATP  | C     | 501 | 36   | 29,33,33     | 0.28 | 0        | 44,52,52    | 0.50 | 1 (2%)   |
| 37  | ADP  | D     | 502 | 36   | 27,29,29     | 1.37 | 4 (14%)  | 42,45,45    | 1.98 | 10 (23%) |
| 35  | ATP  | A     | 501 | 36   | 29,33,33     | 0.28 | 0        | 44,52,52    | 0.47 | 1 (2%)   |
| 35  | ATP  | B     | 501 | 36   | 29,33,33     | 0.28 | 0        | 44,52,52    | 0.47 | 1 (2%)   |
| 35  | ATP  | F     | 501 | 36   | 29,33,33     | 0.28 | 0        | 44,52,52    | 0.48 | 1 (2%)   |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 35  | ATP  | C     | 501 | 36   | -       | 6/22/38/38 | 0/3/3/3 |
| 37  | ADP  | D     | 502 | 36   | -       | 6/16/32/32 | 0/3/3/3 |
| 35  | ATP  | A     | 501 | 36   | -       | 5/22/38/38 | 0/3/3/3 |
| 35  | ATP  | B     | 501 | 36   | -       | 2/22/38/38 | 0/3/3/3 |
| 35  | ATP  | F     | 501 | 36   | -       | 4/22/38/38 | 0/3/3/3 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 37  | D     | 502 | ADP  | C5-C4 | 4.61  | 1.47        | 1.39     |
| 37  | D     | 502 | ADP  | C5-C6 | 2.62  | 1.48        | 1.41     |
| 37  | D     | 502 | ADP  | C8-N7 | 2.35  | 1.36        | 1.31     |
| 37  | D     | 502 | ADP  | C5-N7 | -2.23 | 1.34        | 1.39     |

All (14) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 37  | D     | 502 | ADP  | C5-C4-N3    | -6.25 | 118.60      | 126.75   |
| 37  | D     | 502 | ADP  | N3-C4-N9    | 4.95  | 135.24      | 127.08   |
| 37  | D     | 502 | ADP  | C2-N3-C4    | 3.78  | 120.68      | 111.75   |
| 37  | D     | 502 | ADP  | PA-O3A-PB   | -3.49 | 120.87      | 132.83   |
| 37  | D     | 502 | ADP  | C4-C5-N7    | -3.21 | 106.71      | 110.62   |
| 37  | D     | 502 | ADP  | N3-C2-N1    | -2.96 | 123.97      | 128.60   |
| 37  | D     | 502 | ADP  | C5-N7-C8    | 2.72  | 107.38      | 103.51   |
| 37  | D     | 502 | ADP  | C3'-C2'-C1' | 2.66  | 106.49      | 101.43   |
| 37  | D     | 502 | ADP  | C4-N9-C8    | 2.57  | 108.52      | 105.73   |
| 35  | C     | 501 | ATP  | PB-O3B-PG   | 2.03  | 139.79      | 132.83   |
| 37  | D     | 502 | ADP  | C6-C5-N7    | 2.03  | 135.80      | 132.02   |
| 35  | F     | 501 | ATP  | PB-O3B-PG   | 2.02  | 139.77      | 132.83   |
| 35  | B     | 501 | ATP  | PB-O3B-PG   | 2.02  | 139.75      | 132.83   |
| 35  | A     | 501 | ATP  | PB-O3B-PG   | 2.01  | 139.73      | 132.83   |

There are no chirality outliers.

All (23) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 35  | A     | 501 | ATP  | PB-O3B-PG-O3G |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 35  | B     | 501 | ATP  | C5'-O5'-PA-O2A  |
| 35  | B     | 501 | ATP  | C5'-O5'-PA-O3A  |
| 35  | C     | 501 | ATP  | PB-O3B-PG-O2G   |
| 35  | C     | 501 | ATP  | C5'-O5'-PA-O1A  |
| 35  | C     | 501 | ATP  | C5'-O5'-PA-O2A  |
| 35  | C     | 501 | ATP  | C5'-O5'-PA-O3A  |
| 35  | F     | 501 | ATP  | PB-O3B-PG-O2G   |
| 37  | D     | 502 | ADP  | PA-O3A-PB-O2B   |
| 37  | D     | 502 | ADP  | C5'-O5'-PA-O1A  |
| 37  | D     | 502 | ADP  | O4'-C4'-C5'-O5' |
| 35  | F     | 501 | ATP  | O4'-C4'-C5'-O5' |
| 35  | F     | 501 | ATP  | C3'-C4'-C5'-O5' |
| 37  | D     | 502 | ADP  | C3'-C4'-C5'-O5' |
| 35  | A     | 501 | ATP  | C3'-C4'-C5'-O5' |
| 35  | A     | 501 | ATP  | O4'-C4'-C5'-O5' |
| 35  | F     | 501 | ATP  | PB-O3B-PG-O1G   |
| 35  | A     | 501 | ATP  | PB-O3B-PG-O1G   |
| 35  | A     | 501 | ATP  | PB-O3B-PG-O2G   |
| 37  | D     | 502 | ADP  | C5'-O5'-PA-O3A  |
| 35  | C     | 501 | ATP  | PG-O3B-PB-O1B   |
| 35  | C     | 501 | ATP  | PG-O3B-PB-O2B   |
| 37  | D     | 502 | ADP  | C5'-O5'-PA-O2A  |

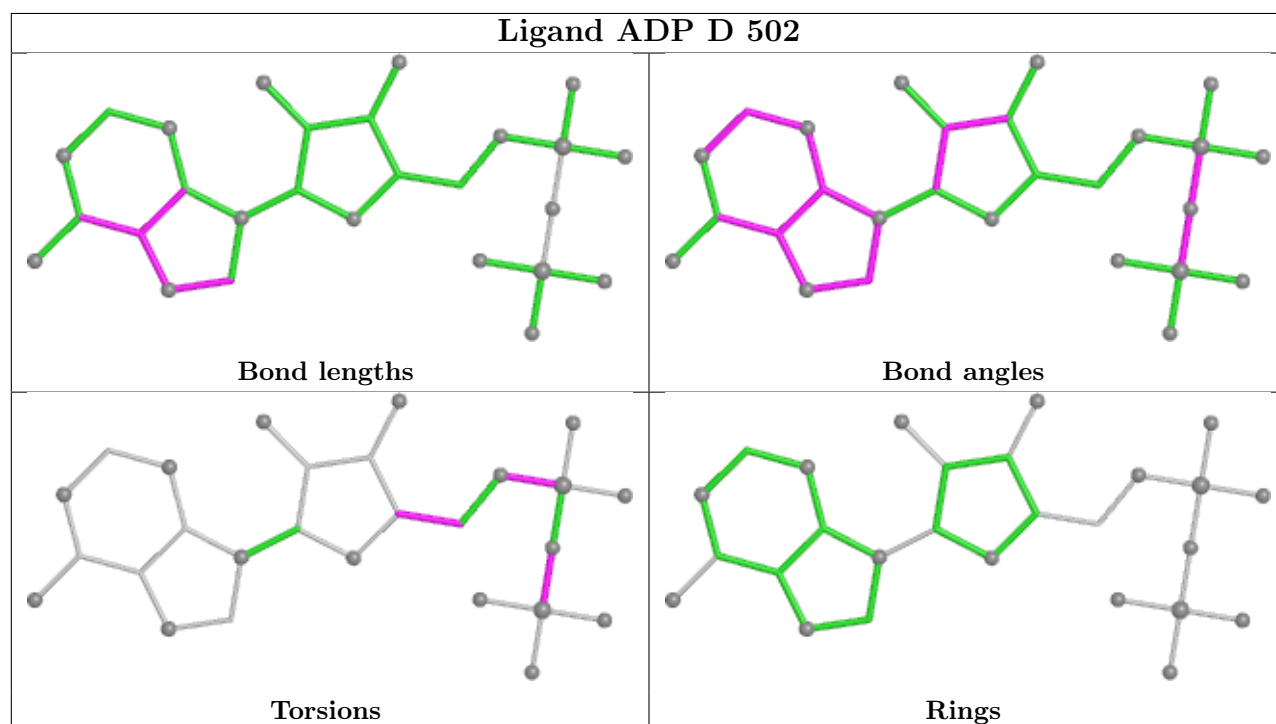
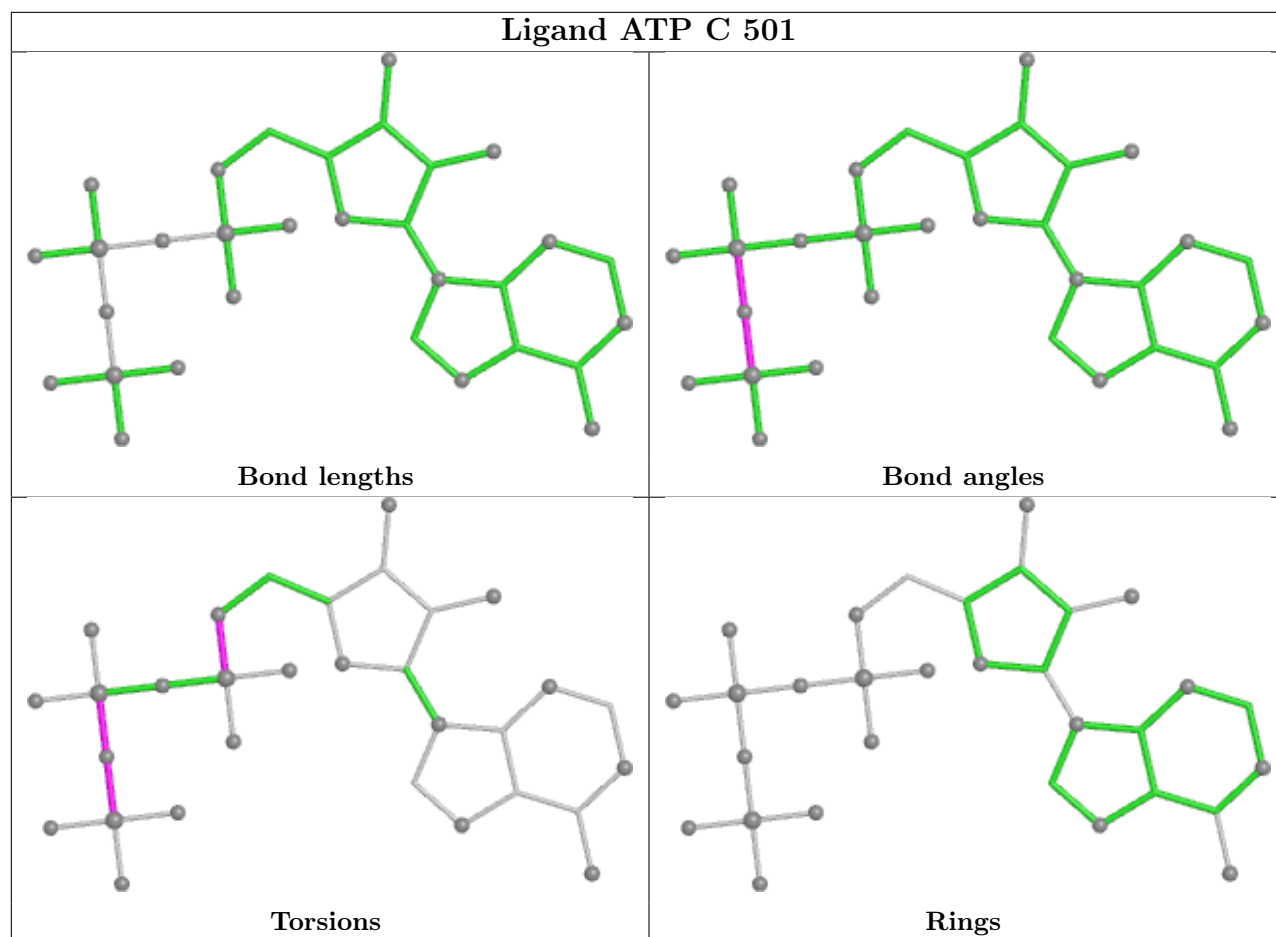
There are no ring outliers.

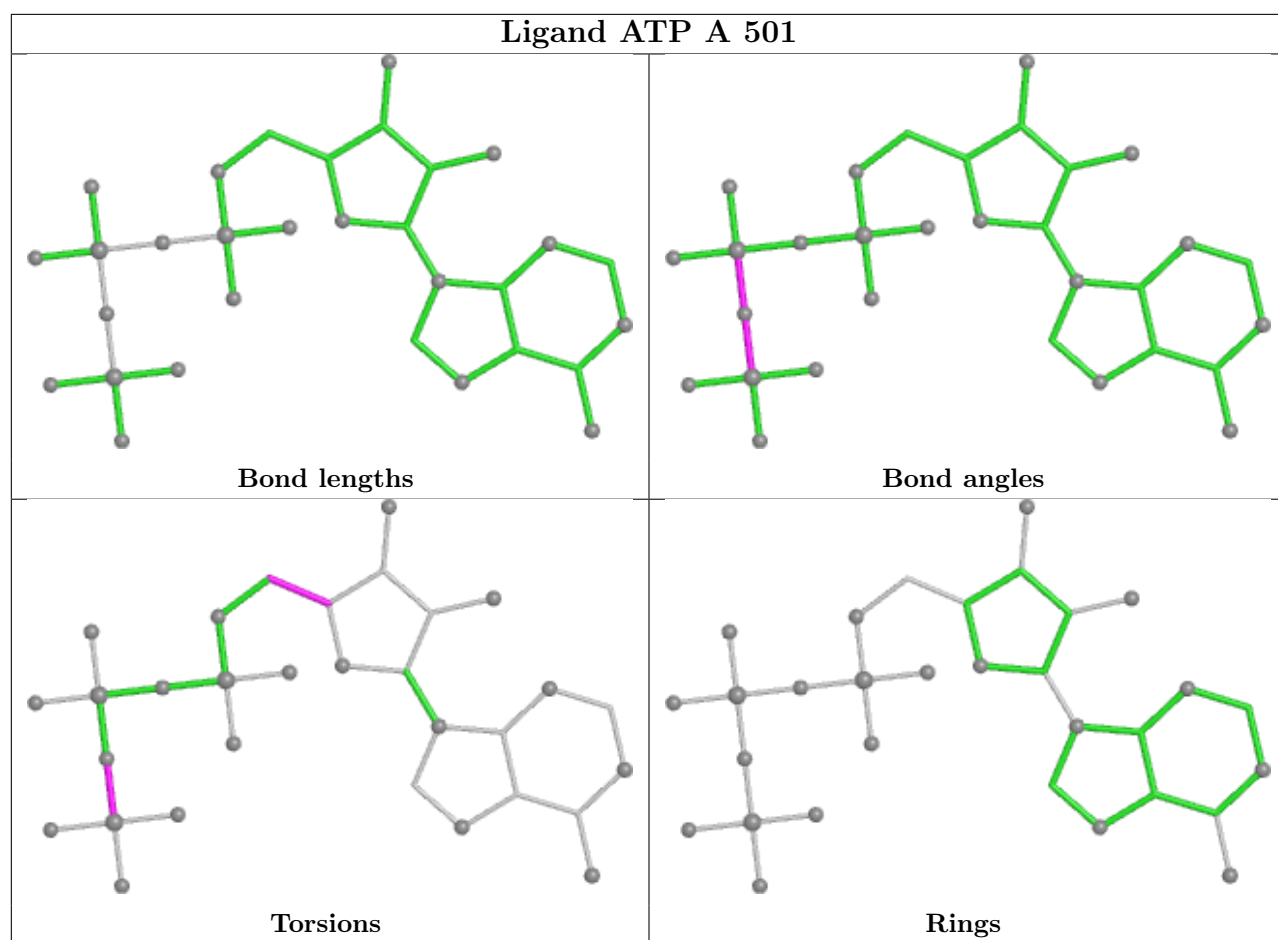
3 monomers are involved in 5 short contacts:

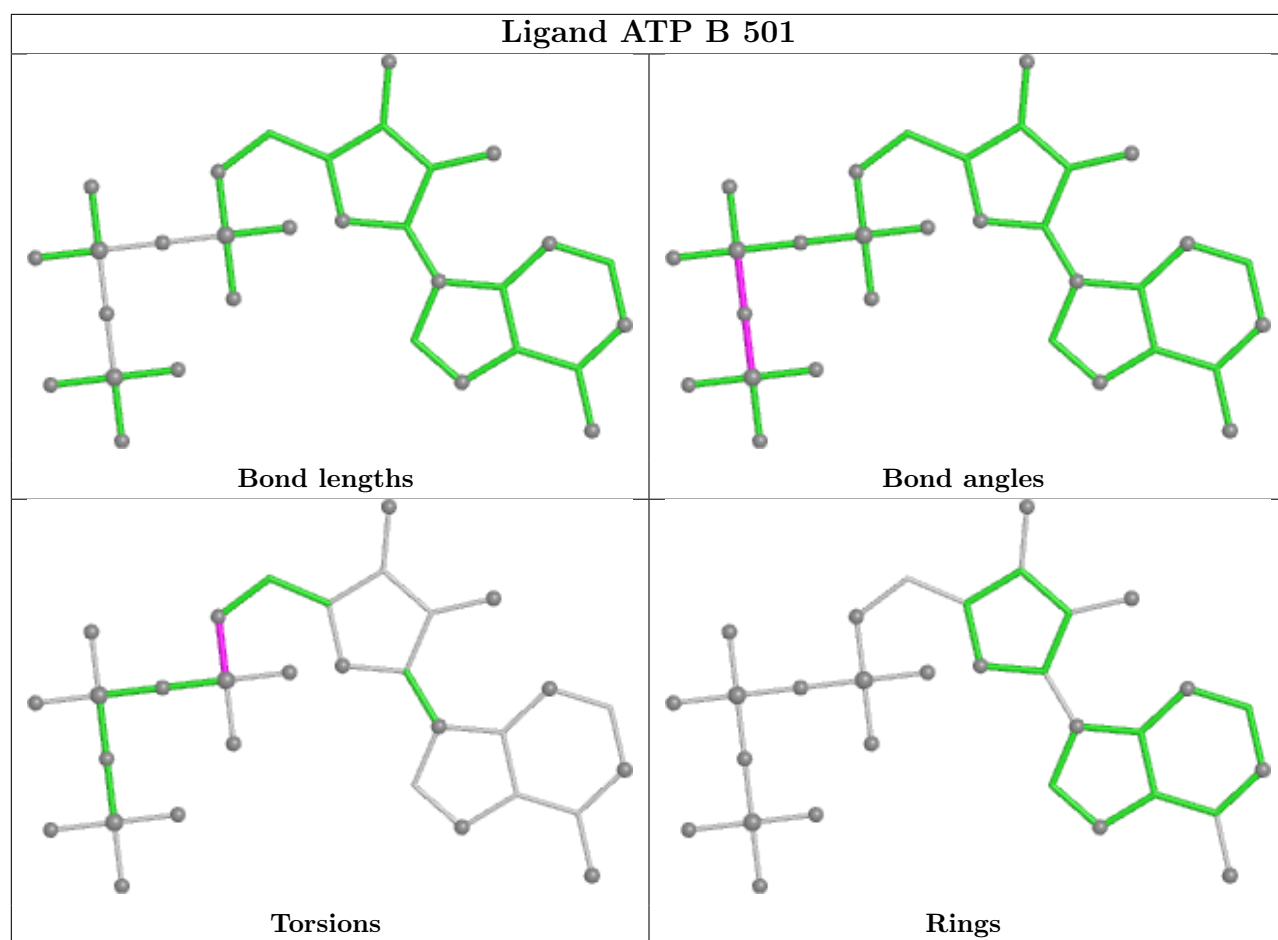
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 35  | C     | 501 | ATP  | 1       | 0            |
| 35  | B     | 501 | ATP  | 2       | 0            |
| 35  | F     | 501 | ATP  | 2       | 0            |

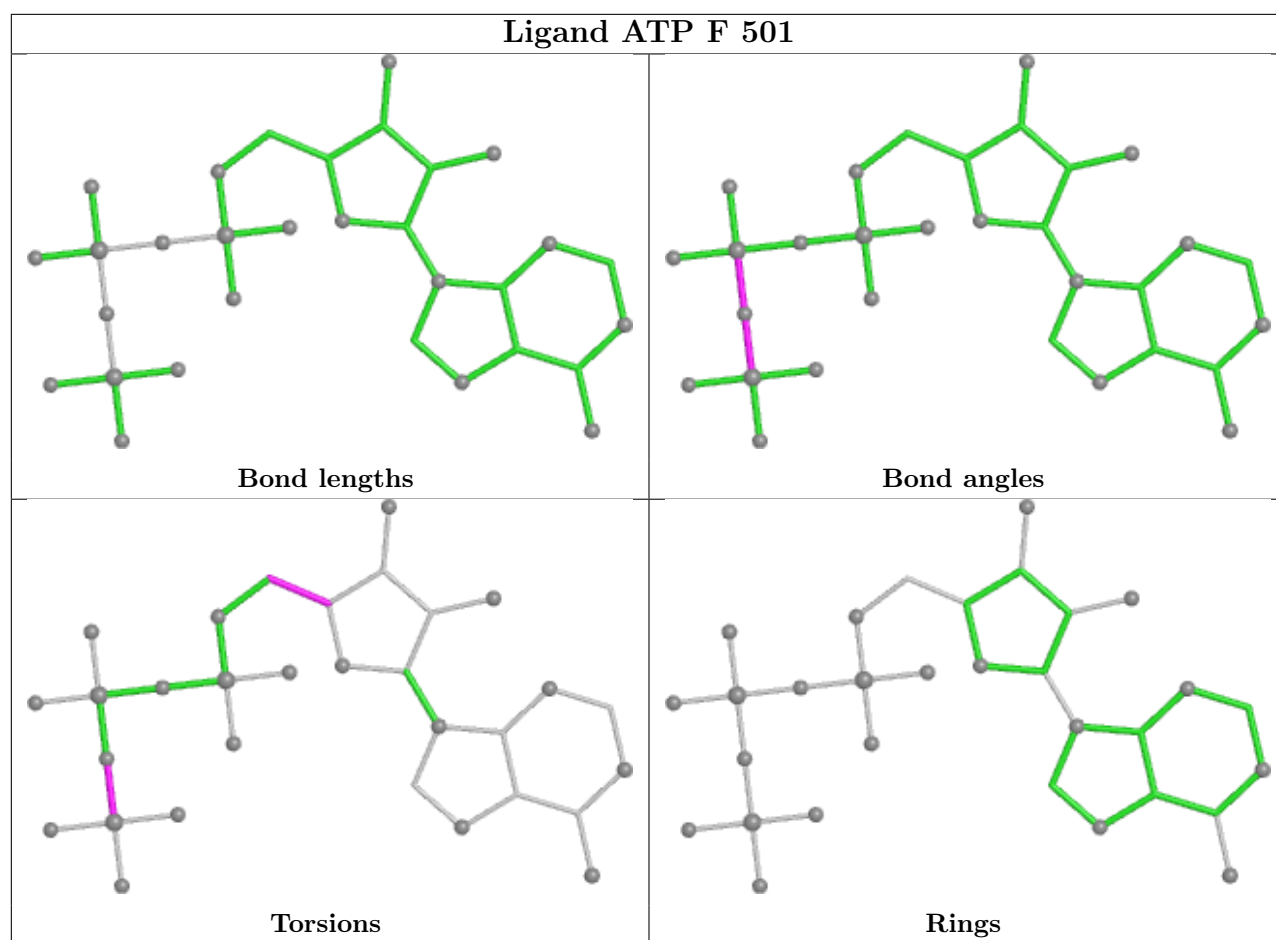
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.









## 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.



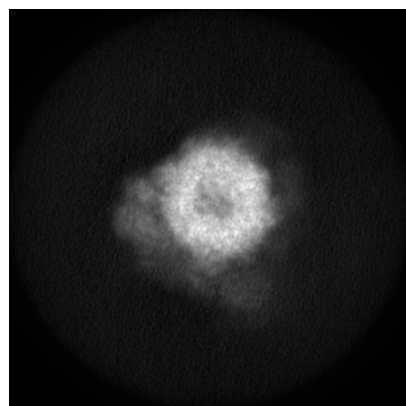
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62080. These allow visual inspection of the internal detail of the map and identification of artifacts.

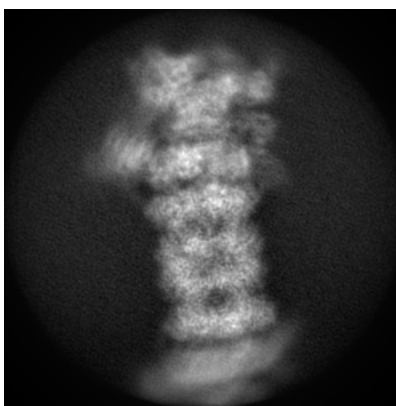
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

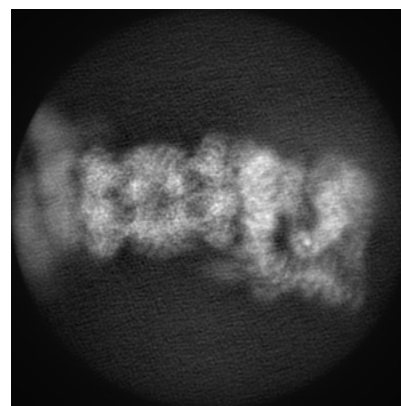
#### 6.1.1 Primary map



X

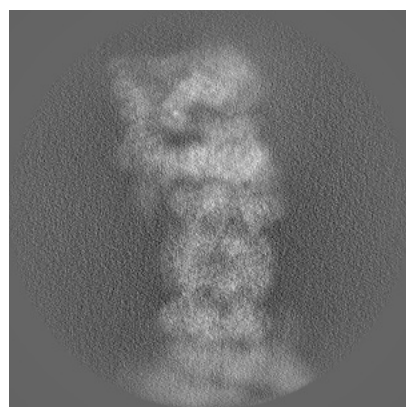


Y

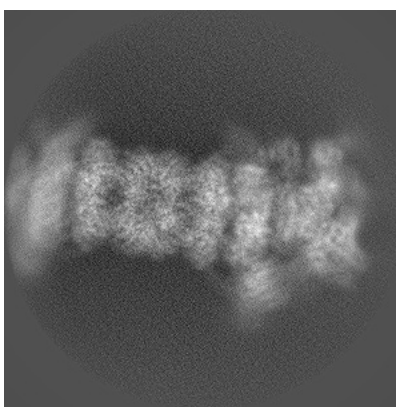


Z

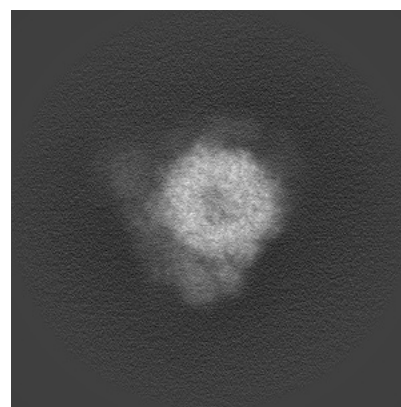
#### 6.1.2 Raw map



X



Y

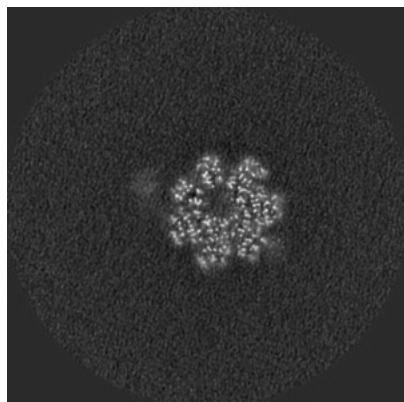


Z

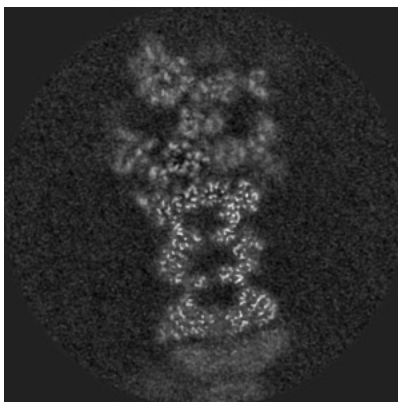
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

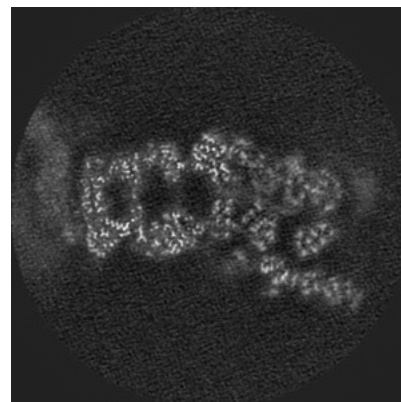
### 6.2.1 Primary map



X Index: 300

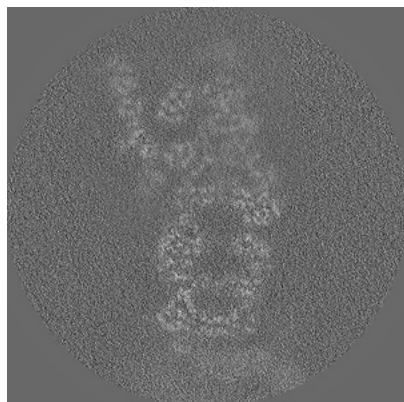


Y Index: 300

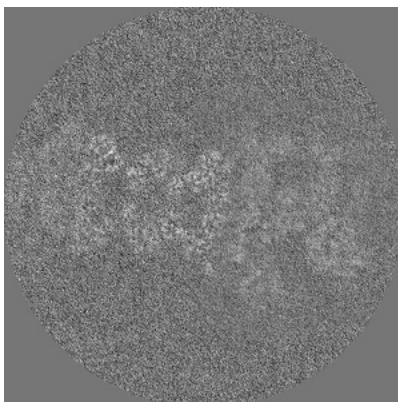


Z Index: 300

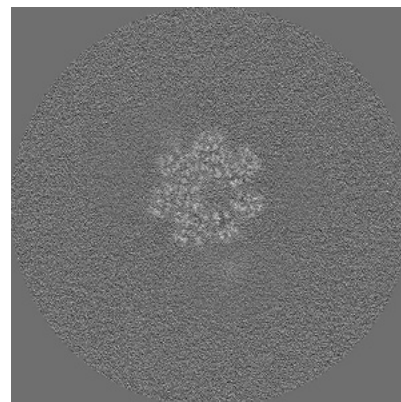
### 6.2.2 Raw map



X Index: 300



Y Index: 300

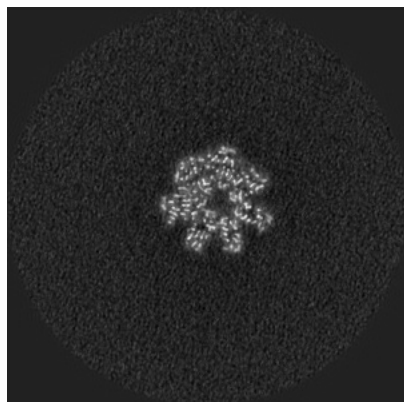


Z Index: 300

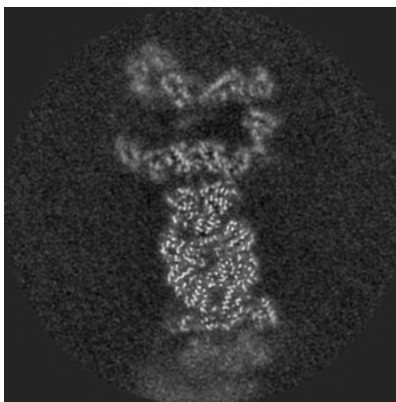
The images above show central slices of the map in three orthogonal directions.

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

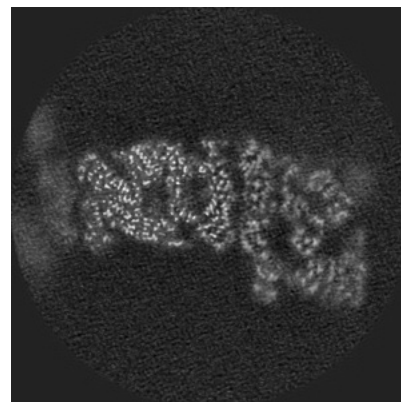
### 6.3.1 Primary map



X Index: 251

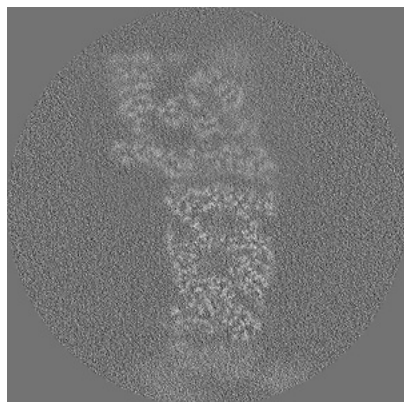


Y Index: 274

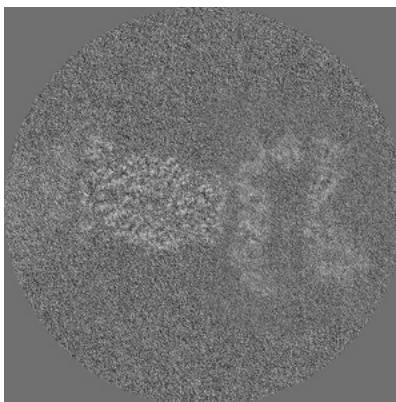


Z Index: 276

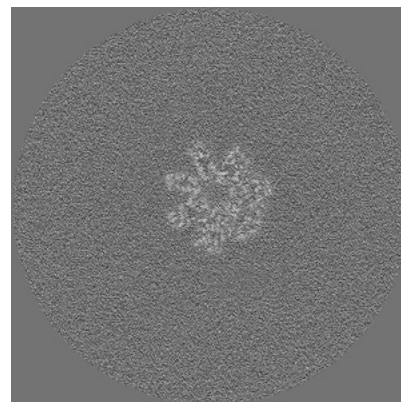
### 6.3.2 Raw map



X Index: 278



Y Index: 275



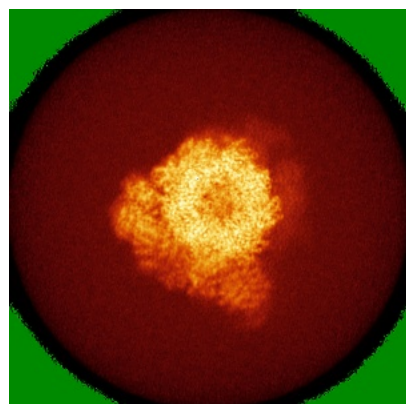
Z Index: 251

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

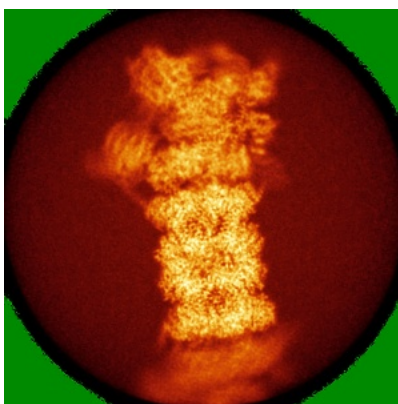


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

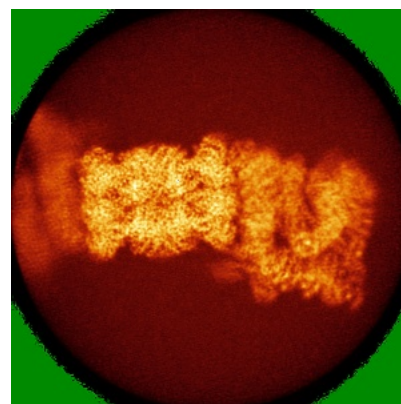
### 6.4.1 Primary map



X

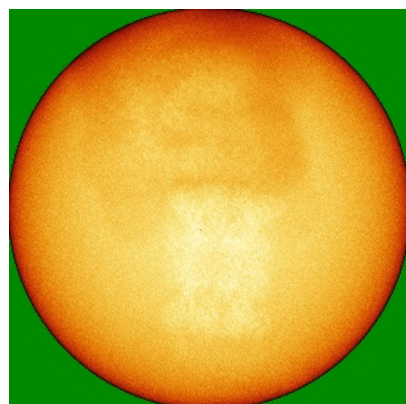


Y

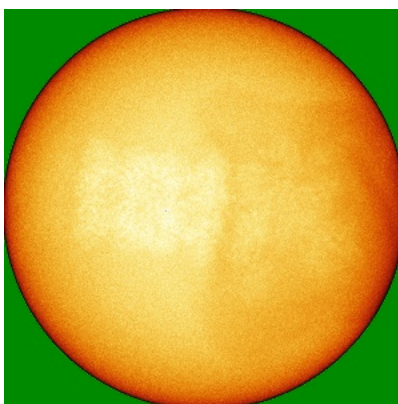


Z

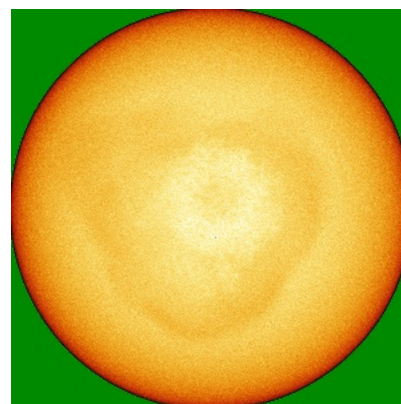
### 6.4.2 Raw map



X



Y

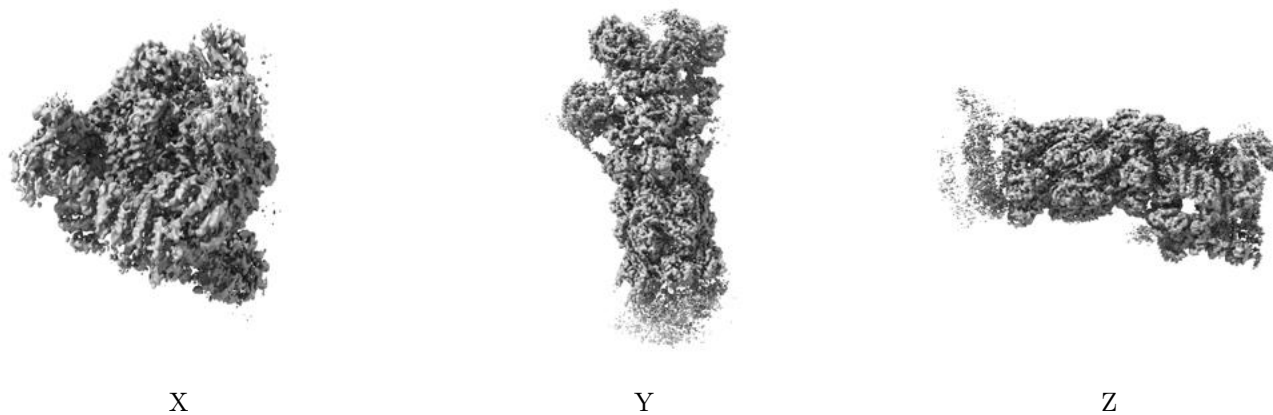


Z

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

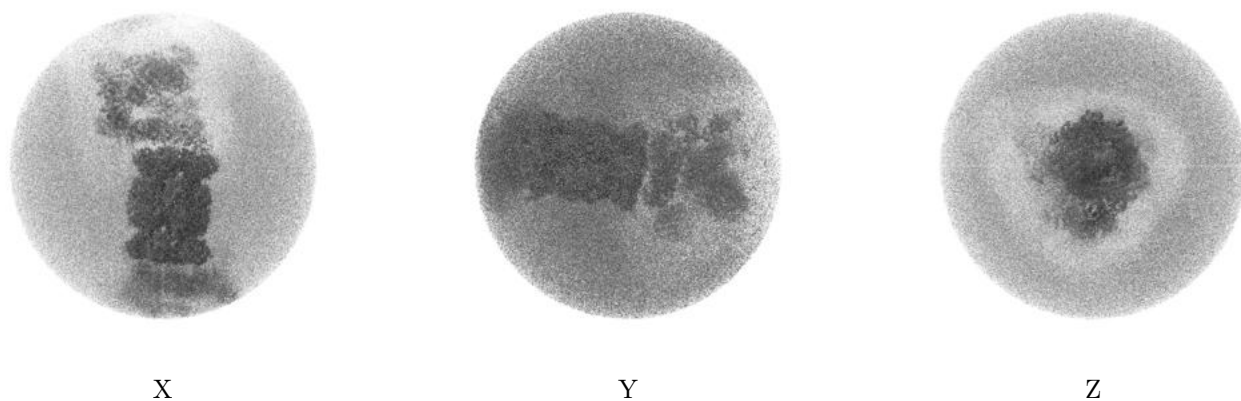
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00617. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

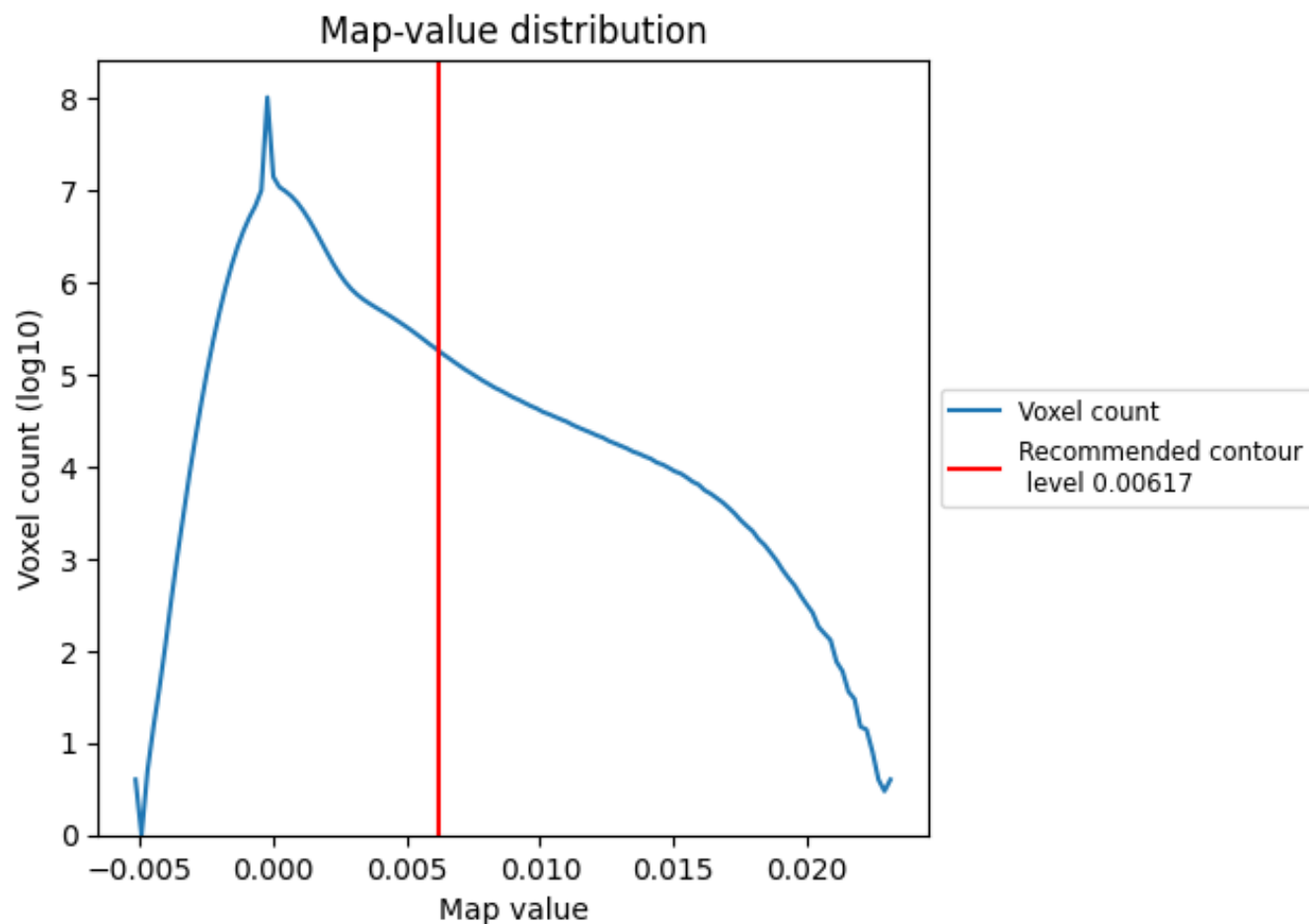
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

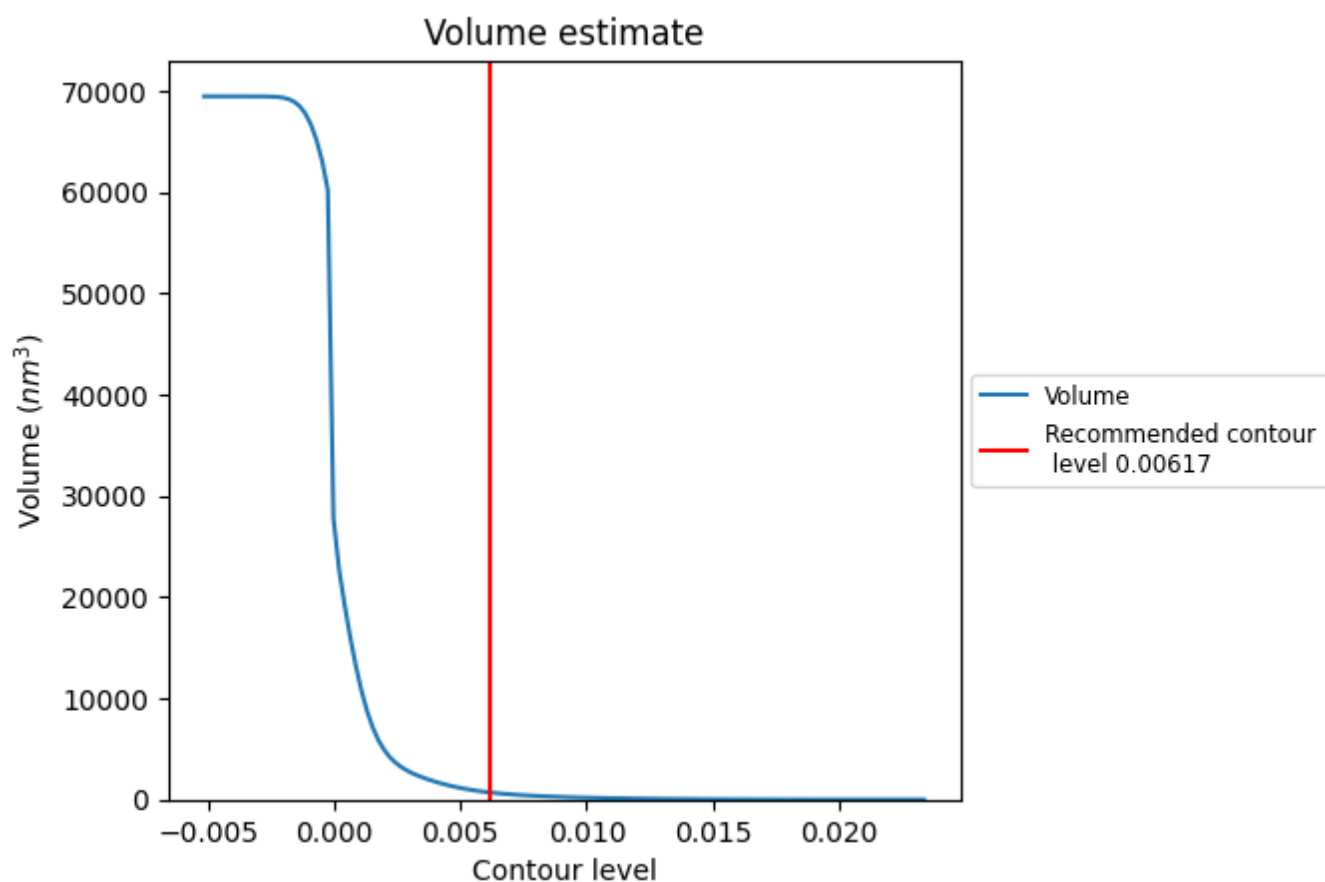
This section contains the results of statistical analysis of the map.

### 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.

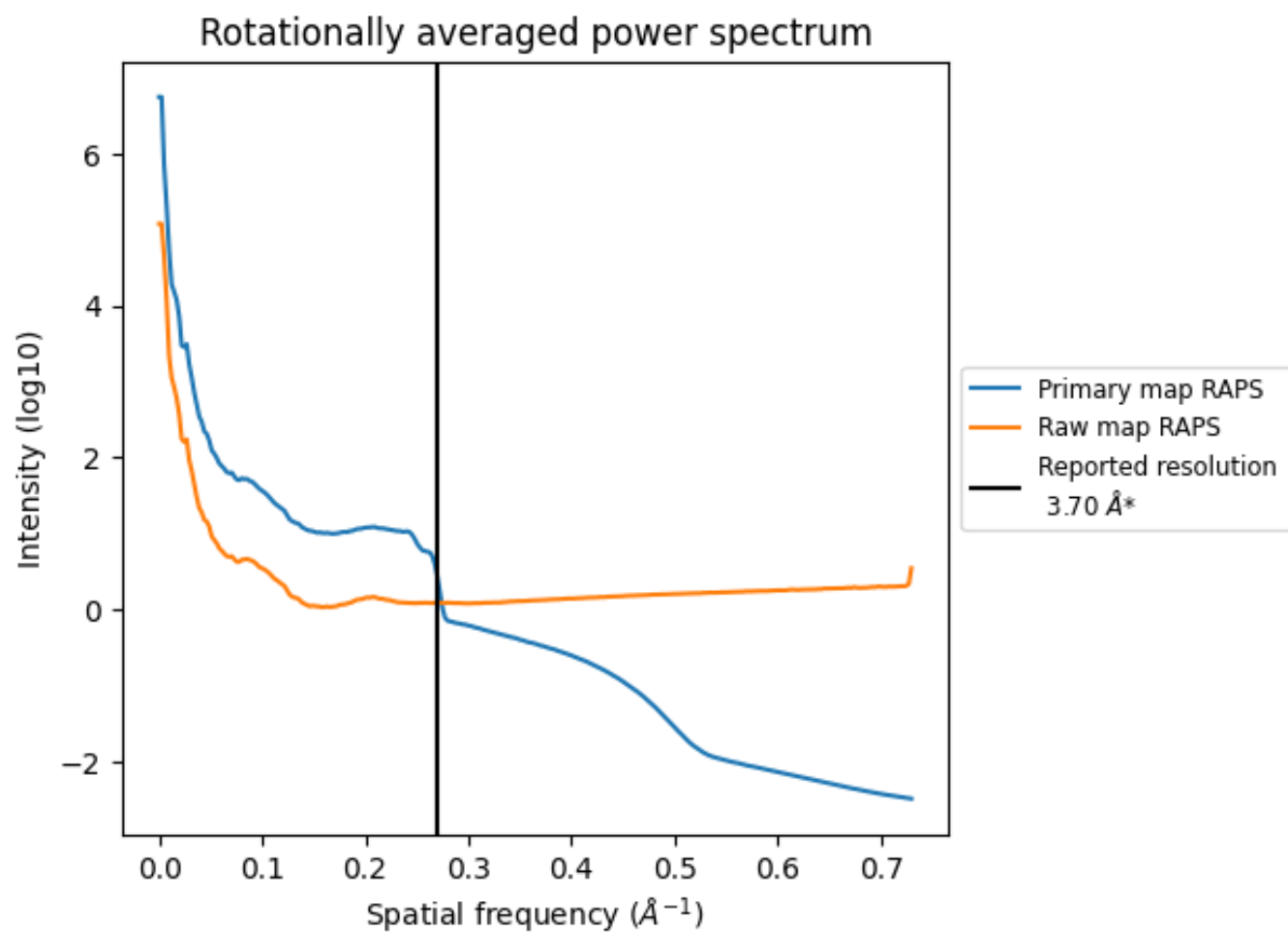
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 698 nm<sup>3</sup>; this corresponds to an approximate mass of 631 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 ⓘ



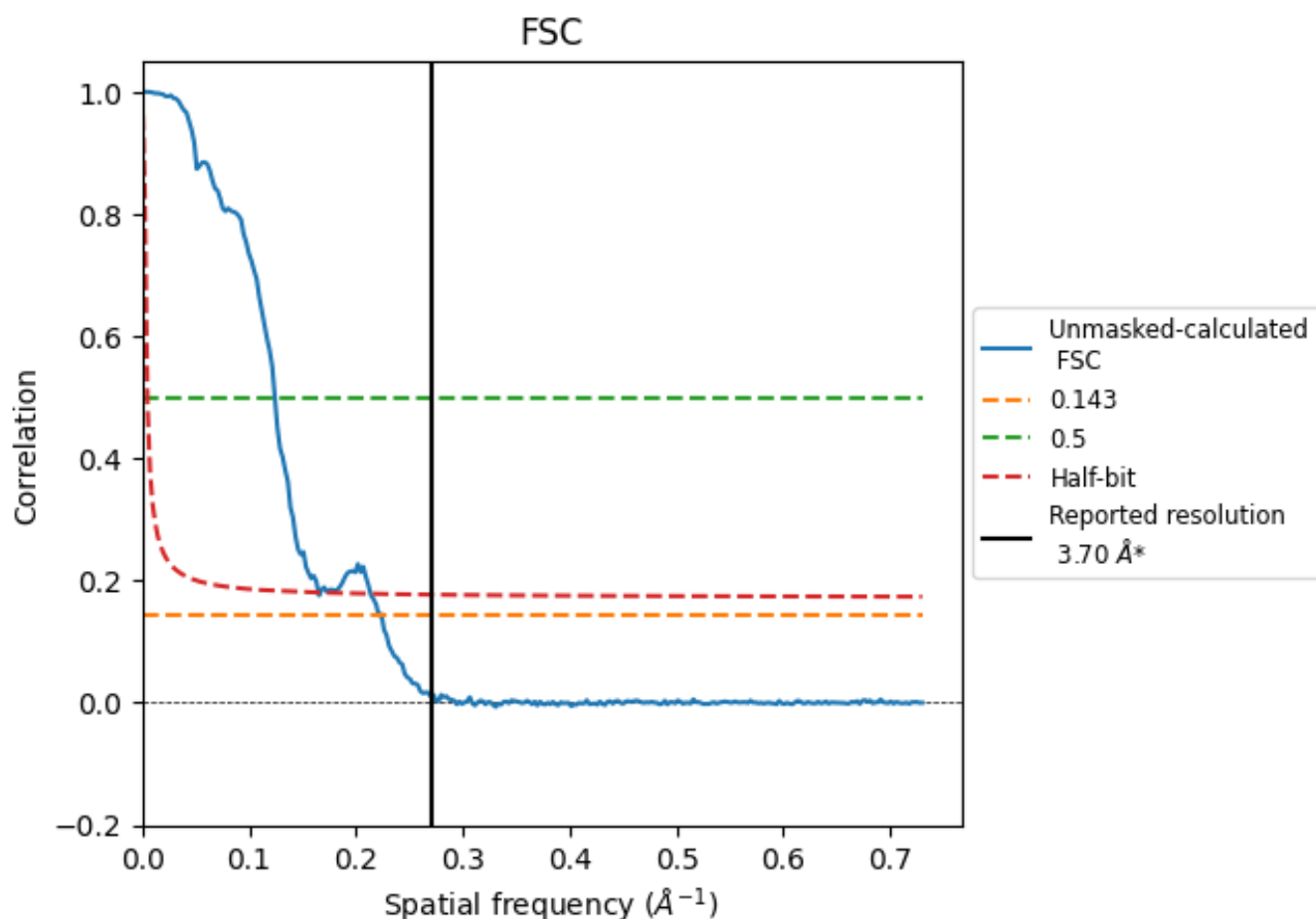
\*Reported resolution corresponds to spatial frequency of 0.270  $\text{\AA}^{-1}$



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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.270  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

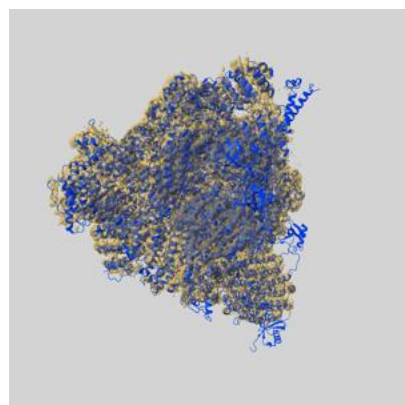
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.70                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 4.52                               | 8.06 | 6.06     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.52 differs from the reported value 3.7 by more than 10 %

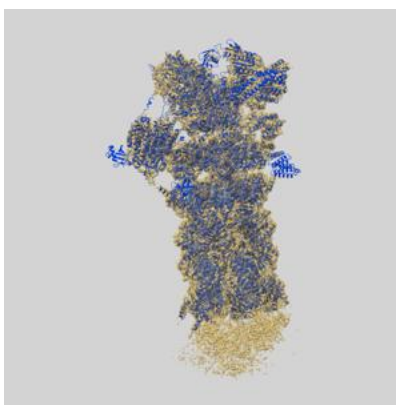
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62080 and PDB model 9K54. Per-residue inclusion information can be found in section [3](#) on page [13](#).

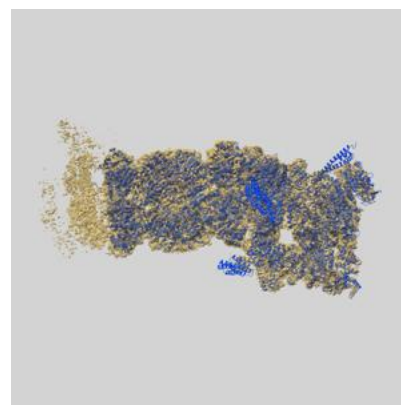
### 9.1 Map-model overlay [i](#)



X



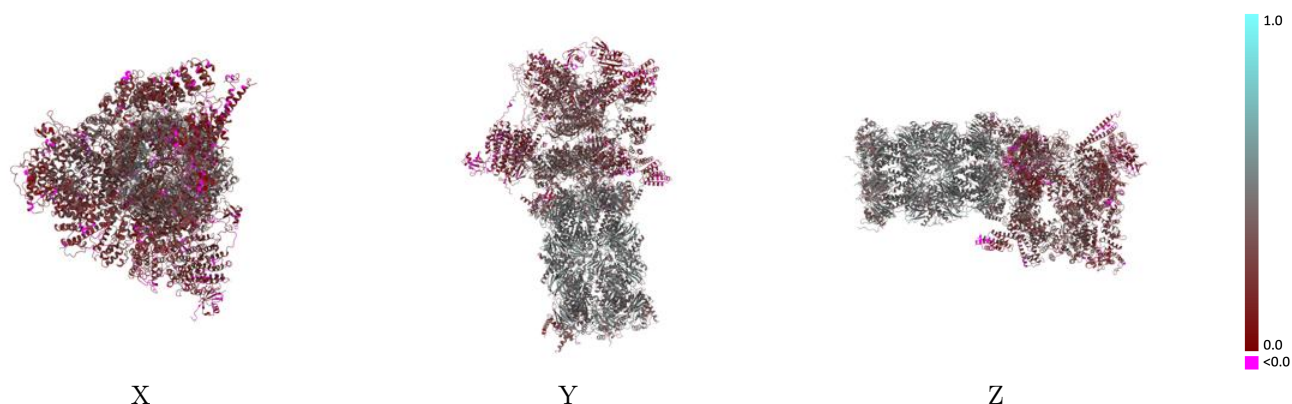
Y



Z

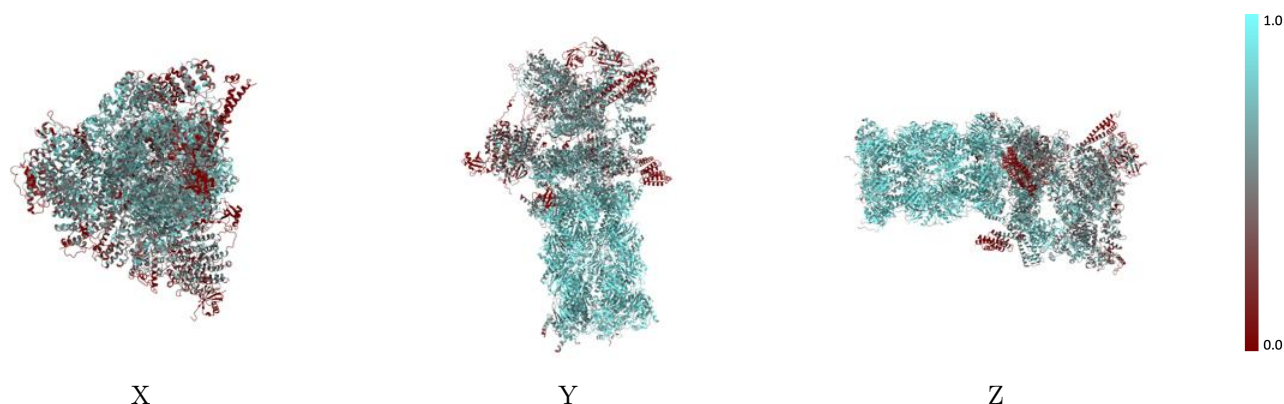
The images above show the 3D surface view of the map at the recommended contour level 0.00617 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



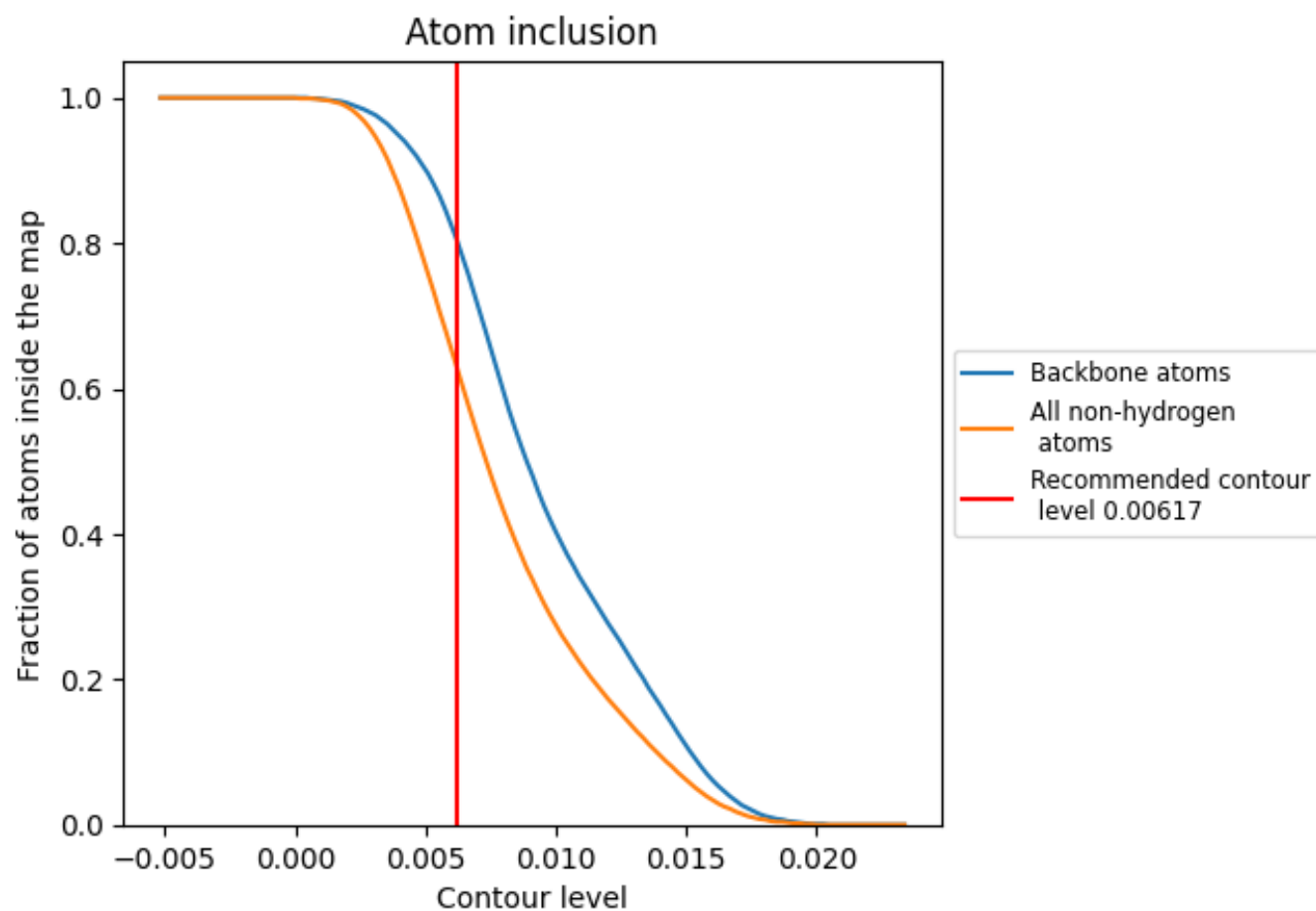
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00617).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ



































The table lists the average atom inclusion at the recommended contour level (0.00617) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.6320   |  0.3450   |
| A     |  0.5760   |  0.3210   |
| B     |  0.5750   |  0.3290   |
| C     |  0.6450   |  0.3490   |
| D     |  0.6240   |  0.3300   |
| E     |  0.3470   |  0.1810   |
| F     |  0.4820   |  0.2760   |
| G     |  0.8160   |  0.4540   |
| H     |  0.8420   |  0.4630   |
| I     |  0.7840   |  0.4480   |
| J     |  0.7720   |  0.4300   |
| K     |  0.7740   |  0.4510   |
| L     |  0.8280   |  0.4630   |
| M     |  0.8100   |  0.4490   |
| N     |  0.8560  |  0.4790  |
| O     |  0.8590 |  0.4720 |
| P     |  0.8650 |  0.4790 |
| Q     |  0.8470 |  0.4750 |
| R     |  0.8690 |  0.4810 |
| S     |  0.8410 |  0.4730 |
| T     |  0.8620 |  0.4830 |
| U     |  0.5050 |  0.2310 |
| V     |  0.5470 |  0.2750 |
| W     |  0.4140 |  0.2390 |
| X     |  0.4890 |  0.2640 |
| Y     |  0.6920 |  0.3050 |
| Z     |  0.5270 |  0.2770 |
| a     |  0.5030 |  0.2180 |
| b     |  0.4200 |  0.1900 |
| c     |  0.5120 |  0.2680 |
| d     |  0.3630 |  0.2050 |
| e     |  0.5080 |  0.3130 |
| f     |  0.3790 |  0.2090 |
| g     |  0.7910 |  0.4480 |
| h     |  0.7910 |  0.4500 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| i     |  0.7320 |  0.4310 |
| j     |  0.6700 |  0.3690 |
| k     |  0.7370 |  0.4330 |
| l     |  0.8110 |  0.4470 |
| m     |  0.7900 |  0.4470 |
| n     |  0.8500 |  0.4750 |
| o     |  0.8450 |  0.4680 |
| p     |  0.8610 |  0.4780 |
| q     |  0.8460 |  0.4760 |
| r     |  0.8710 |  0.4750 |
| s     |  0.8420 |  0.4690 |
| t     |  0.8620 |  0.4670 |
| v     |  0.1610 |  0.2700 |
| w     |  0.0100 |  0.0790 |
| x     |  0.0050 |  0.1600 |
| y     |  0.0080 |  0.0900 |
| z     |  0.1940 |  0.1040 |