



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:40 AM UTC

PDB ID : 3UNF / pdb\_00003unf  
Title : Mouse 20S immunoproteasome in complex with PR-957  
Authors : Huber, E.; Basler, M.; Schwab, R.; Heinemeyer, W.; Kirk, C.; Groettrup, M.; Groll, M.  
Deposited on : 2011-11-15  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

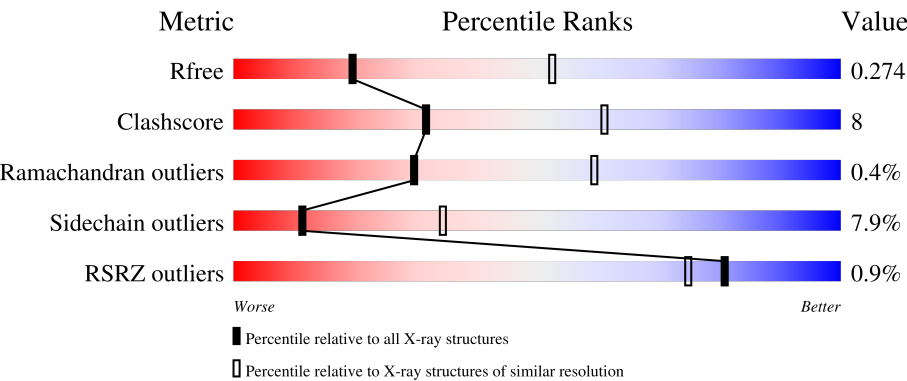
MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
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:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| R <sub>free</sub>     | 180053                      | 2481 (2.90-2.90)                                      |
| Clashscore            | 190562                      | 2690 (2.90-2.90)                                      |
| Ramachandran outliers | 187476                      | 2623 (2.90-2.90)                                      |
| Sidechain outliers    | 187428                      | 2625 (2.90-2.90)                                      |
| RSRZ outliers         | 180081                      | 2481 (2.90-2.90)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                                               |
|-----|-------|--------|----------------------------------------------------------------------------------------------------------------|
| 1   | A     | 234    | <div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>72%24%. .</div></div>  |
| 1   | O     | 234    | <div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>75%21%. .</div></div>  |
| 2   | B     | 261    | <div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>72%20%. 5%</div></div> |
| 2   | P     | 261    | <div><div></div><div><div></div><div></div><div></div><div></div><div></div></div><div>74%19%. 5%</div></div>  |
| 3   | C     | 248    | <div><div>4%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>66%27%. .</div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | Q     | 248    |                  |
| 4   | D     | 241    |                  |
| 4   | R     | 241    |                  |
| 5   | E     | 263    |                  |
| 5   | S     | 263    |                  |
| 6   | F     | 255    |                  |
| 6   | T     | 255    |                  |
| 7   | G     | 246    |                  |
| 7   | U     | 246    |                  |
| 8   | H     | 234    |                  |
| 8   | V     | 234    |                  |
| 9   | I     | 205    |                  |
| 9   | W     | 205    |                  |
| 10  | J     | 201    |                  |
| 10  | X     | 201    |                  |
| 11  | K     | 204    |                  |
| 11  | Y     | 204    |                  |
| 12  | L     | 213    |                  |
| 12  | Z     | 213    |                  |
| 13  | M     | 219    |                  |
| 13  | a     | 219    |                  |
| 14  | N     | 199    |                  |
| 14  | b     | 199    |                  |

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49805 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 230      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1801  | 1150 | 308 | 337 | 6 |         |         |       |
| 1   | O     | 230      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1801  | 1150 | 308 | 337 | 6 |         |         |       |

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 248      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1950  | 1232 | 335 | 373 | 10 |         |         |       |
| 2   | P     | 248      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1950  | 1232 | 335 | 373 | 10 |         |         |       |

- Molecule 3 is a protein called Proteasome subunit alpha type-7.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | C     | 238      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1876  | 1179 | 331 | 361 | 5 |         |         |       |
| 3   | Q     | 238      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1876  | 1179 | 331 | 361 | 5 |         |         |       |

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4   | D     | 233      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1778  | 1116 | 294 | 357 | 11 |         |         |       |
| 4   | R     | 233      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1778  | 1116 | 294 | 357 | 11 |         |         |       |

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 5   | E     | 238      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1872  | 1171 | 336 | 354 | 11 |         |         |       |
| 5   | S     | 238      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1872  | 1171 | 336 | 354 | 11 |         |         |       |

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 6   | F     | 244      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1903  | 1206 | 325 | 361 | 11 |         |         |       |
| 6   | T     | 244      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1903  | 1206 | 325 | 361 | 11 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 7   | G     | 243      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1890  | 1199 | 315 | 363 | 13 |         |         |       |
| 7   | U     | 243      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1890  | 1199 | 315 | 363 | 13 |         |         |       |

- Molecule 8 is a protein called Proteasome subunit beta type-10.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 8   | H     | 219      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1619  | 1010 | 294 | 307 | 8 |         |         |       |
| 8   | V     | 219      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1619  | 1010 | 294 | 307 | 8 |         |         |       |

- Molecule 9 is a protein called Proteasome subunit beta type-3.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 9   | I     | 204      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1592  | 1013 | 265 | 295 | 19 |         |         |       |
| 9   | W     | 204      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1592  | 1013 | 265 | 295 | 19 |         |         |       |

- Molecule 10 is a protein called Proteasome subunit beta type-2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 10  | J     | 196      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1570  | 1006 | 267 | 288 | 9 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 10  | X     | 196      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1570  | 1006 | 267 | 288 | 9 |         |         |       |

- Molecule 11 is a protein called Proteasome subunit beta type-8.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 11  | K     | 201      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1566  | 981 | 268 | 302 | 15 |         |         |       |
| 11  | Y     | 201      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1566  | 981 | 268 | 302 | 15 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 12  | L     | 213      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1654  | 1047 | 284 | 313 | 10 |         |         |       |
| 12  | Z     | 213      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1654  | 1047 | 284 | 313 | 10 |         |         |       |

- Molecule 13 is a protein called Proteasome subunit beta type-4.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 13  | M     | 216      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1685  | 1063 | 291 | 319 | 12 |         |         |       |
| 13  | a     | 216      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1685  | 1063 | 291 | 319 | 12 |         |         |       |

- Molecule 14 is a protein called Proteasome subunit beta type-9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14  | N     | 199      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1498  | 947 | 254 | 289 | 8 |         |         |       |
| 14  | b     | 199      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1498  | 947 | 254 | 289 | 8 |         |         |       |

- Molecule 15 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 15  | A     | 3        | Total | Cl | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 15  | D     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 15  | E     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 15  | H     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 15  | I     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 15  | J     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 15  | L     | 2        | Total Cl<br>2 2 | 0       | 0       |
| 15  | M     | 4        | Total Cl<br>4 4 | 0       | 0       |
| 15  | N     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 15  | O     | 2        | Total Cl<br>2 2 | 0       | 0       |
| 15  | P     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 15  | Q     | 4        | Total Cl<br>4 4 | 0       | 0       |
| 15  | R     | 3        | Total Cl<br>3 3 | 0       | 0       |
| 15  | S     | 2        | Total Cl<br>2 2 | 0       | 0       |
| 15  | U     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 15  | V     | 4        | Total Cl<br>4 4 | 0       | 0       |
| 15  | W     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 15  | X     | 3        | Total Cl<br>3 3 | 0       | 0       |
| 15  | Z     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 15  | a     | 4        | Total Cl<br>4 4 | 0       | 0       |

- Molecule 16 is POTASSIUM ION (CCD ID: K) (formula: K).

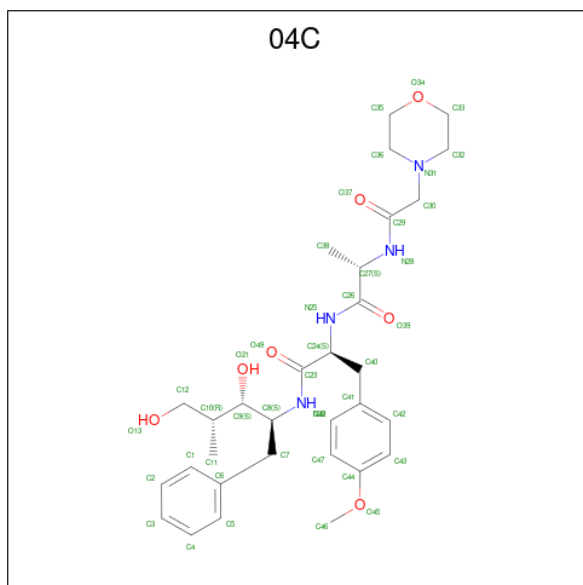
| Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 16  | B     | 1        | Total K<br>1 1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 16  | G     | 1        | Total K<br>1 1 | 0       | 0       |
| 16  | I     | 1        | Total K<br>1 1 | 0       | 0       |
| 16  | K     | 1        | Total K<br>1 1 | 0       | 0       |
| 16  | L     | 1        | Total K<br>1 1 | 0       | 0       |
| 16  | M     | 1        | Total K<br>1 1 | 0       | 0       |
| 16  | S     | 1        | Total K<br>1 1 | 0       | 0       |
| 16  | X     | 1        | Total K<br>1 1 | 0       | 0       |
| 16  | Z     | 3        | Total K<br>3 3 | 0       | 0       |
| 16  | a     | 1        | Total K<br>1 1 | 0       | 0       |
| 16  | b     | 1        | Total K<br>1 1 | 0       | 0       |

- Molecule 17 is 1,2,4-trideoxy-4-methyl-2-{[N-(morpholin-4-ylacetyl)-L-alanyl-O-methyl-L-tyrosyl]amino}-1-phenyl-D-xylitol (CCD ID: 04C) (formula: C<sub>31</sub>H<sub>44</sub>N<sub>4</sub>O<sub>7</sub>).



| Mol | Chain | Residues | Atoms                    | ZeroOcc | AltConf |
|-----|-------|----------|--------------------------|---------|---------|
| 17  | H     | 1        | Total C N O<br>42 31 4 7 | 0       | 0       |

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| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 17  | K     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 42    | 31 | 4 | 7 |         |         |
| 17  | N     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 42    | 31 | 4 | 7 |         |         |
| 17  | V     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 42    | 31 | 4 | 7 |         |         |
| 17  | Y     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 42    | 31 | 4 | 7 |         |         |
| 17  | b     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 42    | 31 | 4 | 7 |         |         |

- Molecule 18 is IODIDE ION (CCD ID: IOD) (formula: I).

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 18  | H     | 1        | Total | I | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 18  | K     | 1        | Total | I | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 18  | N     | 1        | Total | I | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 18  | V     | 1        | Total | I | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 18  | Y     | 1        | Total | I | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 18  | b     | 1        | Total | I | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

- Molecule 19 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 19  | A     | 43       | Total | O  | 0       | 0       |
|     |       |          | 43    | 43 |         |         |
| 19  | B     | 42       | Total | O  | 0       | 0       |
|     |       |          | 42    | 42 |         |         |
| 19  | C     | 29       | Total | O  | 0       | 0       |
|     |       |          | 29    | 29 |         |         |
| 19  | D     | 24       | Total | O  | 0       | 0       |
|     |       |          | 24    | 24 |         |         |
| 19  | E     | 39       | Total | O  | 0       | 0       |
|     |       |          | 39    | 39 |         |         |
| 19  | F     | 37       | Total | O  | 0       | 0       |
|     |       |          | 37    | 37 |         |         |

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| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 19  | G     | 44       | Total O<br>44 44 | 0       | 0       |
| 19  | H     | 40       | Total O<br>40 40 | 0       | 0       |
| 19  | I     | 25       | Total O<br>25 25 | 0       | 0       |
| 19  | J     | 28       | Total O<br>28 28 | 0       | 0       |
| 19  | K     | 32       | Total O<br>32 32 | 0       | 0       |
| 19  | L     | 43       | Total O<br>43 43 | 0       | 0       |
| 19  | M     | 50       | Total O<br>50 50 | 0       | 0       |
| 19  | N     | 29       | Total O<br>29 29 | 0       | 0       |
| 19  | O     | 44       | Total O<br>44 44 | 0       | 0       |
| 19  | P     | 38       | Total O<br>38 38 | 0       | 0       |
| 19  | Q     | 13       | Total O<br>13 13 | 0       | 0       |
| 19  | R     | 24       | Total O<br>24 24 | 0       | 0       |
| 19  | S     | 40       | Total O<br>40 40 | 0       | 0       |
| 19  | T     | 32       | Total O<br>32 32 | 0       | 0       |
| 19  | U     | 38       | Total O<br>38 38 | 0       | 0       |
| 19  | V     | 39       | Total O<br>39 39 | 0       | 0       |
| 19  | W     | 39       | Total O<br>39 39 | 0       | 0       |
| 19  | X     | 20       | Total O<br>20 20 | 0       | 0       |
| 19  | Y     | 36       | Total O<br>36 36 | 0       | 0       |
| 19  | Z     | 49       | Total O<br>49 49 | 0       | 0       |
| 19  | a     | 35       | Total O<br>35 35 | 0       | 0       |

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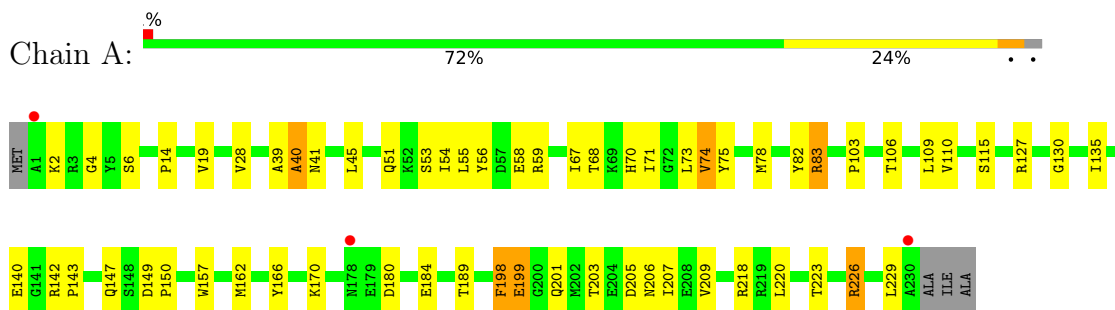
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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 19  | b     | 33       | Total | O  | 0       | 0       |
|     |       |          | 33    | 33 |         |         |

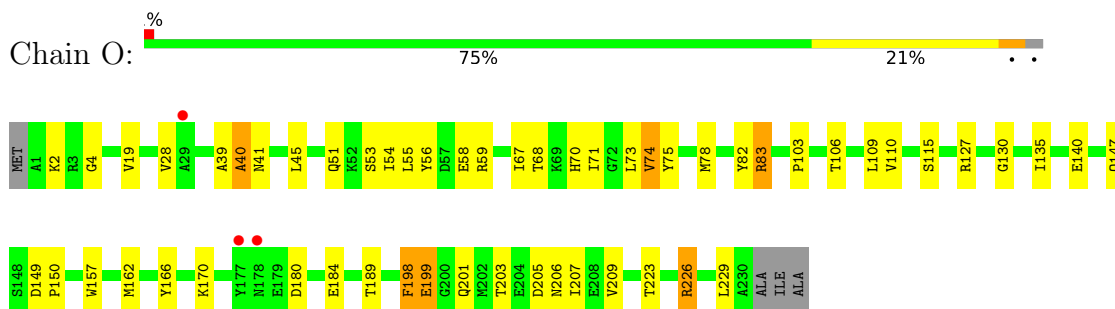
### 3 Residue-property plots [i](#)

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 electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

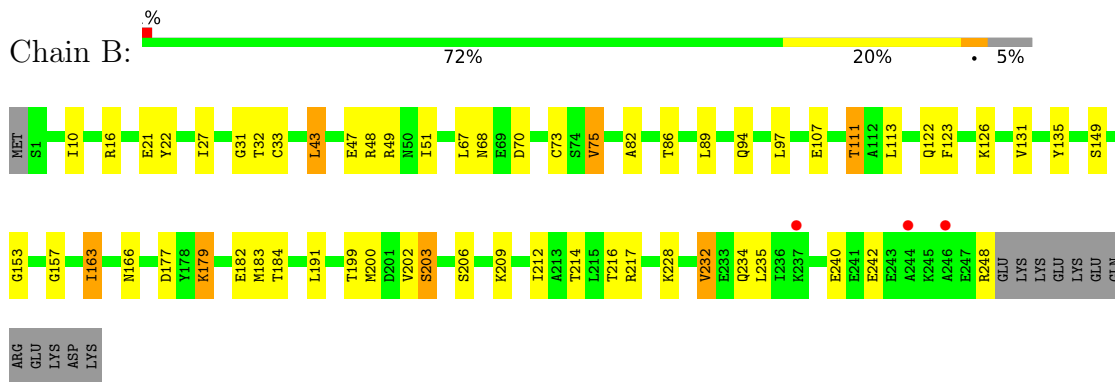
- Molecule 1: Proteasome subunit alpha type-2



- Molecule 1: Proteasome subunit alpha type-2

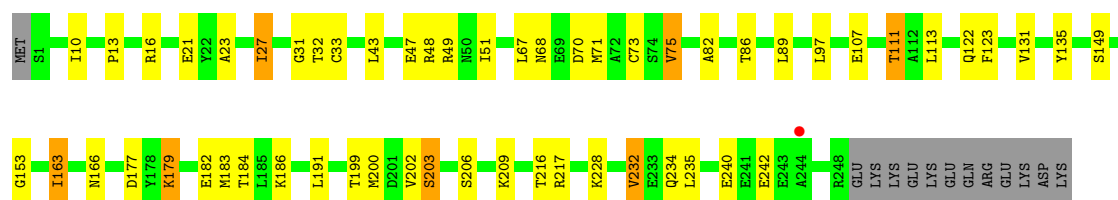


- Molecule 2: Proteasome subunit alpha type-4

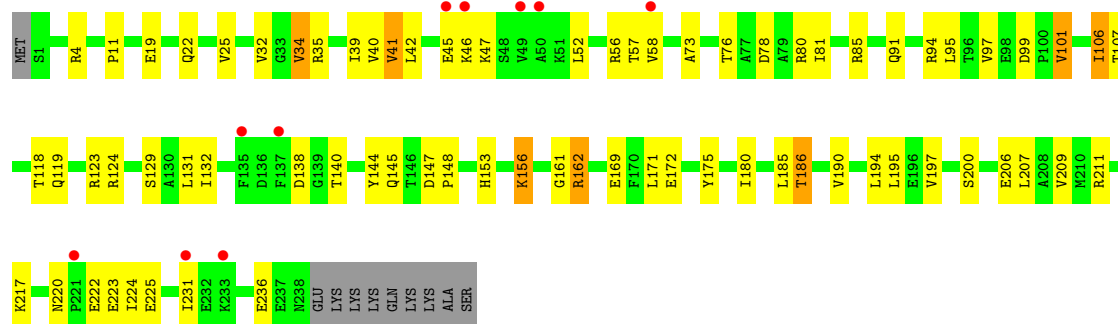


- Molecule 2: Proteasome subunit alpha type-4

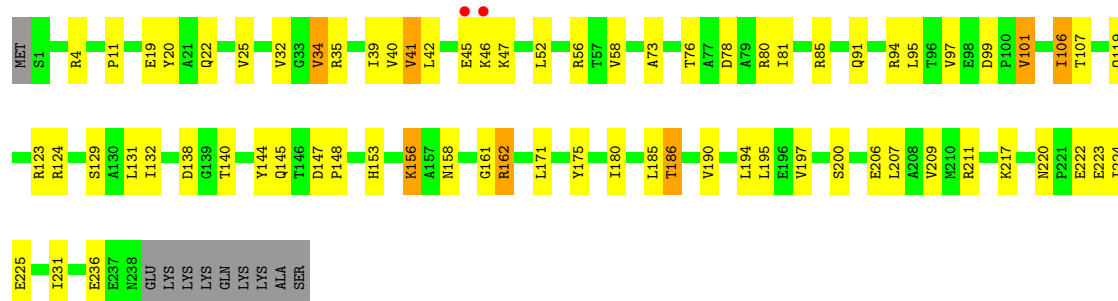




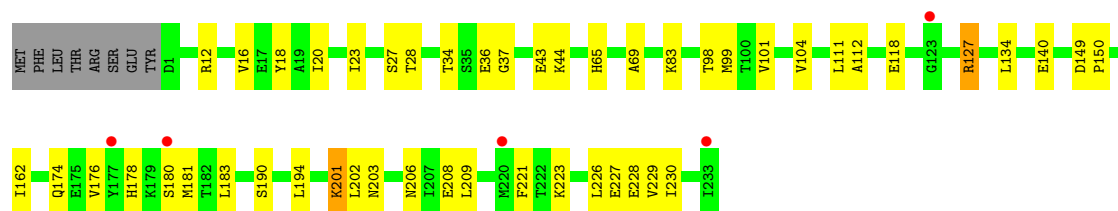
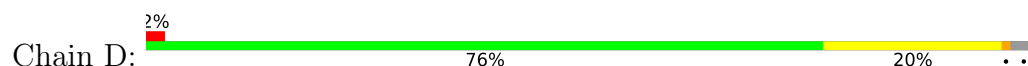
• Molecule 3: Proteasome subunit alpha type-7



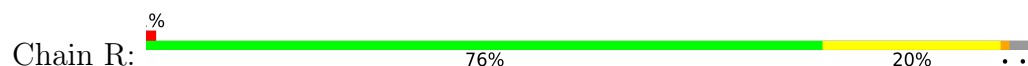
• Molecule 3: Proteasome subunit alpha type-7

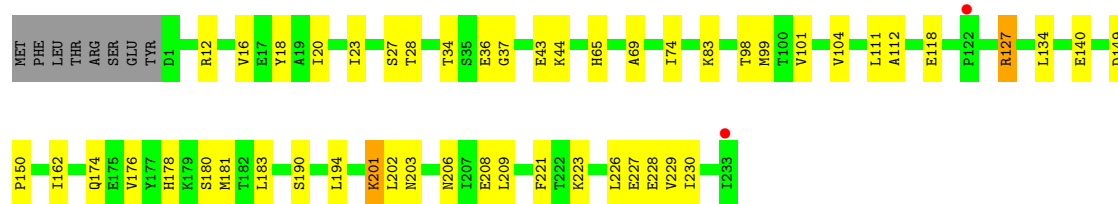


• Molecule 4: Proteasome subunit alpha type-5



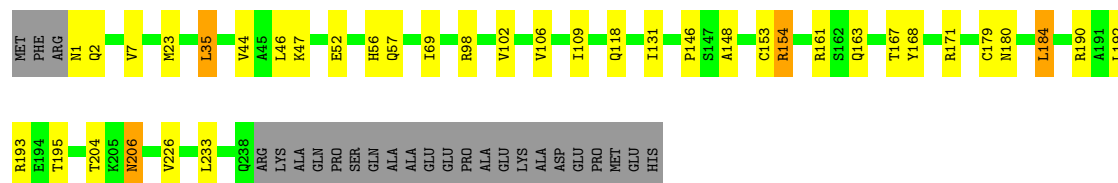
• Molecule 4: Proteasome subunit alpha type-5





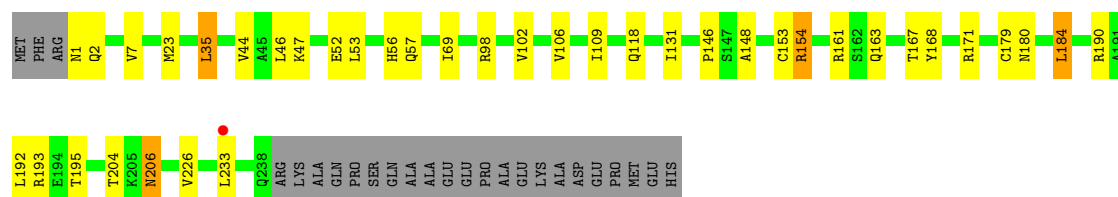
• Molecule 5: Proteasome subunit alpha type-1

Chain E: 76% 13% 10%



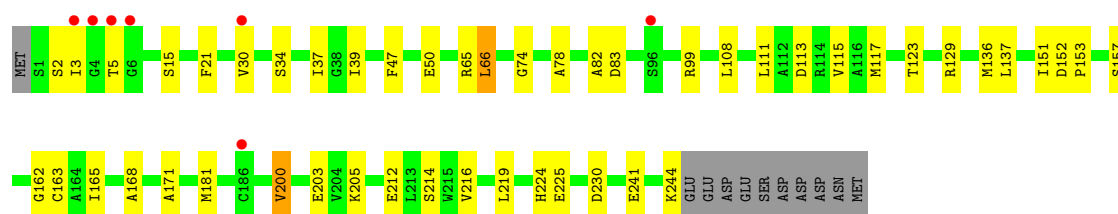
• Molecule 5: Proteasome subunit alpha type-1

Chain S: 76% 13% 10%



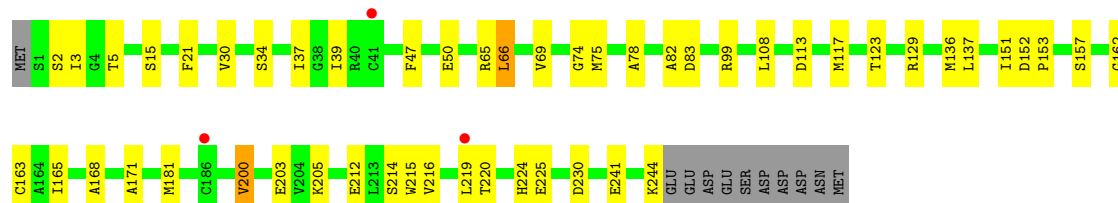
• Molecule 6: Proteasome subunit alpha type-3

Chain F: 3% 76% 18% . .

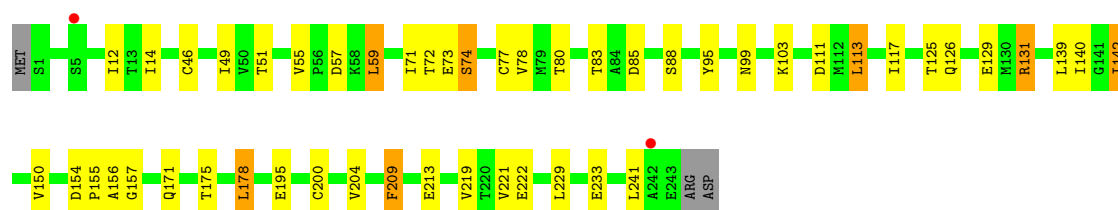
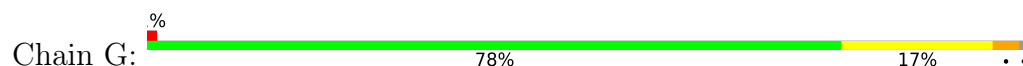


• Molecule 6: Proteasome subunit alpha type-3

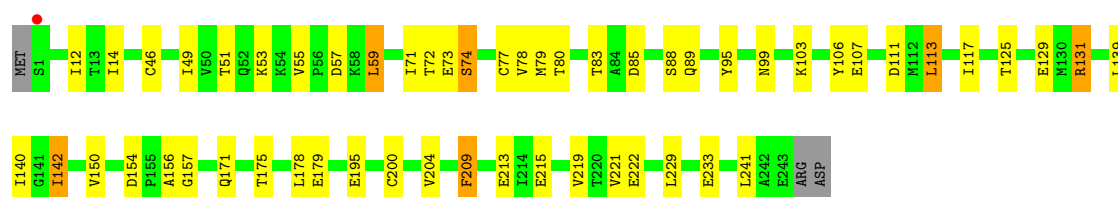
Chain T: .% 76% 19% . .



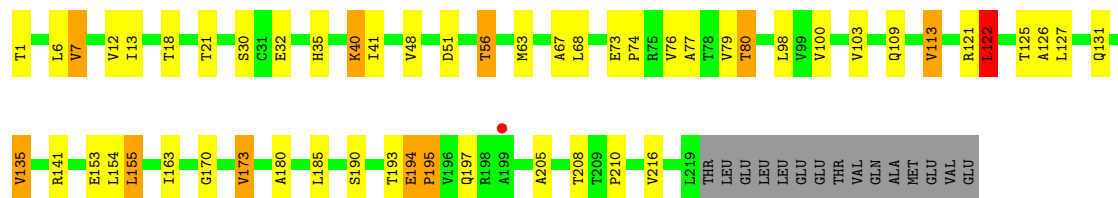
- Molecule 7: Proteasome subunit alpha type-6



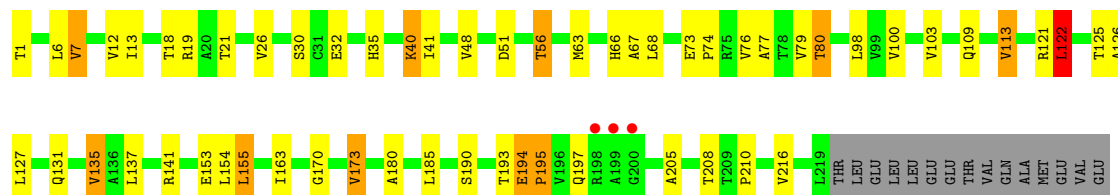
- Molecule 7: Proteasome subunit alpha type-6



- Molecule 8: Proteasome subunit beta type-10



- Molecule 8: Proteasome subunit beta type-10



- Molecule 9: Proteasome subunit beta type-3

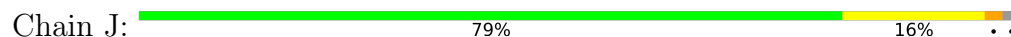




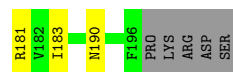
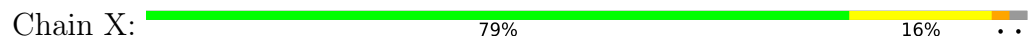
• Molecule 9: Proteasome subunit beta type-3



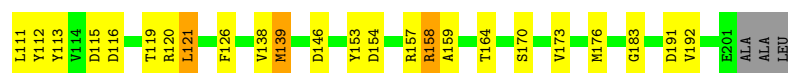
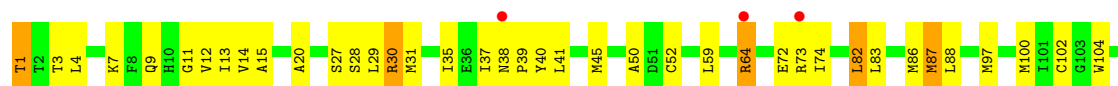
• Molecule 10: Proteasome subunit beta type-2



• Molecule 10: Proteasome subunit beta type-2



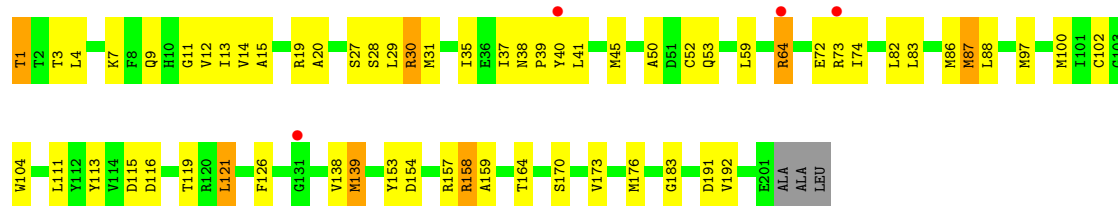
• Molecule 11: Proteasome subunit beta type-8



• Molecule 11: Proteasome subunit beta type-8

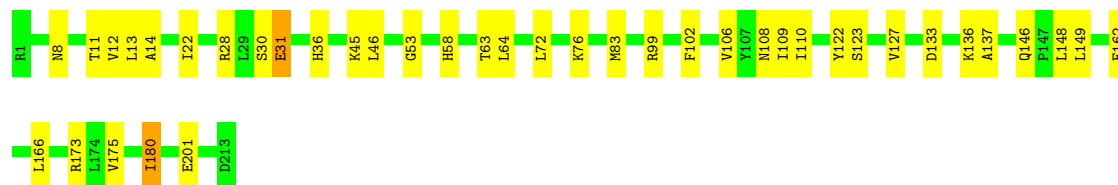






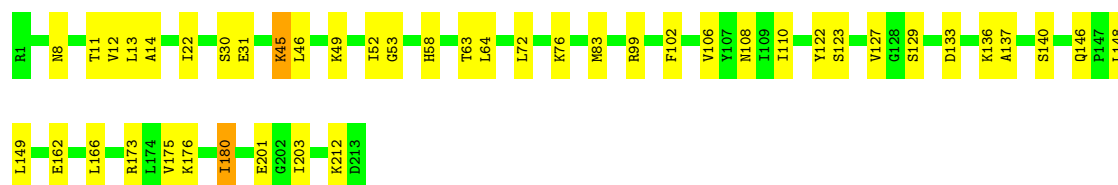
• Molecule 12: Proteasome subunit beta type-1

Chain L: 81% 18% .



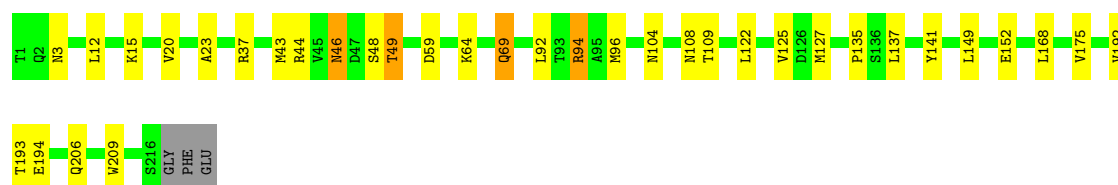
• Molecule 12: Proteasome subunit beta type-1

Chain Z: 79% 20% .



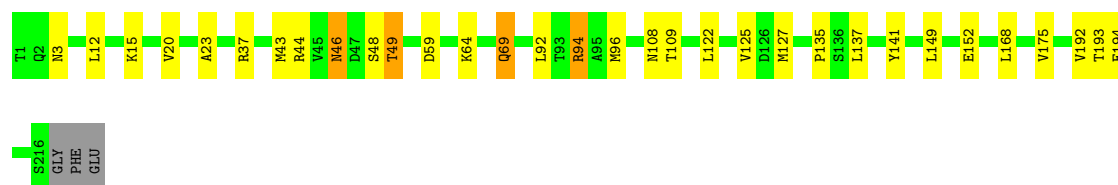
• Molecule 13: Proteasome subunit beta type-4

Chain M: 83% 14% ..

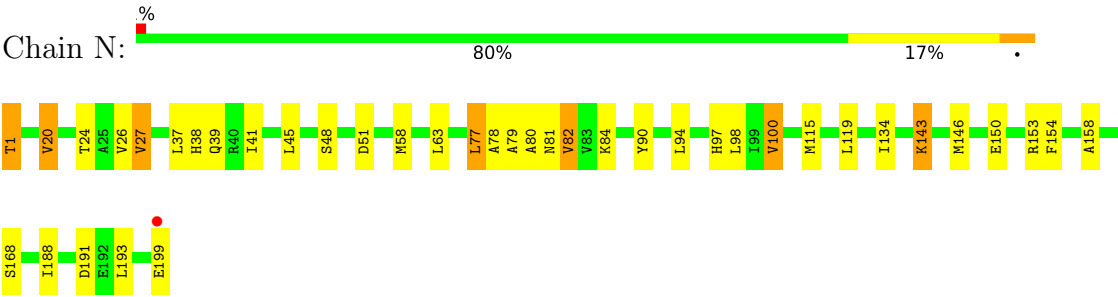


• Molecule 13: Proteasome subunit beta type-4

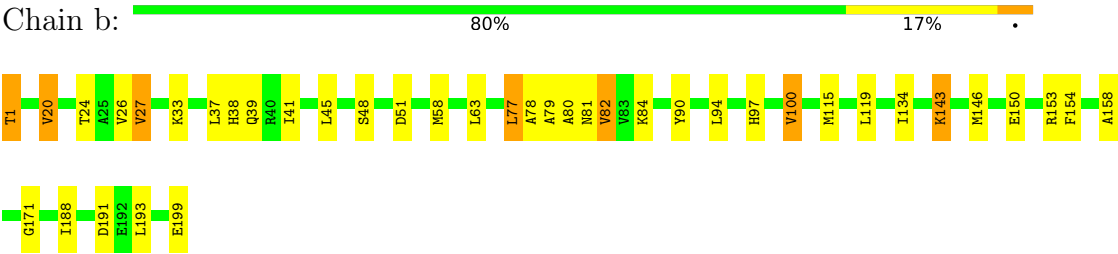
Chain a: 84% 13% ..



• Molecule 14: Proteasome subunit beta type-9



● Molecule 14: Proteasome subunit beta type-9



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 117.30Å 194.60Å 157.70Å<br>90.00° 107.10° 90.00°            | Depositor        |
| Resolution (Å)                                                          | 15.00 – 2.90<br>15.00 – 2.90                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.1 (15.00-2.90)<br>96.5 (15.00-2.90)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.12                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.37 (at 2.90Å)                                             | Xtrriage         |
| Refinement program                                                      | REFMAC 5.6.0119                                             | Depositor        |
| R, $R_{free}$                                                           | 0.235 , 0.275<br>0.234 , 0.274                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 7255 reflections (5.00%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 46.1                                                        | Xtrriage         |
| Anisotropy                                                              | 0.520                                                       | Xtrriage         |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 55.9                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$ | Xtrriage         |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtrriage         |
| $F_o, F_c$ correlation                                                  | 0.91                                                        | EDS              |
| Total number of atoms                                                   | 49805                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 61.0                                                        | wwPDB-VP         |

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5201e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: IOD, CL, 04C, K

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     | 0.52         | 0/1840         | 0.79        | 0/2491          |
| 1   | O     | 0.52         | 0/1840         | 0.79        | 0/2491          |
| 2   | B     | 0.49         | 0/1980         | 0.81        | 0/2667          |
| 2   | P     | 0.49         | 0/1980         | 0.81        | 0/2667          |
| 3   | C     | 0.47         | 0/1903         | 0.82        | 2/2569 (0.1%)   |
| 3   | Q     | 0.47         | 0/1903         | 0.82        | 2/2569 (0.1%)   |
| 4   | D     | 0.52         | 0/1805         | 0.77        | 0/2437          |
| 4   | R     | 0.52         | 0/1805         | 0.77        | 0/2437          |
| 5   | E     | 0.57         | 0/1907         | 0.81        | 0/2578          |
| 5   | S     | 0.57         | 0/1907         | 0.81        | 0/2578          |
| 6   | F     | 0.52         | 0/1938         | 0.81        | 0/2608          |
| 6   | T     | 0.52         | 0/1938         | 0.81        | 0/2608          |
| 7   | G     | 0.50         | 0/1924         | 0.82        | 3/2600 (0.1%)   |
| 7   | U     | 0.49         | 0/1924         | 0.82        | 3/2600 (0.1%)   |
| 8   | H     | 0.60         | 1/1645 (0.1%)  | 0.82        | 1/2235 (0.0%)   |
| 8   | V     | 0.61         | 1/1645 (0.1%)  | 0.83        | 1/2235 (0.0%)   |
| 9   | I     | 0.46         | 0/1621         | 0.80        | 0/2185          |
| 9   | W     | 0.46         | 0/1621         | 0.81        | 1/2185 (0.0%)   |
| 10  | J     | 0.51         | 0/1602         | 0.79        | 0/2167          |
| 10  | X     | 0.51         | 0/1602         | 0.79        | 0/2167          |
| 11  | K     | 0.53         | 1/1597 (0.1%)  | 0.80        | 0/2151          |
| 11  | Y     | 0.53         | 1/1597 (0.1%)  | 0.81        | 2/2151 (0.1%)   |
| 12  | L     | 0.48         | 0/1685         | 0.77        | 0/2271          |
| 12  | Z     | 0.49         | 0/1685         | 0.77        | 0/2271          |
| 13  | M     | 0.50         | 0/1718         | 0.76        | 0/2325          |
| 13  | a     | 0.50         | 0/1718         | 0.76        | 0/2325          |
| 14  | N     | 0.55         | 1/1526 (0.1%)  | 0.85        | 2/2071 (0.1%)   |
| 14  | b     | 0.55         | 1/1526 (0.1%)  | 0.87        | 2/2071 (0.1%)   |
| All | All   | 0.52         | 6/49382 (0.0%) | 0.80        | 19/66710 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 11  | K     | 0                   | 1                   |
| 11  | Y     | 0                   | 1                   |
| 14  | N     | 0                   | 2                   |
| 14  | b     | 0                   | 1                   |
| All | All   | 0                   | 5                   |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 8   | V     | 1   | THR  | C-N   | 10.45 | 1.47        | 1.33     |
| 8   | H     | 1   | THR  | C-N   | 9.98  | 1.46        | 1.33     |
| 11  | Y     | 1   | THR  | C-N   | 7.70  | 1.45        | 1.33     |
| 11  | K     | 1   | THR  | C-N   | 7.06  | 1.44        | 1.33     |
| 14  | N     | 1   | THR  | C-N   | 6.07  | 1.41        | 1.33     |
| 14  | b     | 1   | THR  | C-N   | 5.97  | 1.41        | 1.33     |

All (19) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 14  | b     | 1   | THR  | CA-C-N | 9.48  | 136.14      | 122.77   |
| 14  | b     | 1   | THR  | C-N-CA | 9.48  | 136.14      | 122.77   |
| 14  | N     | 1   | THR  | CA-C-N | 7.91  | 133.92      | 122.77   |
| 14  | N     | 1   | THR  | C-N-CA | 7.91  | 133.92      | 122.77   |
| 3   | C     | 52  | LEU  | N-CA-C | -6.79 | 104.68      | 114.12   |
| 8   | V     | 122 | LEU  | N-CA-C | 6.68  | 114.23      | 108.22   |
| 8   | H     | 122 | LEU  | N-CA-C | 6.48  | 114.05      | 108.22   |
| 11  | Y     | 1   | THR  | CA-C-N | 6.18  | 132.74      | 122.73   |
| 11  | Y     | 1   | THR  | C-N-CA | 6.18  | 132.74      | 122.73   |
| 3   | Q     | 52  | LEU  | N-CA-C | -6.00 | 104.62      | 113.61   |
| 3   | C     | 200 | SER  | N-CA-C | 5.53  | 117.43      | 110.24   |
| 3   | Q     | 200 | SER  | N-CA-C | 5.43  | 117.30      | 110.24   |
| 9   | W     | 117 | LYS  | N-CA-C | 5.26  | 116.04      | 109.57   |
| 7   | U     | 46  | CYS  | N-CA-C | 5.12  | 116.08      | 108.60   |
| 7   | G     | 46  | CYS  | N-CA-C | 5.10  | 116.05      | 108.60   |
| 7   | G     | 55  | VAL  | CA-C-N | 5.07  | 125.10      | 119.32   |
| 7   | G     | 55  | VAL  | C-N-CA | 5.07  | 125.10      | 119.32   |
| 7   | U     | 55  | VAL  | CA-C-N | 5.03  | 125.05      | 119.32   |
| 7   | U     | 55  | VAL  | C-N-CA | 5.03  | 125.05      | 119.32   |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 11  | K     | 1   | THR  | Peptide           |
| 14  | N     | 1   | THR  | Peptide,Mainchain |
| 11  | Y     | 1   | THR  | Peptide           |
| 14  | b     | 1   | THR  | Peptide           |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1801  | 0        | 1800     | 42      | 0            |
| 1   | O     | 1801  | 0        | 1800     | 36      | 0            |
| 2   | B     | 1950  | 0        | 1973     | 30      | 0            |
| 2   | P     | 1950  | 0        | 1973     | 26      | 0            |
| 3   | C     | 1876  | 0        | 1902     | 46      | 0            |
| 3   | Q     | 1876  | 0        | 1902     | 44      | 0            |
| 4   | D     | 1778  | 0        | 1767     | 27      | 0            |
| 4   | R     | 1778  | 0        | 1767     | 29      | 0            |
| 5   | E     | 1872  | 0        | 1859     | 24      | 0            |
| 5   | S     | 1872  | 0        | 1859     | 24      | 0            |
| 6   | F     | 1903  | 0        | 1894     | 31      | 0            |
| 6   | T     | 1903  | 0        | 1894     | 32      | 0            |
| 7   | G     | 1890  | 0        | 1900     | 30      | 0            |
| 7   | U     | 1890  | 0        | 1900     | 34      | 0            |
| 8   | H     | 1619  | 0        | 1640     | 28      | 0            |
| 8   | V     | 1619  | 0        | 1640     | 31      | 0            |
| 9   | I     | 1592  | 0        | 1612     | 35      | 0            |
| 9   | W     | 1592  | 0        | 1612     | 35      | 0            |
| 10  | J     | 1570  | 0        | 1573     | 21      | 0            |
| 10  | X     | 1570  | 0        | 1573     | 20      | 0            |
| 11  | K     | 1566  | 0        | 1516     | 47      | 1            |
| 11  | Y     | 1566  | 0        | 1515     | 47      | 0            |
| 12  | L     | 1654  | 0        | 1652     | 21      | 0            |
| 12  | Z     | 1654  | 0        | 1651     | 26      | 0            |
| 13  | M     | 1685  | 0        | 1664     | 21      | 1            |
| 13  | a     | 1685  | 0        | 1664     | 21      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 14  | N     | 1498  | 0        | 1476     | 24      | 0            |
| 14  | b     | 1498  | 0        | 1476     | 23      | 0            |
| 15  | A     | 3     | 0        | 0        | 0       | 0            |
| 15  | D     | 1     | 0        | 0        | 0       | 0            |
| 15  | E     | 1     | 0        | 0        | 0       | 0            |
| 15  | H     | 1     | 0        | 0        | 0       | 0            |
| 15  | I     | 1     | 0        | 0        | 0       | 0            |
| 15  | J     | 1     | 0        | 0        | 0       | 0            |
| 15  | L     | 2     | 0        | 0        | 0       | 0            |
| 15  | M     | 4     | 0        | 0        | 0       | 0            |
| 15  | N     | 1     | 0        | 0        | 0       | 0            |
| 15  | O     | 2     | 0        | 0        | 0       | 0            |
| 15  | P     | 1     | 0        | 0        | 0       | 0            |
| 15  | Q     | 4     | 0        | 0        | 0       | 0            |
| 15  | R     | 3     | 0        | 0        | 0       | 0            |
| 15  | S     | 2     | 0        | 0        | 0       | 0            |
| 15  | U     | 1     | 0        | 0        | 0       | 0            |
| 15  | V     | 4     | 0        | 0        | 0       | 0            |
| 15  | W     | 1     | 0        | 0        | 0       | 0            |
| 15  | X     | 3     | 0        | 0        | 0       | 0            |
| 15  | Z     | 1     | 0        | 0        | 0       | 0            |
| 15  | a     | 4     | 0        | 0        | 0       | 0            |
| 16  | B     | 1     | 0        | 0        | 0       | 0            |
| 16  | G     | 1     | 0        | 0        | 0       | 0            |
| 16  | I     | 1     | 0        | 0        | 0       | 0            |
| 16  | K     | 1     | 0        | 0        | 0       | 0            |
| 16  | L     | 1     | 0        | 0        | 0       | 0            |
| 16  | M     | 1     | 0        | 0        | 0       | 0            |
| 16  | S     | 1     | 0        | 0        | 0       | 0            |
| 16  | X     | 1     | 0        | 0        | 0       | 0            |
| 16  | Z     | 3     | 0        | 0        | 0       | 0            |
| 16  | a     | 1     | 0        | 0        | 0       | 0            |
| 16  | b     | 1     | 0        | 0        | 0       | 0            |
| 17  | H     | 42    | 0        | 42       | 0       | 0            |
| 17  | K     | 42    | 0        | 42       | 4       | 0            |
| 17  | N     | 42    | 0        | 42       | 3       | 0            |
| 17  | V     | 42    | 0        | 42       | 1       | 0            |
| 17  | Y     | 42    | 0        | 42       | 4       | 0            |
| 17  | b     | 42    | 0        | 42       | 3       | 0            |
| 18  | H     | 1     | 0        | 0        | 0       | 0            |
| 18  | K     | 1     | 0        | 0        | 1       | 0            |
| 18  | N     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 18  | V     | 1     | 0        | 0        | 1       | 0            |
| 18  | Y     | 1     | 0        | 0        | 0       | 0            |
| 18  | b     | 1     | 0        | 0        | 0       | 0            |
| 19  | A     | 43    | 0        | 0        | 2       | 0            |
| 19  | B     | 42    | 0        | 0        | 4       | 0            |
| 19  | C     | 29    | 0        | 0        | 0       | 0            |
| 19  | D     | 24    | 0        | 0        | 0       | 0            |
| 19  | E     | 39    | 0        | 0        | 0       | 0            |
| 19  | F     | 37    | 0        | 0        | 0       | 0            |
| 19  | G     | 44    | 0        | 0        | 1       | 0            |
| 19  | H     | 40    | 0        | 0        | 0       | 0            |
| 19  | I     | 25    | 0        | 0        | 0       | 0            |
| 19  | J     | 28    | 0        | 0        | 0       | 0            |
| 19  | K     | 32    | 0        | 0        | 3       | 0            |
| 19  | L     | 43    | 0        | 0        | 3       | 0            |
| 19  | M     | 50    | 0        | 0        | 1       | 0            |
| 19  | N     | 29    | 0        | 0        | 2       | 0            |
| 19  | O     | 44    | 0        | 0        | 0       | 0            |
| 19  | P     | 38    | 0        | 0        | 0       | 0            |
| 19  | Q     | 13    | 0        | 0        | 0       | 0            |
| 19  | R     | 24    | 0        | 0        | 0       | 0            |
| 19  | S     | 40    | 0        | 0        | 0       | 0            |
| 19  | T     | 32    | 0        | 0        | 0       | 0            |
| 19  | U     | 38    | 0        | 0        | 3       | 0            |
| 19  | V     | 39    | 0        | 0        | 0       | 0            |
| 19  | W     | 39    | 0        | 0        | 0       | 0            |
| 19  | X     | 20    | 0        | 0        | 0       | 0            |
| 19  | Y     | 36    | 0        | 0        | 0       | 0            |
| 19  | Z     | 49    | 0        | 0        | 5       | 0            |
| 19  | a     | 35    | 0        | 0        | 0       | 0            |
| 19  | b     | 33    | 0        | 0        | 0       | 0            |
| All | All   | 49805 | 0        | 48706    | 792     | 1            |

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 8.

All (792) 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) |
|-----------------|------------------|--------------------------|-------------------|
| 5:S:154:ARG:HG2 | 5:S:154:ARG:HH11 | 1.26                     | 0.98              |
| 11:Y:31:MET:HG2 | 17:Y:301:04C:H42 | 1.45                     | 0.98              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:E:154:ARG:HG2  | 5:E:154:ARG:HH11  | 1.27                     | 0.96              |
| 5:E:2:GLN:HE22   | 6:F:5:THR:HA      | 1.29                     | 0.96              |
| 3:C:162:ARG:HG2  | 3:C:162:ARG:HH11  | 1.31                     | 0.95              |
| 3:Q:35:ARG:HH21  | 3:Q:156:LYS:HG3   | 1.32                     | 0.93              |
| 3:Q:162:ARG:HG2  | 3:Q:162:ARG:HH11  | 1.31                     | 0.93              |
| 3:C:35:ARG:HH21  | 3:C:156:LYS:HG3   | 1.32                     | 0.92              |
| 12:Z:110:ILE:HA  | 19:Z:426:HOH:O    | 1.67                     | 0.92              |
| 12:Z:49:LYS:HB3  | 19:Z:415:HOH:O    | 1.72                     | 0.89              |
| 8:H:194:GLU:H    | 8:H:195:PRO:HD3   | 1.37                     | 0.88              |
| 8:V:194:GLU:H    | 8:V:195:PRO:HD3   | 1.37                     | 0.87              |
| 4:R:201:LYS:HE2  | 4:R:201:LYS:H     | 1.42                     | 0.85              |
| 11:K:31:MET:HG2  | 17:K:301:04C:H42  | 1.57                     | 0.84              |
| 12:Z:52:ILE:HA   | 19:Z:426:HOH:O    | 1.76                     | 0.84              |
| 11:K:3:THR:HG22  | 11:K:100:MET:HE2  | 1.62                     | 0.82              |
| 4:D:201:LYS:HE2  | 4:D:201:LYS:H     | 1.44                     | 0.81              |
| 8:H:40:LYS:HE2   | 8:H:73:GLU:HG3    | 1.63                     | 0.81              |
| 11:Y:3:THR:HG22  | 11:Y:100:MET:HE2  | 1.62                     | 0.80              |
| 11:Y:53:GLN:OE1  | 12:Z:129:SER:HA   | 1.82                     | 0.79              |
| 8:V:40:LYS:HE2   | 8:V:73:GLU:HG3    | 1.65                     | 0.77              |
| 11:Y:45:MET:HE2  | 17:Y:301:04C:H44  | 1.67                     | 0.77              |
| 5:E:2:GLN:NE2    | 6:F:5:THR:HA      | 2.00                     | 0.76              |
| 9:W:124:ASP:HB2  | 9:W:128:CYS:H     | 1.50                     | 0.76              |
| 3:C:41:VAL:HB    | 3:C:209:VAL:HG12  | 1.68                     | 0.75              |
| 3:C:162:ARG:HG2  | 3:C:162:ARG:NH1   | 1.95                     | 0.75              |
| 5:S:2:GLN:HE22   | 6:T:5:THR:HA      | 1.51                     | 0.75              |
| 3:Q:41:VAL:HB    | 3:Q:209:VAL:HG12  | 1.68                     | 0.74              |
| 5:S:47:LYS:HB3   | 5:S:56:HIS:HB3    | 1.69                     | 0.74              |
| 12:L:13:LEU:HD11 | 12:L:149:LEU:HD11 | 1.70                     | 0.74              |
| 9:I:124:ASP:HB2  | 9:I:128:CYS:H     | 1.50                     | 0.74              |
| 5:E:47:LYS:HB3   | 5:E:56:HIS:HB3    | 1.69                     | 0.73              |
| 2:P:68:ASN:HD22  | 2:P:70:ASP:H      | 1.37                     | 0.73              |
| 6:T:151:ILE:HG12 | 6:T:157:SER:HB3   | 1.70                     | 0.73              |
| 8:V:163:ILE:HG23 | 8:V:170:GLY:HA2   | 1.70                     | 0.73              |
| 12:Z:13:LEU:HD11 | 12:Z:149:LEU:HD11 | 1.70                     | 0.72              |
| 2:B:68:ASN:HD22  | 2:B:70:ASP:H      | 1.37                     | 0.72              |
| 6:F:151:ILE:HG12 | 6:F:157:SER:HB3   | 1.71                     | 0.72              |
| 5:S:154:ARG:HG2  | 5:S:154:ARG:NH1   | 2.02                     | 0.71              |
| 3:Q:162:ARG:HG2  | 3:Q:162:ARG:NH1   | 1.95                     | 0.71              |
| 8:V:131:GLN:O    | 8:V:135:VAL:HG23  | 1.90                     | 0.71              |
| 8:H:131:GLN:O    | 8:H:135:VAL:HG23  | 1.91                     | 0.70              |
| 8:H:163:ILE:HG23 | 8:H:170:GLY:HA2   | 1.73                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:K:45:MET:HE2   | 17:K:301:04C:H44  | 1.71                     | 0.69              |
| 1:O:83:ARG:HH11   | 1:O:83:ARG:HG2    | 1.56                     | 0.69              |
| 2:P:166:ASN:HB2   | 2:P:199:THR:HG23  | 1.73                     | 0.69              |
| 9:W:115:THR:O     | 9:W:116:PHE:CD2   | 2.46                     | 0.69              |
| 9:I:115:THR:O     | 9:I:116:PHE:CD2   | 2.46                     | 0.69              |
| 11:Y:138:VAL:HG21 | 11:Y:159:ALA:HA   | 1.75                     | 0.69              |
| 11:Y:64:ARG:HG3   | 11:Y:64:ARG:HH11  | 1.57                     | 0.68              |
| 2:B:212:ILE:HG22  | 19:B:434:HOH:O    | 1.92                     | 0.68              |
| 1:O:45:LEU:HB3    | 1:O:74:VAL:HG21   | 1.76                     | 0.68              |
| 1:A:45:LEU:HB3    | 1:A:74:VAL:HG21   | 1.76                     | 0.68              |
| 1:A:83:ARG:HG2    | 1:A:83:ARG:HH11   | 1.57                     | 0.68              |
| 2:B:166:ASN:HB2   | 2:B:199:THR:HG23  | 1.73                     | 0.68              |
| 4:D:221:PHE:HB3   | 4:D:226:LEU:CD1   | 2.24                     | 0.68              |
| 4:R:221:PHE:HB3   | 4:R:226:LEU:CD1   | 2.25                     | 0.67              |
| 6:F:136:MET:HE3   | 6:F:163:CYS:HB3   | 1.77                     | 0.67              |
| 8:H:194:GLU:N     | 8:H:195:PRO:HD3   | 2.09                     | 0.67              |
| 11:K:138:VAL:HG21 | 11:K:159:ALA:HA   | 1.75                     | 0.67              |
| 1:A:127:ARG:HH21  | 7:G:125:THR:HG22  | 1.58                     | 0.67              |
| 5:E:2:GLN:HE22    | 6:F:5:THR:CA      | 2.06                     | 0.66              |
| 12:Z:110:ILE:HG12 | 19:Z:426:HOH:O    | 1.93                     | 0.66              |
| 6:T:136:MET:HE3   | 6:T:163:CYS:HB3   | 1.76                     | 0.66              |
| 8:V:194:GLU:N     | 8:V:195:PRO:HD3   | 2.09                     | 0.66              |
| 10:J:52:ASP:HB3   | 10:J:98:TYR:HD2   | 1.61                     | 0.66              |
| 5:E:148:ALA:HB3   | 6:F:82:ALA:HB1    | 1.77                     | 0.66              |
| 5:E:154:ARG:HG2   | 5:E:154:ARG:NH1   | 2.03                     | 0.66              |
| 11:Y:41:LEU:HB2   | 11:Y:73:ARG:HH22  | 1.60                     | 0.66              |
| 8:V:40:LYS:H      | 8:V:40:LYS:HD3    | 1.61                     | 0.66              |
| 6:T:39:ILE:HG22   | 6:T:162:GLY:HA2   | 1.77                     | 0.65              |
| 5:S:148:ALA:HB3   | 6:T:82:ALA:HB1    | 1.77                     | 0.65              |
| 13:a:59:ASP:HB3   | 13:a:108:ASN:HD21 | 1.62                     | 0.65              |
| 11:K:41:LEU:HB2   | 11:K:73:ARG:HH22  | 1.60                     | 0.65              |
| 1:O:203:THR:H     | 1:O:206:ASN:HD22  | 1.43                     | 0.65              |
| 1:A:203:THR:H     | 1:A:206:ASN:HD22  | 1.43                     | 0.65              |
| 4:R:176:VAL:O     | 4:R:176:VAL:HG12  | 1.96                     | 0.65              |
| 4:R:34:THR:HG22   | 4:R:36:GLU:H      | 1.62                     | 0.65              |
| 10:X:52:ASP:HB3   | 10:X:98:TYR:HD2   | 1.61                     | 0.65              |
| 4:D:176:VAL:HG12  | 4:D:176:VAL:O     | 1.96                     | 0.65              |
| 3:Q:101:VAL:HG11  | 3:Q:106:ILE:HG12  | 1.80                     | 0.64              |
| 6:F:39:ILE:HG22   | 6:F:162:GLY:HA2   | 1.78                     | 0.64              |
| 9:W:44:MET:HE3    | 9:W:70:LEU:HD22   | 1.78                     | 0.64              |
| 12:Z:8:ASN:HD22   | 12:Z:58:HIS:H     | 1.45                     | 0.64              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:H:40:LYS:H     | 8:H:40:LYS:HD3    | 1.61                     | 0.64              |
| 2:B:135:TYR:HE1  | 2:B:149:SER:HB2   | 1.63                     | 0.64              |
| 9:W:144:GLN:H    | 9:W:144:GLN:HE21  | 1.46                     | 0.64              |
| 8:V:205:ALA:O    | 8:V:208:THR:HG23  | 1.97                     | 0.64              |
| 4:D:227:GLU:HA   | 4:D:230:ILE:HG22  | 1.79                     | 0.63              |
| 13:M:59:ASP:HB3  | 13:M:108:ASN:HD21 | 1.62                     | 0.63              |
| 9:I:44:MET:HE3   | 9:I:70:LEU:HD22   | 1.79                     | 0.63              |
| 1:O:149:ASP:HB2  | 1:O:150:PRO:HD2   | 1.80                     | 0.63              |
| 3:C:101:VAL:HG11 | 3:C:106:ILE:HG12  | 1.80                     | 0.63              |
| 2:P:135:TYR:HE1  | 2:P:149:SER:HB2   | 1.63                     | 0.63              |
| 9:I:144:GLN:H    | 9:I:144:GLN:HE21  | 1.47                     | 0.63              |
| 11:K:30:ARG:O    | 11:K:30:ARG:HG2   | 1.99                     | 0.63              |
| 4:D:34:THR:HG22  | 4:D:36:GLU:H      | 1.62                     | 0.63              |
| 12:L:8:ASN:HD22  | 12:L:58:HIS:H     | 1.45                     | 0.63              |
| 8:H:205:ALA:O    | 8:H:208:THR:HG23  | 1.98                     | 0.62              |
| 14:b:20:VAL:CG2  | 14:b:27:VAL:HG22  | 2.29                     | 0.62              |
| 8:H:13:ILE:HG12  | 8:H:155:LEU:HD22  | 1.80                     | 0.62              |
| 14:N:20:VAL:CG2  | 14:N:27:VAL:HG22  | 2.28                     | 0.62              |
| 1:O:67:ILE:HD11  | 1:O:73:LEU:HD12   | 1.81                     | 0.62              |
| 11:K:7:LYS:HB3   | 11:K:12:VAL:HG22  | 1.81                     | 0.62              |
| 1:A:149:ASP:HB2  | 1:A:150:PRO:HD2   | 1.80                     | 0.62              |
| 3:C:162:ARG:HH11 | 3:C:162:ARG:CG    | 2.10                     | 0.62              |
| 4:R:227:GLU:HA   | 4:R:230:ILE:HG22  | 1.80                     | 0.62              |
| 12:Z:12:VAL:HG21 | 12:Z:53:GLY:HA3   | 1.82                     | 0.61              |
| 1:A:67:ILE:HD11  | 1:A:73:LEU:HD12   | 1.81                     | 0.61              |
| 11:Y:7:LYS:HB3   | 11:Y:12:VAL:HG22  | 1.81                     | 0.61              |
| 6:F:117:MET:HE1  | 7:G:88:SER:HA     | 1.82                     | 0.61              |
| 11:Y:30:ARG:O    | 11:Y:30:ARG:HG2   | 2.00                     | 0.61              |
| 4:R:221:PHE:HB3  | 4:R:226:LEU:HD12  | 1.83                     | 0.61              |
| 9:I:86:LEU:O     | 9:I:90:VAL:HG23   | 2.01                     | 0.61              |
| 12:L:14:ALA:HA   | 12:L:22:ILE:O     | 2.01                     | 0.60              |
| 9:W:86:LEU:O     | 9:W:90:VAL:HG23   | 2.01                     | 0.60              |
| 3:C:41:VAL:HG22  | 3:C:190:VAL:HG21  | 1.83                     | 0.60              |
| 11:K:64:ARG:HG2  | 11:K:64:ARG:HH11  | 1.66                     | 0.60              |
| 12:Z:14:ALA:HA   | 12:Z:22:ILE:O     | 2.01                     | 0.60              |
| 3:C:35:ARG:NH2   | 3:C:156:LYS:HG3   | 2.11                     | 0.60              |
| 1:O:4:GLY:HA2    | 7:U:129:GLU:HG2   | 1.82                     | 0.60              |
| 1:O:127:ARG:HH21 | 7:U:125:THR:HG22  | 1.67                     | 0.60              |
| 3:Q:41:VAL:HG22  | 3:Q:190:VAL:HG21  | 1.83                     | 0.59              |
| 4:D:221:PHE:HB3  | 4:D:226:LEU:HD12  | 1.83                     | 0.59              |
| 3:Q:162:ARG:HH11 | 3:Q:162:ARG:CG    | 2.10                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:T:168:ALA:HB3  | 6:T:200:VAL:HG13  | 1.84                     | 0.59              |
| 6:F:47:PHE:HB2   | 6:F:214:SER:HB2   | 1.85                     | 0.59              |
| 1:A:45:LEU:HD13  | 1:A:74:VAL:HG23   | 1.85                     | 0.59              |
| 12:L:12:VAL:HG21 | 12:L:53:GLY:HA3   | 1.84                     | 0.59              |
| 10:J:86:ARG:HE   | 10:J:86:ARG:HA    | 1.67                     | 0.58              |
| 4:D:44:LYS:HE2   | 4:D:208:GLU:HG3   | 1.85                     | 0.58              |
| 6:F:66:LEU:HD22  | 6:F:212:GLU:HB3   | 1.85                     | 0.58              |
| 1:O:45:LEU:HD13  | 1:O:74:VAL:HG23   | 1.85                     | 0.58              |
| 10:X:86:ARG:HE   | 10:X:86:ARG:HA    | 1.67                     | 0.58              |
| 14:N:80:ALA:HB1  | 14:N:119:LEU:HD11 | 1.85                     | 0.58              |
| 6:T:47:PHE:HB2   | 6:T:214:SER:HB2   | 1.85                     | 0.58              |
| 6:T:66:LEU:HD22  | 6:T:212:GLU:HB3   | 1.85                     | 0.58              |
| 11:K:73:ARG:HD2  | 11:K:74:ILE:H     | 1.69                     | 0.58              |
| 6:F:168:ALA:HB3  | 6:F:200:VAL:HG13  | 1.84                     | 0.58              |
| 4:R:44:LYS:HE2   | 4:R:208:GLU:HG3   | 1.85                     | 0.58              |
| 8:V:13:ILE:HG12  | 8:V:155:LEU:HD22  | 1.86                     | 0.57              |
| 3:Q:35:ARG:NH2   | 3:Q:156:LYS:HG3   | 2.11                     | 0.57              |
| 3:Q:39:ILE:HG22  | 3:Q:211:ARG:HA    | 1.87                     | 0.57              |
| 14:b:80:ALA:HB1  | 14:b:119:LEU:HD11 | 1.86                     | 0.57              |
| 8:V:41:ILE:HG21  | 8:V:79:VAL:HG21   | 1.87                     | 0.57              |
| 11:Y:38:ASN:HB2  | 11:Y:73:ARG:NH2   | 2.20                     | 0.57              |
| 11:Y:73:ARG:HD2  | 11:Y:74:ILE:H     | 1.70                     | 0.57              |
| 1:A:45:LEU:HB3   | 1:A:74:VAL:CG2    | 2.35                     | 0.56              |
| 11:K:38:ASN:HB2  | 11:K:73:ARG:NH2   | 2.19                     | 0.56              |
| 3:C:39:ILE:HG22  | 3:C:211:ARG:HA    | 1.87                     | 0.56              |
| 3:C:45:GLU:OE2   | 3:C:194:LEU:HB3   | 2.06                     | 0.56              |
| 3:Q:45:GLU:OE2   | 3:Q:194:LEU:HB3   | 2.06                     | 0.56              |
| 5:S:2:GLN:NE2    | 6:T:5:THR:HA      | 2.19                     | 0.56              |
| 1:A:218:ARG:HG3  | 19:A:430:HOH:O    | 2.04                     | 0.56              |
| 8:H:41:ILE:HG21  | 8:H:79:VAL:HG21   | 1.88                     | 0.56              |
| 8:V:141:ARG:HB2  | 8:V:154:LEU:HD13  | 1.87                     | 0.56              |
| 9:I:184:VAL:HB   | 9:I:199:LEU:HD12  | 1.88                     | 0.56              |
| 13:M:92:LEU:O    | 13:M:96:MET:HG2   | 2.06                     | 0.56              |
| 2:P:135:TYR:CE1  | 2:P:149:SER:HB2   | 2.41                     | 0.56              |
| 5:E:161:ARG:HD2  | 5:E:195:THR:O     | 2.06                     | 0.56              |
| 9:W:184:VAL:HB   | 9:W:199:LEU:HD12  | 1.88                     | 0.56              |
| 1:O:45:LEU:HB3   | 1:O:74:VAL:CG2    | 2.35                     | 0.55              |
| 13:a:92:LEU:O    | 13:a:96:MET:HG2   | 2.06                     | 0.55              |
| 5:S:161:ARG:HD2  | 5:S:195:THR:O     | 2.07                     | 0.55              |
| 13:a:15:LYS:HB3  | 13:a:20:VAL:HG22  | 1.88                     | 0.55              |
| 11:K:37:ILE:HG22 | 11:K:38:ASN:HD22  | 1.72                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 14:N:98:LEU:HD21 | 19:N:310:HOH:O   | 2.05                     | 0.55              |
| 17:N:201:04C:H8  | 17:N:201:04C:H22 | 1.88                     | 0.55              |
| 11:Y:37:ILE:HG22 | 11:Y:38:ASN:HD22 | 1.71                     | 0.55              |
| 3:C:25:VAL:HG21  | 3:C:129:SER:HB2  | 1.87                     | 0.55              |
| 8:V:109:GLN:HG2  | 8:V:121:ARG:HH11 | 1.71                     | 0.55              |
| 2:B:135:TYR:CE1  | 2:B:149:SER:HB2  | 2.41                     | 0.55              |
| 4:R:174:GLN:HE21 | 5:S:52:GLU:HG2   | 1.72                     | 0.55              |
| 8:H:141:ARG:HB2  | 8:H:154:LEU:HD13 | 1.88                     | 0.55              |
| 8:H:194:GLU:N    | 8:H:195:PRO:CD   | 2.70                     | 0.55              |
| 2:P:153:GLY:O    | 3:Q:80:ARG:NH2   | 2.34                     | 0.55              |
| 3:Q:25:VAL:HG21  | 3:Q:129:SER:HB2  | 1.87                     | 0.55              |
| 5:E:44:VAL:HG12  | 5:E:192:LEU:HD22 | 1.89                     | 0.55              |
| 8:H:109:GLN:HG2  | 8:H:121:ARG:HH11 | 1.70                     | 0.55              |
| 9:I:148:MET:HE2  | 9:I:172:ASN:HB2  | 1.89                     | 0.55              |
| 9:W:148:MET:HE2  | 9:W:172:ASN:HB2  | 1.88                     | 0.55              |
| 7:U:57:ASP:OD2   | 7:U:59:LEU:HB2   | 2.06                     | 0.55              |
| 2:B:75:VAL:HG21  | 2:B:82:ALA:HB1   | 1.89                     | 0.54              |
| 8:V:35:HIS:CG    | 8:V:56:THR:HG21  | 2.42                     | 0.54              |
| 7:G:57:ASP:OD2   | 7:G:59:LEU:HB2   | 2.07                     | 0.54              |
| 5:S:193:ARG:HH22 | 5:S:233:LEU:HD12 | 1.73                     | 0.54              |
| 3:Q:32:VAL:HG12  | 3:Q:194:LEU:HD21 | 1.88                     | 0.54              |
| 1:A:39:ALA:O     | 1:A:41:ASN:N     | 2.36                     | 0.54              |
| 3:C:32:VAL:HG12  | 3:C:194:LEU:HD21 | 1.87                     | 0.54              |
| 11:K:3:THR:CG2   | 11:K:100:MET:HE2 | 2.36                     | 0.54              |
| 11:K:112:TYR:HB3 | 19:K:406:HOH:O   | 2.06                     | 0.54              |
| 3:C:58:VAL:HG12  | 3:C:58:VAL:O     | 2.07                     | 0.54              |
| 8:V:40:LYS:HD3   | 8:V:40:LYS:N     | 2.23                     | 0.54              |
| 2:P:75:VAL:HG21  | 2:P:82:ALA:HB1   | 1.90                     | 0.54              |
| 7:U:95:TYR:O     | 7:U:99:ASN:HB2   | 2.08                     | 0.54              |
| 3:C:19:GLU:HA    | 3:C:22:GLN:HE21  | 1.72                     | 0.54              |
| 5:E:193:ARG:HH22 | 5:E:233:LEU:HD12 | 1.73                     | 0.54              |
| 7:G:95:TYR:O     | 7:G:99:ASN:HB2   | 2.08                     | 0.54              |
| 6:T:152:ASP:HB2  | 6:T:153:PRO:HD2  | 1.90                     | 0.54              |
| 8:V:98:LEU:HB2   | 8:V:113:VAL:HG13 | 1.90                     | 0.54              |
| 3:Q:58:VAL:O     | 3:Q:58:VAL:HG12  | 2.07                     | 0.53              |
| 6:T:117:MET:HE1  | 7:U:88:SER:HA    | 1.89                     | 0.53              |
| 14:b:20:VAL:HG23 | 14:b:27:VAL:HG22 | 1.90                     | 0.53              |
| 2:B:212:ILE:CG2  | 19:B:434:HOH:O   | 2.53                     | 0.53              |
| 13:M:15:LYS:HB3  | 13:M:20:VAL:HG22 | 1.88                     | 0.53              |
| 3:Q:19:GLU:HA    | 3:Q:22:GLN:HE21  | 1.72                     | 0.53              |
| 4:D:221:PHE:HB3  | 4:D:226:LEU:HD11 | 1.89                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 11:K:153:TYR:O   | 11:K:157:ARG:HB2 | 2.09                     | 0.53              |
| 8:V:194:GLU:N    | 8:V:195:PRO:CD   | 2.70                     | 0.53              |
| 14:N:45:LEU:HD23 | 17:N:201:04C:H44 | 1.89                     | 0.53              |
| 6:T:34:SER:HB2   | 6:T:50:GLU:HG3   | 1.90                     | 0.53              |
| 5:S:44:VAL:HG12  | 5:S:192:LEU:HD22 | 1.89                     | 0.53              |
| 12:L:109:ILE:HB  | 19:L:442:HOH:O   | 2.08                     | 0.53              |
| 4:R:221:PHE:HB3  | 4:R:226:LEU:HD11 | 1.90                     | 0.53              |
| 11:Y:3:THR:HG22  | 11:Y:100:MET:CE  | 2.36                     | 0.53              |
| 6:F:152:ASP:HB2  | 6:F:153:PRO:HD2  | 1.90                     | 0.53              |
| 8:H:35:HIS:CG    | 8:H:56:THR:HG21  | 2.44                     | 0.53              |
| 4:D:203:ASN:HB3  | 4:D:206:ASN:HB2  | 1.91                     | 0.53              |
| 3:Q:81:ILE:O     | 3:Q:85:ARG:HG2   | 2.09                     | 0.53              |
| 14:b:33:LYS:HZ3  | 17:b:201:04C:H34 | 1.74                     | 0.53              |
| 13:M:15:LYS:HE2  | 13:M:135:PRO:HA  | 1.91                     | 0.53              |
| 14:N:20:VAL:HG23 | 14:N:27:VAL:HG22 | 1.91                     | 0.53              |
| 13:a:15:LYS:HE2  | 13:a:135:PRO:HA  | 1.91                     | 0.53              |
| 3:C:95:LEU:HG    | 10:J:62:LYS:HG2  | 1.89                     | 0.53              |
| 9:I:171:LEU:HD21 | 9:I:199:LEU:HD13 | 1.91                     | 0.53              |
| 11:Y:153:TYR:O   | 11:Y:157:ARG:HB2 | 2.09                     | 0.52              |
| 3:C:81:ILE:O     | 3:C:85:ARG:HG2   | 2.09                     | 0.52              |
| 6:F:34:SER:HB2   | 6:F:50:GLU:HG3   | 1.90                     | 0.52              |
| 3:Q:180:ILE:HA   | 3:Q:186:THR:HG23 | 1.91                     | 0.52              |
| 4:R:16:VAL:O     | 4:R:20:ILE:HG12  | 2.09                     | 0.52              |
| 10:X:35:MET:HG2  | 10:X:45:LEU:HD22 | 1.92                     | 0.52              |
| 9:I:11:MET:HG3   | 9:I:137:VAL:HG12 | 1.91                     | 0.52              |
| 4:D:16:VAL:O     | 4:D:20:ILE:HG12  | 2.09                     | 0.52              |
| 11:Y:97:MET:H    | 11:Y:116:ASP:HB3 | 1.74                     | 0.52              |
| 12:L:99:ARG:HD2  | 12:L:102:PHE:O   | 2.10                     | 0.52              |
| 4:D:27:SER:HB2   | 4:D:43:GLU:HG3   | 1.91                     | 0.52              |
| 2:P:31:GLY:HA2   | 2:P:49:ARG:NH1   | 2.25                     | 0.52              |
| 9:W:11:MET:HG3   | 9:W:137:VAL:HG12 | 1.91                     | 0.52              |
| 9:W:171:LEU:HD21 | 9:W:199:LEU:HD13 | 1.91                     | 0.52              |
| 7:G:77:CYS:HB3   | 7:G:139:LEU:HD23 | 1.92                     | 0.52              |
| 11:K:40:TYR:HE1  | 11:K:73:ARG:HG2  | 1.75                     | 0.52              |
| 11:K:40:TYR:HB3  | 11:K:183:GLY:HA2 | 1.91                     | 0.52              |
| 11:Y:38:ASN:HB2  | 11:Y:73:ARG:CZ   | 2.39                     | 0.52              |
| 2:B:31:GLY:HA2   | 2:B:49:ARG:NH1   | 2.25                     | 0.52              |
| 14:N:84:LYS:HG3  | 14:N:119:LEU:HB2 | 1.92                     | 0.52              |
| 8:V:210:PRO:HB2  | 9:W:200:LYS:HB3  | 1.92                     | 0.52              |
| 6:F:123:THR:O    | 7:G:131:ARG:NH1  | 2.43                     | 0.52              |
| 7:U:77:CYS:HB3   | 7:U:139:LEU:HD23 | 1.92                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:F:78:ALA:HB3   | 6:F:165:ILE:HD12  | 1.92                     | 0.52              |
| 8:H:40:LYS:HD3   | 8:H:40:LYS:N      | 2.23                     | 0.52              |
| 8:H:98:LEU:HB2   | 8:H:113:VAL:HG13  | 1.92                     | 0.52              |
| 11:K:138:VAL:CG2 | 11:K:159:ALA:HA   | 2.40                     | 0.52              |
| 5:S:206:ASN:C    | 5:S:206:ASN:HD22  | 2.18                     | 0.52              |
| 10:X:21:ALA:HB3  | 10:X:29:LYS:HB2   | 1.92                     | 0.52              |
| 11:Y:40:TYR:HB3  | 11:Y:183:GLY:HA2  | 1.91                     | 0.52              |
| 11:K:74:ILE:HD11 | 19:K:422:HOH:O    | 2.10                     | 0.51              |
| 4:R:203:ASN:HB3  | 4:R:206:ASN:HB2   | 1.91                     | 0.51              |
| 11:K:97:MET:H    | 11:K:116:ASP:HB3  | 1.74                     | 0.51              |
| 11:K:115:ASP:HB2 | 11:K:119:THR:HB   | 1.92                     | 0.51              |
| 3:Q:78:ASP:OD1   | 3:Q:124:ARG:NH2   | 2.43                     | 0.51              |
| 12:Z:99:ARG:HD2  | 12:Z:102:PHE:O    | 2.10                     | 0.51              |
| 2:B:153:GLY:O    | 3:C:80:ARG:NH2    | 2.36                     | 0.51              |
| 3:C:78:ASP:OD1   | 3:C:124:ARG:NH2   | 2.44                     | 0.51              |
| 1:O:198:PHE:O    | 1:O:199:GLU:CB    | 2.59                     | 0.51              |
| 8:V:103:VAL:HG11 | 8:V:180:ALA:HA    | 1.91                     | 0.51              |
| 5:E:206:ASN:C    | 5:E:206:ASN:HD22  | 2.18                     | 0.51              |
| 11:K:3:THR:HG22  | 11:K:100:MET:CE   | 2.36                     | 0.51              |
| 10:J:35:MET:HG2  | 10:J:45:LEU:HD22  | 1.92                     | 0.51              |
| 11:K:38:ASN:HB2  | 11:K:73:ARG:CZ    | 2.41                     | 0.51              |
| 11:K:100:MET:SD  | 11:K:126:PHE:HB2  | 2.51                     | 0.51              |
| 4:R:174:GLN:HA   | 5:S:53:LEU:HD21   | 1.92                     | 0.51              |
| 11:Y:115:ASP:HB2 | 11:Y:119:THR:HB   | 1.92                     | 0.51              |
| 11:Y:138:VAL:CG2 | 11:Y:159:ALA:HA   | 2.41                     | 0.51              |
| 12:Z:110:ILE:HB  | 12:Z:122:TYR:HB2  | 1.92                     | 0.51              |
| 14:b:45:LEU:HD23 | 17:b:201:O4C:H44  | 1.91                     | 0.51              |
| 3:C:180:ILE:HA   | 3:C:186:THR:HG23  | 1.91                     | 0.51              |
| 11:Y:40:TYR:HE1  | 11:Y:73:ARG:HG2   | 1.76                     | 0.51              |
| 2:B:67:LEU:HD11  | 2:B:73:CYS:HB3    | 1.93                     | 0.51              |
| 1:O:39:ALA:O     | 1:O:41:ASN:N      | 2.36                     | 0.51              |
| 6:T:78:ALA:HB3   | 6:T:165:ILE:HD12  | 1.92                     | 0.51              |
| 11:Y:100:MET:SD  | 11:Y:126:PHE:HB2  | 2.51                     | 0.51              |
| 8:H:63:MET:HE3   | 8:H:74:PRO:HB3    | 1.93                     | 0.51              |
| 8:H:103:VAL:HG11 | 8:H:180:ALA:HA    | 1.91                     | 0.51              |
| 2:B:94:GLN:HE21  | 9:I:68:PHE:HA     | 1.76                     | 0.51              |
| 6:F:241:GLU:HA   | 6:F:244:LYS:NZ    | 2.25                     | 0.50              |
| 8:H:67:ALA:HB2   | 8:H:74:PRO:HG3    | 1.93                     | 0.50              |
| 13:M:92:LEU:HD23 | 13:M:125:VAL:HG21 | 1.93                     | 0.50              |
| 4:R:27:SER:HB2   | 4:R:43:GLU:HG3    | 1.91                     | 0.50              |
| 14:b:63:LEU:HD21 | 14:b:79:ALA:HA    | 1.93                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:51:GLN:HG2   | 1:A:56:TYR:CD2    | 2.46                     | 0.50              |
| 1:A:198:PHE:O    | 1:A:199:GLU:CB    | 2.59                     | 0.50              |
| 9:W:47:ARG:HG2   | 9:W:111:LEU:HB2   | 1.94                     | 0.50              |
| 1:A:4:GLY:HA2    | 7:G:129:GLU:HG2   | 1.94                     | 0.50              |
| 12:L:8:ASN:ND2   | 12:L:58:HIS:H     | 2.09                     | 0.50              |
| 3:Q:95:LEU:HG    | 10:X:62:LYS:HG2   | 1.93                     | 0.50              |
| 10:X:101:ASN:HB3 | 10:X:132:HIS:CE1  | 2.46                     | 0.50              |
| 14:b:84:LYS:HG3  | 14:b:119:LEU:HB2  | 1.93                     | 0.50              |
| 11:Y:87:MET:HG3  | 11:Y:116:ASP:HA   | 1.93                     | 0.50              |
| 11:K:4:LEU:HD13  | 11:K:139:MET:HE3  | 1.94                     | 0.50              |
| 9:W:3:MET:HE2    | 9:W:125:LEU:HD22  | 1.94                     | 0.50              |
| 9:I:46:ASP:O     | 9:I:47:ARG:CB     | 2.59                     | 0.50              |
| 10:J:101:ASN:HB3 | 10:J:132:HIS:CE1  | 2.46                     | 0.50              |
| 2:P:31:GLY:HA2   | 2:P:49:ARG:HH11   | 1.77                     | 0.50              |
| 10:X:24:ASN:CG   | 10:X:25:ILE:H     | 2.20                     | 0.50              |
| 14:N:146:MET:HE1 | 14:N:154:PHE:HB2  | 1.94                     | 0.49              |
| 2:P:206:SER:HB3  | 2:P:209:LYS:HD2   | 1.94                     | 0.49              |
| 13:a:92:LEU:HD23 | 13:a:125:VAL:HG21 | 1.93                     | 0.49              |
| 10:J:21:ALA:HB3  | 10:J:29:LYS:HB2   | 1.93                     | 0.49              |
| 11:K:72:GLU:HG2  | 11:K:72:GLU:O     | 2.12                     | 0.49              |
| 2:P:67:LEU:HD11  | 2:P:73:CYS:HB3    | 1.93                     | 0.49              |
| 4:R:34:THR:HB    | 4:R:37:GLY:O      | 2.12                     | 0.49              |
| 9:W:46:ASP:O     | 9:W:47:ARG:CB     | 2.59                     | 0.49              |
| 4:D:34:THR:HB    | 4:D:37:GLY:O      | 2.12                     | 0.49              |
| 8:V:67:ALA:HB2   | 8:V:74:PRO:HG3    | 1.94                     | 0.49              |
| 11:Y:40:TYR:CE1  | 11:Y:73:ARG:HG2   | 2.47                     | 0.49              |
| 3:C:35:ARG:HA    | 3:C:40:VAL:HG13   | 1.95                     | 0.49              |
| 9:I:3:MET:HE2    | 9:I:125:LEU:HD22  | 1.94                     | 0.49              |
| 14:N:63:LEU:HD21 | 14:N:79:ALA:HA    | 1.93                     | 0.49              |
| 11:Y:31:MET:CG   | 17:Y:301:04C:H42  | 2.32                     | 0.49              |
| 1:A:220:LEU:HD23 | 19:A:430:HOH:O    | 2.12                     | 0.49              |
| 7:G:171:GLN:O    | 7:G:175:THR:HG23  | 2.12                     | 0.49              |
| 14:b:146:MET:HE1 | 14:b:154:PHE:HB2  | 1.94                     | 0.49              |
| 1:A:106:THR:O    | 1:A:110:VAL:HG23  | 2.13                     | 0.49              |
| 2:B:206:SER:HB3  | 2:B:209:LYS:HD2   | 1.94                     | 0.49              |
| 12:L:22:ILE:HG21 | 12:L:175:VAL:HG21 | 1.95                     | 0.49              |
| 6:T:74:GLY:HA3   | 6:T:224:HIS:CD2   | 2.48                     | 0.49              |
| 9:I:47:ARG:HG2   | 9:I:111:LEU:HB2   | 1.94                     | 0.49              |
| 2:P:13:PRO:HA    | 3:Q:20:TYR:CE2    | 2.46                     | 0.49              |
| 11:Y:3:THR:CG2   | 11:Y:100:MET:HE2  | 2.36                     | 0.49              |
| 9:I:124:ASP:HB3  | 9:I:126:ILE:H     | 1.78                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:L:8:ASN:HA     | 12:L:30:SER:O     | 2.13                     | 0.49              |
| 3:Q:35:ARG:HA     | 3:Q:40:VAL:HG13   | 1.95                     | 0.49              |
| 7:U:171:GLN:O     | 7:U:175:THR:HG23  | 2.12                     | 0.49              |
| 11:Y:4:LEU:HD13   | 11:Y:139:MET:HE3  | 1.93                     | 0.49              |
| 3:C:131:LEU:HD23  | 3:C:145:GLN:HB3   | 1.95                     | 0.48              |
| 11:K:40:TYR:CE1   | 11:K:73:ARG:HG2   | 2.47                     | 0.48              |
| 11:K:87:MET:HG3   | 11:K:116:ASP:HA   | 1.94                     | 0.48              |
| 1:O:106:THR:O     | 1:O:110:VAL:HG23  | 2.13                     | 0.48              |
| 6:F:74:GLY:HA3    | 6:F:224:HIS:CD2   | 2.48                     | 0.48              |
| 10:J:24:ASN:CG    | 10:J:25:ILE:H     | 2.20                     | 0.48              |
| 4:R:34:THR:HG23   | 4:R:181:MET:O     | 2.14                     | 0.48              |
| 7:U:107:GLU:HG3   | 19:U:424:HOH:O    | 2.12                     | 0.48              |
| 11:Y:173:VAL:HG12 | 11:Y:191:ASP:HA   | 1.95                     | 0.48              |
| 12:Z:8:ASN:ND2    | 12:Z:58:HIS:H     | 2.09                     | 0.48              |
| 1:O:51:GLN:HG2    | 1:O:56:TYR:CD2    | 2.49                     | 0.48              |
| 4:R:149:ASP:HB2   | 4:R:150:PRO:CD    | 2.43                     | 0.48              |
| 9:W:124:ASP:HB3   | 9:W:126:ILE:H     | 1.78                     | 0.48              |
| 11:Y:72:GLU:O     | 11:Y:72:GLU:HG2   | 2.12                     | 0.48              |
| 2:B:31:GLY:HA2    | 2:B:49:ARG:HH11   | 1.77                     | 0.48              |
| 4:D:149:ASP:HB2   | 4:D:150:PRO:CD    | 2.42                     | 0.48              |
| 11:K:173:VAL:HG12 | 11:K:191:ASP:HA   | 1.95                     | 0.48              |
| 3:Q:91:GLN:HE21   | 10:X:62:LYS:HG3   | 1.79                     | 0.48              |
| 4:D:34:THR:HG23   | 4:D:181:MET:O     | 2.13                     | 0.48              |
| 8:H:210:PRO:HB2   | 9:I:200:LYS:HB3   | 1.95                     | 0.48              |
| 10:X:44:LEU:HD11  | 10:X:102:LEU:HD13 | 1.96                     | 0.48              |
| 7:G:72:THR:HG22   | 7:G:74:SER:H      | 1.79                     | 0.48              |
| 9:I:46:ASP:O      | 9:I:47:ARG:HB2    | 2.13                     | 0.48              |
| 5:S:2:GLN:HE22    | 6:T:5:THR:H       | 1.62                     | 0.48              |
| 6:T:108:LEU:HD11  | 6:T:137:LEU:HB3   | 1.96                     | 0.48              |
| 9:W:46:ASP:O      | 9:W:47:ARG:HB2    | 2.14                     | 0.48              |
| 2:B:89:LEU:HG     | 2:B:113:LEU:HD13  | 1.96                     | 0.48              |
| 4:D:65:HIS:CE1    | 4:D:98:THR:HB     | 2.49                     | 0.47              |
| 9:I:113:PRO:O     | 9:I:114:LYS:HB2   | 2.14                     | 0.47              |
| 10:J:181:ARG:HG2  | 10:J:190:ASN:HA   | 1.96                     | 0.47              |
| 1:O:147:GLN:HE21  | 1:O:157:TRP:HE1   | 1.62                     | 0.47              |
| 2:P:47:GLU:HG3    | 2:P:200:MET:HE3   | 1.96                     | 0.47              |
| 6:T:152:ASP:HB2   | 6:T:153:PRO:CD    | 2.44                     | 0.47              |
| 12:Z:22:ILE:HG21  | 12:Z:175:VAL:HG21 | 1.95                     | 0.47              |
| 6:F:152:ASP:HB2   | 6:F:153:PRO:CD    | 2.45                     | 0.47              |
| 10:X:143:LEU:HD13 | 10:X:163:CYS:SG   | 2.55                     | 0.47              |
| 13:a:46:ASN:ND2   | 13:a:48:SER:H     | 2.12                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:b:38:HIS:CD2   | 14:b:39:GLN:H     | 2.33                     | 0.47              |
| 12:L:110:ILE:HB   | 12:L:122:TYR:HB2  | 1.96                     | 0.47              |
| 3:Q:175:TYR:CZ    | 3:Q:180:ILE:HD11  | 2.50                     | 0.47              |
| 5:S:2:GLN:HE22    | 6:T:5:THR:CA      | 2.23                     | 0.47              |
| 7:U:12:ILE:HG13   | 7:U:14:ILE:HG12   | 1.96                     | 0.47              |
| 6:F:168:ALA:HB1   | 6:F:171:ALA:HB3   | 1.96                     | 0.47              |
| 9:I:122:SER:HB3   | 9:I:136:VAL:HB    | 1.96                     | 0.47              |
| 10:J:80:ALA:O     | 10:J:84:THR:HG23  | 2.13                     | 0.47              |
| 14:N:38:HIS:CD2   | 14:N:39:GLN:H     | 2.33                     | 0.47              |
| 6:F:108:LEU:HD11  | 6:F:137:LEU:HB3   | 1.96                     | 0.47              |
| 10:J:143:LEU:HD13 | 10:J:163:CYS:SG   | 2.55                     | 0.47              |
| 3:Q:131:LEU:HD23  | 3:Q:145:GLN:HB3   | 1.95                     | 0.47              |
| 12:Z:8:ASN:HA     | 12:Z:30:SER:O     | 2.13                     | 0.47              |
| 2:B:47:GLU:HG3    | 2:B:200:MET:HE3   | 1.96                     | 0.47              |
| 2:P:89:LEU:HG     | 2:P:113:LEU:HD13  | 1.97                     | 0.47              |
| 4:R:65:HIS:CE1    | 4:R:98:THR:HB     | 2.49                     | 0.47              |
| 9:W:113:PRO:O     | 9:W:114:LYS:HB2   | 2.15                     | 0.47              |
| 7:G:12:ILE:HG13   | 7:G:14:ILE:HG12   | 1.96                     | 0.47              |
| 12:L:46:LEU:HB3   | 12:L:72:LEU:HD11  | 1.97                     | 0.47              |
| 12:L:137:ALA:H    | 12:L:146:GLN:HE21 | 1.63                     | 0.47              |
| 9:W:122:SER:HB3   | 9:W:136:VAL:HB    | 1.97                     | 0.47              |
| 1:A:40:ALA:HB2    | 1:A:180:ASP:HA    | 1.97                     | 0.47              |
| 2:B:122:GLN:HG3   | 3:C:124:ARG:HG3   | 1.95                     | 0.47              |
| 14:N:168:SER:O    | 17:N:201:04C:H33  | 2.14                     | 0.47              |
| 3:Q:19:GLU:HA     | 3:Q:22:GLN:NE2    | 2.30                     | 0.47              |
| 6:T:168:ALA:HB1   | 6:T:171:ALA:HB3   | 1.96                     | 0.47              |
| 12:Z:46:LEU:HB3   | 12:Z:72:LEU:HD11  | 1.96                     | 0.47              |
| 9:I:61:THR:O      | 9:I:65:ARG:HG3    | 2.14                     | 0.47              |
| 5:S:168:TYR:OH    | 5:S:190:ARG:HD2   | 2.15                     | 0.47              |
| 2:P:86:THR:HA     | 2:P:89:LEU:HD12   | 1.97                     | 0.47              |
| 9:W:61:THR:O      | 9:W:65:ARG:HG3    | 2.14                     | 0.47              |
| 11:Y:72:GLU:O     | 11:Y:73:ARG:HB3   | 2.14                     | 0.47              |
| 12:Z:137:ALA:H    | 12:Z:146:GLN:HE21 | 1.63                     | 0.47              |
| 1:A:147:GLN:HE21  | 1:A:157:TRP:HE1   | 1.62                     | 0.46              |
| 5:E:106:VAL:HA    | 5:E:109:ILE:HD12  | 1.96                     | 0.46              |
| 14:N:188:ILE:HG22 | 14:N:193:LEU:HD12 | 1.97                     | 0.46              |
| 3:Q:11:PRO:HA     | 4:R:18:TYR:CD2    | 2.51                     | 0.46              |
| 5:S:167:THR:O     | 5:S:171:ARG:HG3   | 2.15                     | 0.46              |
| 3:C:175:TYR:CZ    | 3:C:180:ILE:HD11  | 2.50                     | 0.46              |
| 10:J:161:ARG:HE   | 10:J:161:ARG:HB2  | 1.52                     | 0.46              |
| 11:K:20:ALA:HB3   | 11:K:28:SER:HB3   | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:K:72:GLU:O     | 11:K:73:ARG:HB3   | 2.14                     | 0.46              |
| 5:S:106:VAL:HA    | 5:S:109:ILE:HD12  | 1.96                     | 0.46              |
| 2:B:86:THR:HA     | 2:B:89:LEU:HD12   | 1.97                     | 0.46              |
| 4:D:149:ASP:HB2   | 4:D:150:PRO:HD2   | 1.98                     | 0.46              |
| 1:O:147:GLN:HG3   | 1:O:162:MET:HE1   | 1.97                     | 0.46              |
| 14:b:48:SER:HB3   | 14:b:51:ASP:HB2   | 1.98                     | 0.46              |
| 10:J:44:LEU:HD11  | 10:J:102:LEU:HD13 | 1.96                     | 0.46              |
| 14:N:90:TYR:HB2   | 14:N:94:LEU:HD12  | 1.96                     | 0.46              |
| 8:V:63:MET:HE3    | 8:V:74:PRO:HB3    | 1.97                     | 0.46              |
| 10:X:181:ARG:HG2  | 10:X:190:ASN:HA   | 1.97                     | 0.46              |
| 11:Y:59:LEU:HA    | 11:Y:86:MET:HE1   | 1.96                     | 0.46              |
| 14:b:97:HIS:CG    | 14:b:115:MET:HB3  | 2.51                     | 0.46              |
| 14:b:188:ILE:HG22 | 14:b:193:LEU:HD12 | 1.97                     | 0.46              |
| 5:E:167:THR:O     | 5:E:171:ARG:HG3   | 2.15                     | 0.46              |
| 11:K:59:LEU:HA    | 11:K:86:MET:HE1   | 1.96                     | 0.46              |
| 14:N:97:HIS:CG    | 14:N:115:MET:HB3  | 2.50                     | 0.46              |
| 10:X:80:ALA:O     | 10:X:84:THR:HG23  | 2.14                     | 0.46              |
| 3:C:19:GLU:HA     | 3:C:22:GLN:NE2    | 2.30                     | 0.46              |
| 7:G:140:ILE:HG22  | 7:G:150:VAL:HG22  | 1.98                     | 0.46              |
| 7:G:142:ILE:HD13  | 7:G:221:VAL:HA    | 1.98                     | 0.46              |
| 9:I:153:TRP:CH2   | 9:I:155:PRO:HA    | 2.51                     | 0.46              |
| 7:U:49:ILE:HG13   | 19:U:413:HOH:O    | 2.15                     | 0.46              |
| 11:Y:19:ARG:O     | 17:Y:301:04C:H34  | 2.16                     | 0.46              |
| 1:A:70:HIS:CE1    | 1:A:103:PRO:HB3   | 2.51                     | 0.46              |
| 6:F:3:ILE:HD12    | 6:F:15:SER:HB2    | 1.97                     | 0.46              |
| 12:L:64:LEU:CD2   | 12:L:108:ASN:HD21 | 2.28                     | 0.46              |
| 14:N:134:ILE:HG21 | 14:N:158:ALA:O    | 2.15                     | 0.46              |
| 11:Y:20:ALA:HB3   | 11:Y:28:SER:HB3   | 1.97                     | 0.46              |
| 12:Z:64:LEU:CD2   | 12:Z:108:ASN:HD21 | 2.28                     | 0.46              |
| 14:b:90:TYR:HB2   | 14:b:94:LEU:HD12  | 1.96                     | 0.46              |
| 14:b:134:ILE:HG21 | 14:b:158:ALA:O    | 2.15                     | 0.46              |
| 1:O:70:HIS:CE1    | 1:O:103:PRO:HB3   | 2.51                     | 0.46              |
| 9:W:97:LYS:HG3    | 9:W:102:TYR:CE1   | 2.50                     | 0.46              |
| 11:Y:154:ASP:O    | 11:Y:158:ARG:HB2  | 2.16                     | 0.46              |
| 8:H:153:GLU:HG3   | 8:H:154:LEU:N     | 2.31                     | 0.46              |
| 9:I:97:LYS:HG3    | 9:I:102:TYR:CE1   | 2.51                     | 0.46              |
| 11:K:11:GLY:HA2   | 11:K:104:TRP:HZ3  | 1.81                     | 0.46              |
| 7:U:229:LEU:O     | 7:U:233:GLU:HB2   | 2.16                     | 0.46              |
| 11:Y:4:LEU:CD2    | 11:Y:159:ALA:HB3  | 2.46                     | 0.46              |
| 1:A:75:TYR:HB3    | 1:A:82:TYR:CD1    | 2.51                     | 0.46              |
| 7:G:229:LEU:O     | 7:G:233:GLU:HB2   | 2.16                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:I:163:PHE:CE1  | 9:I:197:ARG:HD3   | 2.51                     | 0.46              |
| 10:J:38:MET:HE1  | 10:J:60:ILE:HG22  | 1.98                     | 0.46              |
| 13:M:46:ASN:ND2  | 13:M:49:THR:H     | 2.14                     | 0.46              |
| 1:O:40:ALA:HB2   | 1:O:180:ASP:HA    | 1.98                     | 0.46              |
| 6:T:34:SER:OG    | 6:T:65:ARG:NH1    | 2.49                     | 0.46              |
| 8:H:48:VAL:HB    | 8:H:51:ASP:HB2    | 1.99                     | 0.45              |
| 9:I:35:THR:HG22  | 9:I:37:ASP:H      | 1.82                     | 0.45              |
| 9:I:47:ARG:HG3   | 9:I:189:ILE:CG2   | 2.47                     | 0.45              |
| 11:K:50:ALA:CB   | 12:L:127:VAL:HG12 | 2.46                     | 0.45              |
| 11:K:83:LEU:HD11 | 11:K:97:MET:HE1   | 1.98                     | 0.45              |
| 13:M:46:ASN:ND2  | 13:M:48:SER:H     | 2.13                     | 0.45              |
| 1:O:75:TYR:HB3   | 1:O:82:TYR:CD1    | 2.51                     | 0.45              |
| 5:E:168:TYR:OH   | 5:E:190:ARG:HD2   | 2.15                     | 0.45              |
| 1:O:149:ASP:HB2  | 1:O:150:PRO:CD    | 2.46                     | 0.45              |
| 1:A:149:ASP:HB2  | 1:A:150:PRO:CD    | 2.46                     | 0.45              |
| 7:U:72:THR:HG22  | 7:U:74:SER:H      | 1.81                     | 0.45              |
| 13:a:193:THR:OG1 | 13:a:194:GLU:N    | 2.49                     | 0.45              |
| 3:C:97:VAL:HG12  | 3:C:99:ASP:H      | 1.82                     | 0.45              |
| 14:N:48:SER:HB3  | 14:N:51:ASP:HB2   | 1.98                     | 0.45              |
| 4:R:149:ASP:HB2  | 4:R:150:PRO:HD2   | 1.98                     | 0.45              |
| 7:U:140:ILE:HG22 | 7:U:150:VAL:HG22  | 1.98                     | 0.45              |
| 8:V:48:VAL:HB    | 8:V:51:ASP:HB2    | 1.97                     | 0.45              |
| 9:W:35:THR:HG22  | 9:W:37:ASP:H      | 1.81                     | 0.45              |
| 6:F:34:SER:OG    | 6:F:65:ARG:NH1    | 2.50                     | 0.45              |
| 7:G:71:ILE:HG21  | 7:G:113:LEU:HD11  | 1.99                     | 0.45              |
| 6:T:2:SER:HA     | 6:T:21:PHE:CE2    | 2.52                     | 0.45              |
| 9:W:153:TRP:CH2  | 9:W:155:PRO:HA    | 2.51                     | 0.45              |
| 14:b:33:LYS:NZ   | 17:b:201:04C:H34  | 2.31                     | 0.45              |
| 1:A:83:ARG:NH2   | 7:G:157:GLY:O     | 2.50                     | 0.45              |
| 2:B:214:THR:HG22 | 19:B:434:HOH:O    | 2.17                     | 0.45              |
| 11:K:154:ASP:O   | 11:K:158:ARG:HB2  | 2.16                     | 0.45              |
| 6:T:3:ILE:HD12   | 6:T:15:SER:HB2    | 1.99                     | 0.45              |
| 1:A:147:GLN:HG3  | 1:A:162:MET:HE1   | 1.97                     | 0.45              |
| 7:U:142:ILE:HD13 | 7:U:221:VAL:HA    | 1.97                     | 0.45              |
| 12:Z:45:LYS:HB2  | 12:Z:203:ILE:HD13 | 1.97                     | 0.45              |
| 1:A:73:LEU:HD21  | 1:A:135:ILE:HG12  | 1.99                     | 0.45              |
| 11:K:4:LEU:CD2   | 11:K:159:ALA:HB3  | 2.46                     | 0.45              |
| 1:O:147:GLN:HE21 | 1:O:157:TRP:NE1   | 2.15                     | 0.45              |
| 7:U:72:THR:HG22  | 7:U:73:GLU:N      | 2.32                     | 0.45              |
| 7:U:154:ASP:HB3  | 7:U:156:ALA:H     | 1.82                     | 0.45              |
| 4:D:83:LYS:HD2   | 4:D:111:LEU:HD11  | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:N:78:ALA:O     | 14:N:82:VAL:HG13  | 2.17                     | 0.45              |
| 6:T:99:ARG:NH1    | 13:a:69:GLN:OE1   | 2.50                     | 0.45              |
| 7:U:195:GLU:HG2   | 7:U:241:LEU:HG    | 1.99                     | 0.45              |
| 1:A:53:SER:HB3    | 1:A:56:TYR:CD1    | 2.52                     | 0.45              |
| 2:B:43:LEU:HB2    | 19:B:434:HOH:O    | 2.16                     | 0.45              |
| 5:E:2:GLN:HE22    | 6:F:5:THR:N       | 2.14                     | 0.45              |
| 5:E:35:LEU:HD13   | 5:E:184:LEU:HD22  | 1.99                     | 0.45              |
| 7:G:200:CYS:O     | 7:G:204:VAL:HG23  | 2.17                     | 0.45              |
| 12:L:123:SER:CB   | 12:L:136:LYS:HG2  | 2.47                     | 0.45              |
| 11:Y:87:MET:HE2   | 11:Y:97:MET:HB3   | 1.99                     | 0.45              |
| 11:Y:113:TYR:HD2  | 11:Y:121:LEU:HD12 | 1.82                     | 0.45              |
| 13:a:46:ASN:ND2   | 13:a:49:THR:H     | 2.14                     | 0.45              |
| 3:C:107:THR:HG21  | 3:C:144:TYR:HB3   | 1.99                     | 0.44              |
| 2:P:32:THR:HG21   | 2:P:199:THR:HG21  | 1.99                     | 0.44              |
| 9:W:163:PHE:CE1   | 9:W:197:ARG:HD3   | 2.51                     | 0.44              |
| 12:Z:123:SER:CB   | 12:Z:136:LYS:HG2  | 2.47                     | 0.44              |
| 13:M:12:LEU:HB2   | 13:M:23:ALA:HB3   | 1.99                     | 0.44              |
| 7:U:200:CYS:O     | 7:U:204:VAL:HG23  | 2.17                     | 0.44              |
| 9:W:47:ARG:HG3    | 9:W:189:ILE:CG2   | 2.46                     | 0.44              |
| 9:W:171:LEU:CD2   | 9:W:199:LEU:HD13  | 2.47                     | 0.44              |
| 11:Y:11:GLY:HA2   | 11:Y:104:TRP:HZ3  | 1.81                     | 0.44              |
| 6:F:2:SER:HA      | 6:F:21:PHE:CE2    | 2.52                     | 0.44              |
| 11:K:113:TYR:HD2  | 11:K:121:LEU:HD12 | 1.82                     | 0.44              |
| 13:M:149:LEU:HD11 | 13:M:175:VAL:HG21 | 1.99                     | 0.44              |
| 13:M:193:THR:OG1  | 13:M:194:GLU:N    | 2.50                     | 0.44              |
| 7:U:71:ILE:HG21   | 7:U:113:LEU:HD11  | 1.99                     | 0.44              |
| 1:A:147:GLN:HE21  | 1:A:157:TRP:NE1   | 2.15                     | 0.44              |
| 12:L:76:LYS:HB2   | 12:L:76:LYS:HE3   | 1.87                     | 0.44              |
| 13:M:59:ASP:CB    | 13:M:108:ASN:HD21 | 2.27                     | 0.44              |
| 6:T:83:ASP:OD2    | 6:T:129:ARG:NH2   | 2.51                     | 0.44              |
| 8:V:153:GLU:HG3   | 8:V:154:LEU:N     | 2.31                     | 0.44              |
| 14:b:78:ALA:O     | 14:b:82:VAL:HG13  | 2.16                     | 0.44              |
| 3:C:119:GLN:HG3   | 4:D:127:ARG:HG3   | 1.99                     | 0.44              |
| 5:E:154:ARG:NH1   | 5:E:154:ARG:CG    | 2.77                     | 0.44              |
| 2:P:71:MET:HE3    | 2:P:71:MET:HB2    | 1.89                     | 0.44              |
| 7:U:72:THR:HG21   | 19:U:424:HOH:O    | 2.18                     | 0.44              |
| 11:Y:83:LEU:HD11  | 11:Y:97:MET:HE1   | 1.99                     | 0.44              |
| 3:C:107:THR:HG23  | 3:C:132:ILE:HD13  | 1.99                     | 0.44              |
| 9:I:171:LEU:CD2   | 9:I:199:LEU:HD13  | 2.47                     | 0.44              |
| 2:P:16:ARG:HD2    | 2:P:21:GLU:OE2    | 2.18                     | 0.44              |
| 3:Q:97:VAL:HG12   | 3:Q:99:ASP:H      | 1.82                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:W:27:PHE:HB3    | 9:W:35:THR:HB     | 1.99                     | 0.44              |
| 13:a:149:LEU:HD11 | 13:a:175:VAL:HG21 | 1.99                     | 0.44              |
| 2:B:32:THR:HG21   | 2:B:199:THR:HG21  | 1.99                     | 0.44              |
| 1:O:53:SER:HB3    | 1:O:56:TYR:CD1    | 2.52                     | 0.44              |
| 3:Q:107:THR:HG21  | 3:Q:144:TYR:HB3   | 1.99                     | 0.44              |
| 17:V:301:04C:H37  | 18:V:302:IOD:I    | 2.88                     | 0.44              |
| 4:D:69:ALA:HB3    | 4:D:134:LEU:HB2   | 2.00                     | 0.44              |
| 7:G:195:GLU:HG2   | 7:G:241:LEU:HG    | 2.00                     | 0.44              |
| 2:P:202:VAL:O     | 2:P:203:SER:HB3   | 2.18                     | 0.44              |
| 9:W:106:PRO:HG2   | 9:W:123:LEU:HB2   | 1.99                     | 0.44              |
| 10:X:38:MET:HE1   | 10:X:60:ILE:HG22  | 1.99                     | 0.44              |
| 2:B:16:ARG:HD2    | 2:B:21:GLU:OE2    | 2.18                     | 0.44              |
| 2:B:107:GLU:O     | 2:B:111:THR:OG1   | 2.34                     | 0.44              |
| 11:K:87:MET:HE2   | 11:K:97:MET:HB3   | 1.99                     | 0.44              |
| 3:Q:119:GLN:HG3   | 4:R:127:ARG:HG3   | 2.00                     | 0.44              |
| 3:Q:224:ILE:HG13  | 3:Q:225:GLU:N     | 2.33                     | 0.44              |
| 14:b:80:ALA:HA    | 14:b:100:VAL:HG11 | 1.99                     | 0.44              |
| 14:N:80:ALA:HA    | 14:N:100:VAL:HG11 | 1.98                     | 0.43              |
| 5:S:2:GLN:HE22    | 6:T:5:THR:N       | 2.16                     | 0.43              |
| 13:M:96:MET:HE3   | 13:M:127:MET:HA   | 2.00                     | 0.43              |
| 4:R:83:LYS:HD2    | 4:R:111:LEU:HD11  | 2.00                     | 0.43              |
| 1:A:6:SER:O       | 2:B:126:LYS:NZ    | 2.51                     | 0.43              |
| 1:A:71:ILE:HG21   | 1:A:109:LEU:HD22  | 2.01                     | 0.43              |
| 7:G:155:PRO:HD3   | 19:G:425:HOH:O    | 2.17                     | 0.43              |
| 11:K:14:VAL:O     | 11:K:176:MET:HA   | 2.18                     | 0.43              |
| 3:Q:34:VAL:CG1    | 3:Q:190:VAL:HG22  | 2.48                     | 0.43              |
| 12:Z:72:LEU:HD23  | 12:Z:83:MET:HE3   | 2.00                     | 0.43              |
| 8:H:63:MET:CE     | 8:H:74:PRO:HB3    | 2.48                     | 0.43              |
| 9:I:19:VAL:HG23   | 9:I:189:ILE:HB    | 2.01                     | 0.43              |
| 11:K:164:THR:HG22 | 11:K:170:SER:HB3  | 2.01                     | 0.43              |
| 12:L:72:LEU:HD23  | 12:L:83:MET:HE3   | 1.99                     | 0.43              |
| 13:M:104:ASN:ND2  | 19:M:437:HOH:O    | 2.50                     | 0.43              |
| 1:O:68:THR:HG23   | 1:O:70:HIS:H      | 1.83                     | 0.43              |
| 2:P:123:PHE:HB3   | 3:Q:123:ARG:HB3   | 2.00                     | 0.43              |
| 4:R:99:MET:HE3    | 4:R:104:VAL:HG22  | 2.00                     | 0.43              |
| 1:A:78:MET:CE     | 1:A:130:GLY:HA3   | 2.48                     | 0.43              |
| 2:B:202:VAL:O     | 2:B:203:SER:HB3   | 2.18                     | 0.43              |
| 1:O:78:MET:CE     | 1:O:130:GLY:HA3   | 2.48                     | 0.43              |
| 12:Z:140:SER:HB2  | 19:Z:423:HOH:O    | 2.17                     | 0.43              |
| 1:A:68:THR:HG23   | 1:A:70:HIS:H      | 1.83                     | 0.43              |
| 1:A:83:ARG:HH11   | 1:A:83:ARG:CG     | 2.30                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:11:PRO:HA    | 4:D:18:TYR:CD2   | 2.53                     | 0.43              |
| 3:C:25:VAL:HG23  | 3:C:73:ALA:O     | 2.19                     | 0.43              |
| 6:F:83:ASP:OD2   | 6:F:129:ARG:NH2  | 2.52                     | 0.43              |
| 9:I:27:PHE:HB3   | 9:I:35:THR:HB    | 1.99                     | 0.43              |
| 10:J:23:SER:HB2  | 10:J:28:MET:HE2  | 2.01                     | 0.43              |
| 2:P:107:GLU:O    | 2:P:111:THR:OG1  | 2.34                     | 0.43              |
| 6:T:123:THR:O    | 7:U:131:ARG:NH1  | 2.52                     | 0.43              |
| 6:T:241:GLU:HA   | 6:T:244:LYS:NZ   | 2.33                     | 0.43              |
| 13:a:96:MET:HE3  | 13:a:127:MET:HA  | 2.00                     | 0.43              |
| 1:A:58:GLU:HG2   | 1:A:205:ASP:HB3  | 2.01                     | 0.43              |
| 13:M:46:ASN:C    | 13:M:46:ASN:HD22 | 2.27                     | 0.43              |
| 5:S:35:LEU:HD13  | 5:S:184:LEU:HD22 | 1.99                     | 0.43              |
| 8:V:18:THR:HB    | 8:V:30:SER:HA    | 2.01                     | 0.43              |
| 1:A:110:VAL:HG22 | 1:A:135:ILE:HD13 | 2.00                     | 0.43              |
| 3:C:34:VAL:CG1   | 3:C:190:VAL:HG22 | 2.48                     | 0.43              |
| 11:K:4:LEU:C     | 11:K:100:MET:HE1 | 2.44                     | 0.43              |
| 11:K:15:ALA:HB2  | 11:K:176:MET:HG3 | 2.00                     | 0.43              |
| 1:O:162:MET:HA   | 1:O:166:TYR:HB2  | 2.00                     | 0.43              |
| 3:Q:25:VAL:O     | 3:Q:161:GLY:HA2  | 2.19                     | 0.43              |
| 5:S:23:MET:HA    | 5:S:146:PRO:HG2  | 2.01                     | 0.43              |
| 9:I:29:ILE:O     | 9:I:31:ALA:N     | 2.52                     | 0.43              |
| 2:P:122:GLN:HG3  | 3:Q:124:ARG:HG3  | 2.01                     | 0.43              |
| 3:C:25:VAL:O     | 3:C:161:GLY:HA2  | 2.19                     | 0.43              |
| 7:G:85:ASP:OD1   | 7:G:131:ARG:NH2  | 2.52                     | 0.43              |
| 1:O:73:LEU:HD21  | 1:O:135:ILE:HG12 | 1.99                     | 0.43              |
| 11:Y:38:ASN:HB3  | 11:Y:39:PRO:HD2  | 2.01                     | 0.43              |
| 13:a:46:ASN:C    | 13:a:46:ASN:HD22 | 2.27                     | 0.43              |
| 13:a:94:ARG:NE   | 13:a:94:ARG:HA   | 2.34                     | 0.43              |
| 1:A:55:LEU:HD21  | 7:G:178:LEU:HB3  | 2.01                     | 0.42              |
| 2:B:123:PHE:HB3  | 3:C:123:ARG:HB3  | 2.00                     | 0.42              |
| 2:B:228:LYS:O    | 2:B:232:VAL:HG23 | 2.19                     | 0.42              |
| 5:E:23:MET:HA    | 5:E:146:PRO:HG2  | 2.01                     | 0.42              |
| 10:J:16:ALA:HA   | 10:J:179:SER:O   | 2.18                     | 0.42              |
| 17:K:301:04C:H41 | 17:K:301:04C:H29 | 1.85                     | 0.42              |
| 13:M:94:ARG:HA   | 13:M:94:ARG:NE   | 2.34                     | 0.42              |
| 3:Q:107:THR:HG23 | 3:Q:132:ILE:HD13 | 1.99                     | 0.42              |
| 4:R:69:ALA:HB3   | 4:R:134:LEU:HB2  | 2.00                     | 0.42              |
| 7:U:85:ASP:OD1   | 7:U:131:ARG:NH2  | 2.52                     | 0.42              |
| 11:Y:14:VAL:O    | 11:Y:176:MET:HA  | 2.18                     | 0.42              |
| 11:Y:15:ALA:HB2  | 11:Y:176:MET:HG3 | 2.00                     | 0.42              |
| 11:Y:45:MET:HG2  | 11:Y:52:CYS:HB3  | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:127:ARG:HG3   | 7:G:126:GLN:HG3   | 2.01                     | 0.42              |
| 5:E:102:VAL:O     | 5:E:106:VAL:HG23  | 2.19                     | 0.42              |
| 2:P:228:LYS:O     | 2:P:232:VAL:HG23  | 2.19                     | 0.42              |
| 9:W:70:LEU:HD11   | 9:W:81:ILE:HG21   | 2.01                     | 0.42              |
| 13:a:59:ASP:CB    | 13:a:108:ASN:HD21 | 2.27                     | 0.42              |
| 3:C:220:ASN:C     | 3:C:222:GLU:N     | 2.77                     | 0.42              |
| 3:C:224:ILE:HG13  | 3:C:225:GLU:N     | 2.33                     | 0.42              |
| 4:D:190:SER:O     | 4:D:194:LEU:HB2   | 2.19                     | 0.42              |
| 9:I:70:LEU:HD11   | 9:I:81:ILE:HG21   | 2.01                     | 0.42              |
| 4:R:190:SER:O     | 4:R:194:LEU:HB2   | 2.19                     | 0.42              |
| 5:S:102:VAL:O     | 5:S:106:VAL:HG23  | 2.18                     | 0.42              |
| 8:V:122:LEU:HD13  | 8:V:125:THR:HB    | 2.01                     | 0.42              |
| 9:W:19:VAL:HG23   | 9:W:189:ILE:HB    | 2.01                     | 0.42              |
| 10:X:16:ALA:HA    | 10:X:179:SER:O    | 2.19                     | 0.42              |
| 2:B:33:CYS:HB3    | 2:B:163:ILE:HD12  | 2.02                     | 0.42              |
| 1:O:55:LEU:HG     | 7:U:179:GLU:HG3   | 2.01                     | 0.42              |
| 1:O:110:VAL:HG22  | 1:O:135:ILE:HD13  | 2.00                     | 0.42              |
| 4:R:178:HIS:C     | 4:R:180:SER:H     | 2.27                     | 0.42              |
| 4:D:99:MET:HE3    | 4:D:104:VAL:HG22  | 2.00                     | 0.42              |
| 6:F:99:ARG:NH1    | 13:M:69:GLN:OE1   | 2.52                     | 0.42              |
| 7:G:129:GLU:CD    | 7:G:129:GLU:H     | 2.27                     | 0.42              |
| 7:G:154:ASP:HB3   | 7:G:156:ALA:H     | 1.83                     | 0.42              |
| 2:P:13:PRO:HA     | 3:Q:20:TYR:CD2    | 2.53                     | 0.42              |
| 7:U:113:LEU:O     | 7:U:117:ILE:HG12  | 2.19                     | 0.42              |
| 11:Y:164:THR:HG22 | 11:Y:170:SER:HB3  | 2.01                     | 0.42              |
| 3:C:147:ASP:HB2   | 3:C:148:PRO:HD2   | 2.01                     | 0.42              |
| 1:O:58:GLU:HG2    | 1:O:205:ASP:HB3   | 2.01                     | 0.42              |
| 2:P:33:CYS:HB3    | 2:P:163:ILE:HD12  | 2.02                     | 0.42              |
| 3:Q:11:PRO:HA     | 4:R:18:TYR:CE2    | 2.54                     | 0.42              |
| 7:U:71:ILE:HD11   | 7:U:77:CYS:SG     | 2.60                     | 0.42              |
| 10:X:23:SER:HB2   | 10:X:28:MET:HE2   | 2.01                     | 0.42              |
| 11:Y:102:CYS:SG   | 11:Y:111:LEU:HD13 | 2.60                     | 0.42              |
| 1:A:147:GLN:HG3   | 1:A:162:MET:CE    | 2.50                     | 0.42              |
| 1:A:162:MET:HA    | 1:A:166:TYR:HB2   | 2.00                     | 0.42              |
| 1:A:198:PHE:O     | 1:A:199:GLU:HB2   | 2.20                     | 0.42              |
| 8:H:18:THR:HB     | 8:H:30:SER:HA     | 2.01                     | 0.42              |
| 13:M:209:TRP:CH2  | 14:b:171:GLY:HA2  | 2.54                     | 0.42              |
| 3:Q:25:VAL:HG23   | 3:Q:73:ALA:O      | 2.19                     | 0.42              |
| 7:U:49:ILE:HG21   | 7:U:78:VAL:HB     | 2.01                     | 0.42              |
| 9:W:29:ILE:O      | 9:W:31:ALA:N      | 2.52                     | 0.42              |
| 11:Y:64:ARG:HD3   | 11:Y:64:ARG:HA    | 1.88                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:I:6:ASN:ND2    | 9:I:56:ALA:H      | 2.18                     | 0.42              |
| 17:K:301:04C:O13 | 18:K:302:IOD:I    | 3.08                     | 0.42              |
| 3:Q:220:ASN:C    | 3:Q:222:GLU:N     | 2.77                     | 0.42              |
| 5:S:69:ILE:HG22  | 5:S:131:ILE:HG12  | 2.02                     | 0.42              |
| 11:Y:4:LEU:C     | 11:Y:100:MET:HE1  | 2.44                     | 0.42              |
| 13:a:59:ASP:HB3  | 13:a:108:ASN:ND2  | 2.31                     | 0.42              |
| 5:E:118:GLN:HG3  | 6:F:129:ARG:HG3   | 2.01                     | 0.42              |
| 7:G:71:ILE:HD11  | 7:G:77:CYS:SG     | 2.60                     | 0.42              |
| 8:H:77:ALA:O     | 8:H:80:THR:HG22   | 2.19                     | 0.42              |
| 14:N:24:THR:HB   | 13:a:141:TYR:HE1  | 1.84                     | 0.42              |
| 5:S:118:GLN:HG3  | 6:T:129:ARG:HG3   | 2.02                     | 0.42              |
| 7:U:49:ILE:CG2   | 7:U:78:VAL:HB     | 2.50                     | 0.42              |
| 5:E:46:LEU:HB2   | 5:E:192:LEU:HD11  | 2.02                     | 0.42              |
| 9:I:183:GLY:HA2  | 9:I:201:ALA:HB3   | 2.02                     | 0.42              |
| 10:J:4:LEU:HB2   | 10:J:132:HIS:HB2  | 2.02                     | 0.42              |
| 3:Q:147:ASP:HB2  | 3:Q:148:PRO:HD2   | 2.01                     | 0.42              |
| 9:W:6:ASN:ND2    | 9:W:56:ALA:H      | 2.18                     | 0.42              |
| 13:a:12:LEU:HB2  | 13:a:23:ALA:HB3   | 2.00                     | 0.42              |
| 12:L:136:LYS:HA  | 12:L:146:GLN:HE22 | 1.85                     | 0.41              |
| 7:U:129:GLU:CD   | 7:U:129:GLU:H     | 2.28                     | 0.41              |
| 8:V:77:ALA:O     | 8:V:80:THR:HG22   | 2.20                     | 0.41              |
| 8:H:122:LEU:CD1  | 8:H:125:THR:HB    | 2.50                     | 0.41              |
| 8:H:126:ALA:HB3  | 8:H:135:VAL:HG22  | 2.02                     | 0.41              |
| 9:I:1:SER:HB3    | 9:I:4:SER:HB2     | 2.02                     | 0.41              |
| 4:R:20:ILE:HA    | 4:R:23:ILE:HD12   | 2.01                     | 0.41              |
| 8:V:173:VAL:HG13 | 8:V:190:SER:HB3   | 2.01                     | 0.41              |
| 1:A:74:VAL:HG12  | 1:A:75:TYR:H      | 1.85                     | 0.41              |
| 3:C:94:ARG:HB3   | 10:J:62:LYS:CE    | 2.51                     | 0.41              |
| 6:F:39:ILE:HG22  | 6:F:162:GLY:CA    | 2.46                     | 0.41              |
| 7:G:113:LEU:O    | 7:G:117:ILE:HG12  | 2.19                     | 0.41              |
| 7:G:209:PHE:HB2  | 7:G:213:GLU:HB2   | 2.01                     | 0.41              |
| 13:M:122:LEU:HG  | 13:M:137:LEU:HD12 | 2.02                     | 0.41              |
| 14:N:77:LEU:HD22 | 14:N:81:ASN:ND2   | 2.35                     | 0.41              |
| 1:O:71:ILE:HG21  | 1:O:109:LEU:HD22  | 2.01                     | 0.41              |
| 1:O:83:ARG:NH2   | 7:U:157:GLY:O     | 2.53                     | 0.41              |
| 5:S:46:LEU:HB2   | 5:S:192:LEU:HD11  | 2.02                     | 0.41              |
| 8:V:122:LEU:CD1  | 8:V:125:THR:HB    | 2.49                     | 0.41              |
| 10:X:4:LEU:HB2   | 10:X:132:HIS:HB2  | 2.02                     | 0.41              |
| 4:D:178:HIS:C    | 4:D:180:SER:H     | 2.27                     | 0.41              |
| 6:F:113:ASP:O    | 6:F:117:MET:HG2   | 2.20                     | 0.41              |
| 7:G:72:THR:HG22  | 7:G:73:GLU:N      | 2.34                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 11:K:102:CYS:SG  | 11:K:111:LEU:HD13 | 2.60                     | 0.41              |
| 13:M:46:ASN:HD21 | 13:M:49:THR:CG2   | 2.33                     | 0.41              |
| 5:E:2:GLN:HE22   | 6:F:5:THR:H       | 1.68                     | 0.41              |
| 9:I:90:VAL:HG21  | 9:I:108:ILE:HD11  | 2.03                     | 0.41              |
| 9:I:106:PRO:HG2  | 9:I:123:LEU:HB2   | 2.02                     | 0.41              |
| 11:K:38:ASN:HB3  | 11:K:39:PRO:HD2   | 2.01                     | 0.41              |
| 13:M:141:TYR:HE1 | 14:b:24:THR:HB    | 1.85                     | 0.41              |
| 4:R:20:ILE:HD13  | 4:R:150:PRO:HD2   | 2.02                     | 0.41              |
| 7:U:53:LYS:HB2   | 7:U:215:GLU:HG3   | 2.03                     | 0.41              |
| 7:U:79:MET:HE1   | 7:U:89:GLN:HE21   | 1.86                     | 0.41              |
| 7:U:106:TYR:OH   | 8:V:66:HIS:HE1    | 2.04                     | 0.41              |
| 11:Y:50:ALA:CB   | 12:Z:127:VAL:HG12 | 2.51                     | 0.41              |
| 13:a:43:MET:SD   | 13:a:64:LYS:HG3   | 2.60                     | 0.41              |
| 14:b:41:ILE:HD13 | 14:b:79:ALA:HB2   | 2.02                     | 0.41              |
| 14:b:143:LYS:O   | 14:b:146:MET:HG3  | 2.21                     | 0.41              |
| 3:C:42:LEU:O     | 3:C:207:LEU:HB2   | 2.21                     | 0.41              |
| 1:O:83:ARG:HH11  | 1:O:83:ARG:CG     | 2.29                     | 0.41              |
| 3:Q:42:LEU:O     | 3:Q:207:LEU:HB2   | 2.21                     | 0.41              |
| 3:Q:94:ARG:HB3   | 10:X:62:LYS:CE    | 2.51                     | 0.41              |
| 6:T:39:ILE:HG22  | 6:T:162:GLY:CA    | 2.45                     | 0.41              |
| 8:V:7:VAL:HG22   | 8:V:12:VAL:HG12   | 2.02                     | 0.41              |
| 1:A:142:ARG:HA   | 1:A:143:PRO:HD3   | 1.95                     | 0.41              |
| 3:C:25:VAL:HG21  | 3:C:129:SER:CB    | 2.50                     | 0.41              |
| 7:G:49:ILE:HG21  | 7:G:78:VAL:HB     | 2.02                     | 0.41              |
| 11:K:45:MET:HG2  | 11:K:52:CYS:HB3   | 2.01                     | 0.41              |
| 1:O:147:GLN:HG3  | 1:O:162:MET:CE    | 2.50                     | 0.41              |
| 7:U:209:PHE:HB2  | 7:U:213:GLU:HB2   | 2.01                     | 0.41              |
| 9:W:117:LYS:HA   | 9:W:118:PRO:HD3   | 1.92                     | 0.41              |
| 13:a:122:LEU:HG  | 13:a:137:LEU:HD12 | 2.02                     | 0.41              |
| 2:B:157:GLY:HA3  | 3:C:57:THR:HG21   | 2.02                     | 0.41              |
| 3:C:47:LYS:HE3   | 3:C:206:GLU:HB2   | 2.03                     | 0.41              |
| 4:D:174:GLN:HE21 | 5:E:52:GLU:HG2    | 1.85                     | 0.41              |
| 7:G:51:THR:OG1   | 7:G:78:VAL:HG21   | 2.20                     | 0.41              |
| 8:H:173:VAL:HG13 | 8:H:190:SER:HB3   | 2.02                     | 0.41              |
| 12:L:28:ARG:NH2  | 19:L:425:HOH:O    | 2.52                     | 0.41              |
| 6:T:69:VAL:HG21  | 6:T:75:MET:HE3    | 2.03                     | 0.41              |
| 9:W:183:GLY:HA2  | 9:W:201:ALA:HB3   | 2.03                     | 0.41              |
| 9:I:144:GLN:HE21 | 9:I:144:GLN:N     | 2.16                     | 0.41              |
| 10:J:43:LEU:HD12 | 10:J:183:ILE:HD11 | 2.02                     | 0.41              |
| 10:J:119:ASP:HB3 | 10:J:121:LEU:H    | 1.85                     | 0.41              |
| 13:M:43:MET:SD   | 13:M:64:LYS:HG3   | 2.60                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 14:N:24:THR:HB   | 13:a:141:TYR:CE1  | 2.55                     | 0.41              |
| 14:N:41:ILE:HD13 | 14:N:79:ALA:HB2   | 2.02                     | 0.41              |
| 1:O:68:THR:HG22  | 1:O:71:ILE:HB     | 2.03                     | 0.41              |
| 1:O:74:VAL:HG12  | 1:O:75:TYR:H      | 1.85                     | 0.41              |
| 2:P:179:LYS:O    | 2:P:183:MET:HG2   | 2.21                     | 0.41              |
| 7:U:51:THR:OG1   | 7:U:78:VAL:HG21   | 2.21                     | 0.41              |
| 8:V:19:ARG:HG3   | 8:V:26:VAL:HG13   | 2.03                     | 0.41              |
| 9:W:90:VAL:HG21  | 9:W:108:ILE:HD11  | 2.03                     | 0.41              |
| 14:b:146:MET:HE2 | 14:b:150:GLU:HB3  | 2.02                     | 0.41              |
| 3:C:118:THR:O    | 4:D:127:ARG:NH1   | 2.54                     | 0.41              |
| 3:C:169:GLU:HA   | 3:C:172:GLU:HG3   | 2.03                     | 0.41              |
| 8:V:126:ALA:HB3  | 8:V:135:VAL:HG22  | 2.02                     | 0.41              |
| 8:H:7:VAL:HG22   | 8:H:12:VAL:HG12   | 2.03                     | 0.40              |
| 11:K:82:LEU:O    | 11:K:86:MET:HG3   | 2.22                     | 0.40              |
| 14:N:143:LYS:O   | 14:N:146:MET:HG3  | 2.21                     | 0.40              |
| 3:Q:47:LYS:HE3   | 3:Q:206:GLU:HB2   | 2.03                     | 0.40              |
| 4:R:74:ILE:H     | 4:R:74:ILE:HD12   | 1.86                     | 0.40              |
| 10:X:169:LYS:HG2 | 10:X:170:ARG:HG2  | 2.03                     | 0.40              |
| 12:Z:76:LYS:HB2  | 12:Z:76:LYS:HE3   | 1.87                     | 0.40              |
| 13:a:46:ASN:HD21 | 13:a:49:THR:CG2   | 2.34                     | 0.40              |
| 1:A:223:THR:HG23 | 1:A:226:ARG:HH21  | 1.86                     | 0.40              |
| 3:C:91:GLN:HE21  | 10:J:62:LYS:HG3   | 1.85                     | 0.40              |
| 4:D:20:ILE:HA    | 4:D:23:ILE:HD12   | 2.01                     | 0.40              |
| 12:L:180:ILE:HA  | 19:L:429:HOH:O    | 2.20                     | 0.40              |
| 1:O:223:THR:HG23 | 1:O:226:ARG:HH21  | 1.86                     | 0.40              |
| 10:X:43:LEU:HD12 | 10:X:183:ILE:HD11 | 2.03                     | 0.40              |
| 14:b:77:LEU:HD22 | 14:b:81:ASN:ND2   | 2.36                     | 0.40              |
| 1:A:14:PRO:HA    | 2:B:22:TYR:CD2    | 2.57                     | 0.40              |
| 2:B:179:LYS:O    | 2:B:183:MET:HG2   | 2.21                     | 0.40              |
| 3:C:211:ARG:H    | 3:C:211:ARG:HG2   | 1.73                     | 0.40              |
| 6:F:111:LEU:O    | 6:F:115:VAL:HG23  | 2.21                     | 0.40              |
| 7:G:49:ILE:CG2   | 7:G:78:VAL:HB     | 2.51                     | 0.40              |
| 11:K:120:ARG:HG3 | 19:K:406:HOH:O    | 2.21                     | 0.40              |
| 14:N:45:LEU:HG   | 19:N:310:HOH:O    | 2.21                     | 0.40              |
| 2:P:23:ALA:O     | 2:P:27:ILE:HD12   | 2.21                     | 0.40              |
| 6:T:215:TRP:HB3  | 6:T:220:THR:HG21  | 2.04                     | 0.40              |
| 8:V:137:LEU:HD13 | 8:V:141:ARG:HE    | 1.86                     | 0.40              |
| 9:W:1:SER:HB3    | 9:W:4:SER:HB2     | 2.02                     | 0.40              |
| 12:Z:136:LYS:HA  | 12:Z:146:GLN:HE22 | 1.85                     | 0.40              |
| 1:A:68:THR:HG22  | 1:A:71:ILE:HB     | 2.03                     | 0.40              |
| 4:D:20:ILE:HD13  | 4:D:150:PRO:HD2   | 2.02                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:E:69:ILE:HG22  | 5:E:131:ILE:HG12  | 2.02                     | 0.40              |
| 3:Q:145:GLN:HG2  | 3:Q:158:ASN:HD22  | 1.86                     | 0.40              |
| 6:T:113:ASP:O    | 6:T:117:MET:HG2   | 2.20                     | 0.40              |
| 10:X:161:ARG:HE  | 10:X:161:ARG:HB2  | 1.49                     | 0.40              |
| 12:Z:13:LEU:HD11 | 12:Z:149:LEU:CD1  | 2.47                     | 0.40              |
| 12:Z:176:LYS:O   | 12:Z:180:ILE:HG13 | 2.22                     | 0.40              |
| 3:C:94:ARG:HB3   | 10:J:62:LYS:HE3   | 2.03                     | 0.40              |
| 12:L:31:GLU:HB2  | 12:L:36:HIS:CD2   | 2.56                     | 0.40              |
| 14:N:146:MET:HE2 | 14:N:150:GLU:HB3  | 2.03                     | 0.40              |
| 1:O:198:PHE:O    | 1:O:199:GLU:HB2   | 2.20                     | 0.40              |
| 9:W:141:CYS:HB3  | 9:W:177:ASP:HB2   | 2.03                     | 0.40              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1         | Atom-2                  | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-------------------------|--------------------------|-------------------|
| 11:K:146:ASP:O | 13:M:206:GLN:NE2[2_655] | 2.08                     | 0.12              |

## 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 X-ray entries followed by that with respect to entries of similar resolution.

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     | 228/234 (97%) | 217 (95%) | 8 (4%)  | 3 (1%)   | 9           | 32  |
| 1   | O     | 228/234 (97%) | 217 (95%) | 8 (4%)  | 3 (1%)   | 9           | 32  |
| 2   | B     | 246/261 (94%) | 240 (98%) | 5 (2%)  | 1 (0%)   | 30          | 59  |
| 2   | P     | 246/261 (94%) | 240 (98%) | 5 (2%)  | 1 (0%)   | 30          | 59  |
| 3   | C     | 236/248 (95%) | 222 (94%) | 14 (6%) | 0        | 100         | 100 |
| 3   | Q     | 236/248 (95%) | 221 (94%) | 15 (6%) | 0        | 100         | 100 |
| 4   | D     | 231/241 (96%) | 222 (96%) | 8 (4%)  | 1 (0%)   | 30          | 59  |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 4   | R     | 231/241 (96%)   | 222 (96%)  | 8 (4%)   | 1 (0%)   | 30          | 59  |
| 5   | E     | 236/263 (90%)   | 227 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 5   | S     | 236/263 (90%)   | 227 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 6   | F     | 242/255 (95%)   | 234 (97%)  | 7 (3%)   | 1 (0%)   | 30          | 59  |
| 6   | T     | 242/255 (95%)   | 234 (97%)  | 7 (3%)   | 1 (0%)   | 30          | 59  |
| 7   | G     | 241/246 (98%)   | 236 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 7   | U     | 241/246 (98%)   | 237 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 8   | H     | 217/234 (93%)   | 206 (95%)  | 9 (4%)   | 2 (1%)   | 14          | 41  |
| 8   | V     | 217/234 (93%)   | 206 (95%)  | 9 (4%)   | 2 (1%)   | 14          | 41  |
| 9   | I     | 202/205 (98%)   | 191 (95%)  | 9 (4%)   | 2 (1%)   | 12          | 39  |
| 9   | W     | 202/205 (98%)   | 191 (95%)  | 9 (4%)   | 2 (1%)   | 12          | 39  |
| 10  | J     | 194/201 (96%)   | 187 (96%)  | 6 (3%)   | 1 (0%)   | 24          | 54  |
| 10  | X     | 194/201 (96%)   | 187 (96%)  | 6 (3%)   | 1 (0%)   | 24          | 54  |
| 11  | K     | 199/204 (98%)   | 189 (95%)  | 10 (5%)  | 0        | 100         | 100 |
| 11  | Y     | 199/204 (98%)   | 189 (95%)  | 10 (5%)  | 0        | 100         | 100 |
| 12  | L     | 211/213 (99%)   | 206 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 12  | Z     | 211/213 (99%)   | 205 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 13  | M     | 214/219 (98%)   | 205 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 13  | a     | 214/219 (98%)   | 205 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 14  | N     | 197/199 (99%)   | 195 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 14  | b     | 197/199 (99%)   | 195 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| All | All   | 6188/6446 (96%) | 5953 (96%) | 213 (3%) | 22 (0%)  | 30          | 59  |

All (22) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | F     | 216 | VAL  |
| 9   | I     | 30  | GLN  |
| 6   | T     | 216 | VAL  |
| 9   | W     | 30  | GLN  |
| 1   | A     | 40  | ALA  |
| 1   | A     | 198 | PHE  |
| 1   | A     | 199 | GLU  |
| 2   | B     | 203 | SER  |
| 10  | J     | 24  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 40  | ALA  |
| 1   | O     | 198 | PHE  |
| 1   | O     | 199 | GLU  |
| 2   | P     | 203 | SER  |
| 10  | X     | 24  | ASN  |
| 4   | D     | 112 | ALA  |
| 9   | I     | 47  | ARG  |
| 4   | R     | 112 | ALA  |
| 9   | W     | 47  | ARG  |
| 8   | H     | 195 | PRO  |
| 8   | V     | 195 | PRO  |
| 8   | H     | 194 | GLU  |
| 8   | V     | 194 | GLU  |

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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     | 189/191 (99%) | 172 (91%) | 17 (9%)  | 9           | 28 |
| 1   | O     | 189/191 (99%) | 172 (91%) | 17 (9%)  | 9           | 28 |
| 2   | B     | 208/221 (94%) | 185 (89%) | 23 (11%) | 6           | 20 |
| 2   | P     | 208/221 (94%) | 185 (89%) | 23 (11%) | 6           | 20 |
| 3   | C     | 202/211 (96%) | 180 (89%) | 22 (11%) | 6           | 20 |
| 3   | Q     | 202/211 (96%) | 180 (89%) | 22 (11%) | 6           | 20 |
| 4   | D     | 195/203 (96%) | 181 (93%) | 14 (7%)  | 13          | 39 |
| 4   | R     | 195/203 (96%) | 181 (93%) | 14 (7%)  | 13          | 39 |
| 5   | E     | 204/224 (91%) | 190 (93%) | 14 (7%)  | 14          | 41 |
| 5   | S     | 204/224 (91%) | 190 (93%) | 14 (7%)  | 14          | 41 |
| 6   | F     | 200/211 (95%) | 190 (95%) | 10 (5%)  | 22          | 53 |
| 6   | T     | 200/211 (95%) | 190 (95%) | 10 (5%)  | 22          | 53 |
| 7   | G     | 207/210 (99%) | 194 (94%) | 13 (6%)  | 16          | 45 |
| 7   | U     | 207/210 (99%) | 194 (94%) | 13 (6%)  | 16          | 45 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 8   | H     | 169/183 (92%)   | 149 (88%)  | 20 (12%) | 5           | 17 |
| 8   | V     | 169/183 (92%)   | 149 (88%)  | 20 (12%) | 5           | 17 |
| 9   | I     | 174/175 (99%)   | 163 (94%)  | 11 (6%)  | 16          | 45 |
| 9   | W     | 174/175 (99%)   | 163 (94%)  | 11 (6%)  | 16          | 45 |
| 10  | J     | 166/171 (97%)   | 156 (94%)  | 10 (6%)  | 17          | 47 |
| 10  | X     | 166/171 (97%)   | 156 (94%)  | 10 (6%)  | 17          | 47 |
| 11  | K     | 165/166 (99%)   | 151 (92%)  | 14 (8%)  | 10          | 31 |
| 11  | Y     | 165/166 (99%)   | 151 (92%)  | 14 (8%)  | 10          | 31 |
| 12  | L     | 178/178 (100%)  | 166 (93%)  | 12 (7%)  | 15          | 43 |
| 12  | Z     | 178/178 (100%)  | 165 (93%)  | 13 (7%)  | 13          | 38 |
| 13  | M     | 178/180 (99%)   | 167 (94%)  | 11 (6%)  | 16          | 46 |
| 13  | a     | 178/180 (99%)   | 167 (94%)  | 11 (6%)  | 16          | 46 |
| 14  | N     | 155/155 (100%)  | 143 (92%)  | 12 (8%)  | 12          | 35 |
| 14  | b     | 155/155 (100%)  | 143 (92%)  | 12 (8%)  | 12          | 35 |
| All | All   | 5180/5358 (97%) | 4773 (92%) | 407 (8%) | 11          | 34 |

All (407) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 2   | LYS  |
| 1   | A     | 19  | VAL  |
| 1   | A     | 28  | VAL  |
| 1   | A     | 54  | ILE  |
| 1   | A     | 59  | ARG  |
| 1   | A     | 74  | VAL  |
| 1   | A     | 83  | ARG  |
| 1   | A     | 115 | SER  |
| 1   | A     | 140 | GLU  |
| 1   | A     | 170 | LYS  |
| 1   | A     | 184 | GLU  |
| 1   | A     | 189 | THR  |
| 1   | A     | 201 | GLN  |
| 1   | A     | 207 | ILE  |
| 1   | A     | 209 | VAL  |
| 1   | A     | 226 | ARG  |
| 1   | A     | 229 | LEU  |
| 2   | B     | 10  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 27  | ILE  |
| 2   | B     | 43  | LEU  |
| 2   | B     | 48  | ARG  |
| 2   | B     | 51  | ILE  |
| 2   | B     | 75  | VAL  |
| 2   | B     | 97  | LEU  |
| 2   | B     | 111 | THR  |
| 2   | B     | 131 | VAL  |
| 2   | B     | 163 | ILE  |
| 2   | B     | 177 | ASP  |
| 2   | B     | 179 | LYS  |
| 2   | B     | 182 | GLU  |
| 2   | B     | 184 | THR  |
| 2   | B     | 191 | LEU  |
| 2   | B     | 216 | THR  |
| 2   | B     | 217 | ARG  |
| 2   | B     | 232 | VAL  |
| 2   | B     | 234 | GLN  |
| 2   | B     | 235 | LEU  |
| 2   | B     | 240 | GLU  |
| 2   | B     | 242 | GLU  |
| 2   | B     | 248 | ARG  |
| 3   | C     | 4   | ARG  |
| 3   | C     | 34  | VAL  |
| 3   | C     | 41  | VAL  |
| 3   | C     | 46  | LYS  |
| 3   | C     | 56  | ARG  |
| 3   | C     | 76  | THR  |
| 3   | C     | 101 | VAL  |
| 3   | C     | 106 | ILE  |
| 3   | C     | 138 | ASP  |
| 3   | C     | 140 | THR  |
| 3   | C     | 153 | HIS  |
| 3   | C     | 156 | LYS  |
| 3   | C     | 162 | ARG  |
| 3   | C     | 171 | LEU  |
| 3   | C     | 185 | LEU  |
| 3   | C     | 186 | THR  |
| 3   | C     | 195 | LEU  |
| 3   | C     | 197 | VAL  |
| 3   | C     | 217 | LYS  |
| 3   | C     | 223 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 231 | ILE  |
| 3   | C     | 236 | GLU  |
| 4   | D     | 12  | ARG  |
| 4   | D     | 28  | THR  |
| 4   | D     | 101 | VAL  |
| 4   | D     | 118 | GLU  |
| 4   | D     | 127 | ARG  |
| 4   | D     | 140 | GLU  |
| 4   | D     | 162 | ILE  |
| 4   | D     | 183 | LEU  |
| 4   | D     | 201 | LYS  |
| 4   | D     | 202 | LEU  |
| 4   | D     | 209 | LEU  |
| 4   | D     | 223 | LYS  |
| 4   | D     | 228 | GLU  |
| 4   | D     | 229 | VAL  |
| 5   | E     | 1   | ASN  |
| 5   | E     | 7   | VAL  |
| 5   | E     | 35  | LEU  |
| 5   | E     | 57  | GLN  |
| 5   | E     | 98  | ARG  |
| 5   | E     | 153 | CYS  |
| 5   | E     | 154 | ARG  |
| 5   | E     | 163 | GLN  |
| 5   | E     | 179 | CYS  |
| 5   | E     | 180 | ASN  |
| 5   | E     | 184 | LEU  |
| 5   | E     | 204 | THR  |
| 5   | E     | 206 | ASN  |
| 5   | E     | 226 | VAL  |
| 6   | F     | 30  | VAL  |
| 6   | F     | 37  | ILE  |
| 6   | F     | 66  | LEU  |
| 6   | F     | 181 | MET  |
| 6   | F     | 200 | VAL  |
| 6   | F     | 203 | GLU  |
| 6   | F     | 205 | LYS  |
| 6   | F     | 219 | LEU  |
| 6   | F     | 225 | GLU  |
| 6   | F     | 230 | ASP  |
| 7   | G     | 59  | LEU  |
| 7   | G     | 74  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | G     | 80  | THR  |
| 7   | G     | 83  | THR  |
| 7   | G     | 103 | LYS  |
| 7   | G     | 111 | ASP  |
| 7   | G     | 113 | LEU  |
| 7   | G     | 131 | ARG  |
| 7   | G     | 142 | ILE  |
| 7   | G     | 178 | LEU  |
| 7   | G     | 209 | PHE  |
| 7   | G     | 219 | VAL  |
| 7   | G     | 222 | GLU  |
| 8   | H     | 6   | LEU  |
| 8   | H     | 7   | VAL  |
| 8   | H     | 21  | THR  |
| 8   | H     | 32  | GLU  |
| 8   | H     | 40  | LYS  |
| 8   | H     | 56  | THR  |
| 8   | H     | 68  | LEU  |
| 8   | H     | 76  | VAL  |
| 8   | H     | 80  | THR  |
| 8   | H     | 100 | VAL  |
| 8   | H     | 113 | VAL  |
| 8   | H     | 122 | LEU  |
| 8   | H     | 127 | LEU  |
| 8   | H     | 135 | VAL  |
| 8   | H     | 155 | LEU  |
| 8   | H     | 173 | VAL  |
| 8   | H     | 185 | LEU  |
| 8   | H     | 193 | THR  |
| 8   | H     | 197 | GLN  |
| 8   | H     | 216 | VAL  |
| 9   | I     | 33  | MET  |
| 9   | I     | 36  | THR  |
| 9   | I     | 84  | TYR  |
| 9   | I     | 115 | THR  |
| 9   | I     | 117 | LYS  |
| 9   | I     | 125 | LEU  |
| 9   | I     | 131 | VAL  |
| 9   | I     | 142 | SER  |
| 9   | I     | 144 | GLN  |
| 9   | I     | 171 | LEU  |
| 9   | I     | 192 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | J     | 1   | MET  |
| 10  | J     | 8   | GLN  |
| 10  | J     | 45  | LEU  |
| 10  | J     | 47  | VAL  |
| 10  | J     | 84  | THR  |
| 10  | J     | 85  | ARG  |
| 10  | J     | 103 | LEU  |
| 10  | J     | 143 | LEU  |
| 10  | J     | 154 | GLU  |
| 10  | J     | 161 | ARG  |
| 11  | K     | 9   | GLN  |
| 11  | K     | 13  | ILE  |
| 11  | K     | 27  | SER  |
| 11  | K     | 29  | LEU  |
| 11  | K     | 30  | ARG  |
| 11  | K     | 35  | ILE  |
| 11  | K     | 64  | ARG  |
| 11  | K     | 82  | LEU  |
| 11  | K     | 87  | MET  |
| 11  | K     | 88  | LEU  |
| 11  | K     | 121 | LEU  |
| 11  | K     | 139 | MET  |
| 11  | K     | 158 | ARG  |
| 11  | K     | 192 | VAL  |
| 12  | L     | 11  | THR  |
| 12  | L     | 31  | GLU  |
| 12  | L     | 45  | LYS  |
| 12  | L     | 63  | THR  |
| 12  | L     | 106 | VAL  |
| 12  | L     | 133 | ASP  |
| 12  | L     | 148 | LEU  |
| 12  | L     | 162 | GLU  |
| 12  | L     | 166 | LEU  |
| 12  | L     | 173 | ARG  |
| 12  | L     | 180 | ILE  |
| 12  | L     | 201 | GLU  |
| 13  | M     | 3   | ASN  |
| 13  | M     | 37  | ARG  |
| 13  | M     | 44  | ARG  |
| 13  | M     | 46  | ASN  |
| 13  | M     | 49  | THR  |
| 13  | M     | 69  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | M     | 94  | ARG  |
| 13  | M     | 109 | THR  |
| 13  | M     | 152 | GLU  |
| 13  | M     | 168 | LEU  |
| 13  | M     | 192 | VAL  |
| 14  | N     | 20  | VAL  |
| 14  | N     | 26  | VAL  |
| 14  | N     | 27  | VAL  |
| 14  | N     | 37  | LEU  |
| 14  | N     | 58  | MET  |
| 14  | N     | 77  | LEU  |
| 14  | N     | 82  | VAL  |
| 14  | N     | 100 | VAL  |
| 14  | N     | 143 | LYS  |
| 14  | N     | 153 | ARG  |
| 14  | N     | 191 | ASP  |
| 14  | N     | 199 | GLU  |
| 1   | O     | 2   | LYS  |
| 1   | O     | 19  | VAL  |
| 1   | O     | 28  | VAL  |
| 1   | O     | 54  | ILE  |
| 1   | O     | 59  | ARG  |
| 1   | O     | 74  | VAL  |
| 1   | O     | 83  | ARG  |
| 1   | O     | 115 | SER  |
| 1   | O     | 140 | GLU  |
| 1   | O     | 170 | LYS  |
| 1   | O     | 184 | GLU  |
| 1   | O     | 189 | THR  |
| 1   | O     | 201 | GLN  |
| 1   | O     | 207 | ILE  |
| 1   | O     | 209 | VAL  |
| 1   | O     | 226 | ARG  |
| 1   | O     | 229 | LEU  |
| 2   | P     | 10  | ILE  |
| 2   | P     | 27  | ILE  |
| 2   | P     | 43  | LEU  |
| 2   | P     | 48  | ARG  |
| 2   | P     | 51  | ILE  |
| 2   | P     | 75  | VAL  |
| 2   | P     | 97  | LEU  |
| 2   | P     | 111 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | P     | 131 | VAL  |
| 2   | P     | 163 | ILE  |
| 2   | P     | 177 | ASP  |
| 2   | P     | 179 | LYS  |
| 2   | P     | 182 | GLU  |
| 2   | P     | 184 | THR  |
| 2   | P     | 186 | LYS  |
| 2   | P     | 191 | LEU  |
| 2   | P     | 216 | THR  |
| 2   | P     | 217 | ARG  |
| 2   | P     | 232 | VAL  |
| 2   | P     | 234 | GLN  |
| 2   | P     | 235 | LEU  |
| 2   | P     | 240 | GLU  |
| 2   | P     | 242 | GLU  |
| 3   | Q     | 4   | ARG  |
| 3   | Q     | 34  | VAL  |
| 3   | Q     | 41  | VAL  |
| 3   | Q     | 46  | LYS  |
| 3   | Q     | 56  | ARG  |
| 3   | Q     | 76  | THR  |
| 3   | Q     | 101 | VAL  |
| 3   | Q     | 106 | ILE  |
| 3   | Q     | 138 | ASP  |
| 3   | Q     | 140 | THR  |
| 3   | Q     | 153 | HIS  |
| 3   | Q     | 156 | LYS  |
| 3   | Q     | 162 | ARG  |
| 3   | Q     | 171 | LEU  |
| 3   | Q     | 185 | LEU  |
| 3   | Q     | 186 | THR  |
| 3   | Q     | 195 | LEU  |
| 3   | Q     | 197 | VAL  |
| 3   | Q     | 217 | LYS  |
| 3   | Q     | 223 | GLU  |
| 3   | Q     | 231 | ILE  |
| 3   | Q     | 236 | GLU  |
| 4   | R     | 12  | ARG  |
| 4   | R     | 28  | THR  |
| 4   | R     | 101 | VAL  |
| 4   | R     | 118 | GLU  |
| 4   | R     | 127 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | R     | 140 | GLU  |
| 4   | R     | 162 | ILE  |
| 4   | R     | 183 | LEU  |
| 4   | R     | 201 | LYS  |
| 4   | R     | 202 | LEU  |
| 4   | R     | 209 | LEU  |
| 4   | R     | 223 | LYS  |
| 4   | R     | 228 | GLU  |
| 4   | R     | 229 | VAL  |
| 5   | S     | 1   | ASN  |
| 5   | S     | 7   | VAL  |
| 5   | S     | 35  | LEU  |
| 5   | S     | 57  | GLN  |
| 5   | S     | 98  | ARG  |
| 5   | S     | 153 | CYS  |
| 5   | S     | 154 | ARG  |
| 5   | S     | 163 | GLN  |
| 5   | S     | 179 | CYS  |
| 5   | S     | 180 | ASN  |
| 5   | S     | 184 | LEU  |
| 5   | S     | 204 | THR  |
| 5   | S     | 206 | ASN  |
| 5   | S     | 226 | VAL  |
| 6   | T     | 30  | VAL  |
| 6   | T     | 37  | ILE  |
| 6   | T     | 66  | LEU  |
| 6   | T     | 181 | MET  |
| 6   | T     | 200 | VAL  |
| 6   | T     | 203 | GLU  |
| 6   | T     | 205 | LYS  |
| 6   | T     | 219 | LEU  |
| 6   | T     | 225 | GLU  |
| 6   | T     | 230 | ASP  |
| 7   | U     | 59  | LEU  |
| 7   | U     | 74  | SER  |
| 7   | U     | 80  | THR  |
| 7   | U     | 83  | THR  |
| 7   | U     | 103 | LYS  |
| 7   | U     | 111 | ASP  |
| 7   | U     | 113 | LEU  |
| 7   | U     | 131 | ARG  |
| 7   | U     | 142 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | U     | 178 | LEU  |
| 7   | U     | 209 | PHE  |
| 7   | U     | 219 | VAL  |
| 7   | U     | 222 | GLU  |
| 8   | V     | 6   | LEU  |
| 8   | V     | 7   | VAL  |
| 8   | V     | 21  | THR  |
| 8   | V     | 32  | GLU  |
| 8   | V     | 40  | LYS  |
| 8   | V     | 56  | THR  |
| 8   | V     | 68  | LEU  |
| 8   | V     | 76  | VAL  |
| 8   | V     | 80  | THR  |
| 8   | V     | 100 | VAL  |
| 8   | V     | 113 | VAL  |
| 8   | V     | 122 | LEU  |
| 8   | V     | 127 | LEU  |
| 8   | V     | 135 | VAL  |
| 8   | V     | 155 | LEU  |
| 8   | V     | 173 | VAL  |
| 8   | V     | 185 | LEU  |
| 8   | V     | 193 | THR  |
| 8   | V     | 197 | GLN  |
| 8   | V     | 216 | VAL  |
| 9   | W     | 33  | MET  |
| 9   | W     | 36  | THR  |
| 9   | W     | 84  | TYR  |
| 9   | W     | 115 | THR  |
| 9   | W     | 117 | LYS  |
| 9   | W     | 125 | LEU  |
| 9   | W     | 131 | VAL  |
| 9   | W     | 142 | SER  |
| 9   | W     | 144 | GLN  |
| 9   | W     | 171 | LEU  |
| 9   | W     | 192 | ASP  |
| 10  | X     | 1   | MET  |
| 10  | X     | 8   | GLN  |
| 10  | X     | 45  | LEU  |
| 10  | X     | 47  | VAL  |
| 10  | X     | 84  | THR  |
| 10  | X     | 85  | ARG  |
| 10  | X     | 103 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | X     | 143 | LEU  |
| 10  | X     | 154 | GLU  |
| 10  | X     | 161 | ARG  |
| 11  | Y     | 9   | GLN  |
| 11  | Y     | 13  | ILE  |
| 11  | Y     | 27  | SER  |
| 11  | Y     | 29  | LEU  |
| 11  | Y     | 30  | ARG  |
| 11  | Y     | 35  | ILE  |
| 11  | Y     | 64  | ARG  |
| 11  | Y     | 82  | LEU  |
| 11  | Y     | 87  | MET  |
| 11  | Y     | 88  | LEU  |
| 11  | Y     | 121 | LEU  |
| 11  | Y     | 139 | MET  |
| 11  | Y     | 158 | ARG  |
| 11  | Y     | 192 | VAL  |
| 12  | Z     | 11  | THR  |
| 12  | Z     | 31  | GLU  |
| 12  | Z     | 45  | LYS  |
| 12  | Z     | 63  | THR  |
| 12  | Z     | 106 | VAL  |
| 12  | Z     | 133 | ASP  |
| 12  | Z     | 148 | LEU  |
| 12  | Z     | 162 | GLU  |
| 12  | Z     | 166 | LEU  |
| 12  | Z     | 173 | ARG  |
| 12  | Z     | 180 | ILE  |
| 12  | Z     | 201 | GLU  |
| 12  | Z     | 212 | LYS  |
| 13  | a     | 3   | ASN  |
| 13  | a     | 37  | ARG  |
| 13  | a     | 44  | ARG  |
| 13  | a     | 46  | ASN  |
| 13  | a     | 49  | THR  |
| 13  | a     | 69  | GLN  |
| 13  | a     | 94  | ARG  |
| 13  | a     | 109 | THR  |
| 13  | a     | 152 | GLU  |
| 13  | a     | 168 | LEU  |
| 13  | a     | 192 | VAL  |
| 14  | b     | 20  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | b     | 26  | VAL  |
| 14  | b     | 27  | VAL  |
| 14  | b     | 37  | LEU  |
| 14  | b     | 58  | MET  |
| 14  | b     | 77  | LEU  |
| 14  | b     | 82  | VAL  |
| 14  | b     | 100 | VAL  |
| 14  | b     | 143 | LYS  |
| 14  | b     | 153 | ARG  |
| 14  | b     | 191 | ASP  |
| 14  | b     | 199 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (140) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 62  | HIS  |
| 1   | A     | 94  | GLN  |
| 1   | A     | 111 | GLN  |
| 1   | A     | 139 | ASN  |
| 1   | A     | 147 | GLN  |
| 1   | A     | 165 | ASN  |
| 1   | A     | 178 | ASN  |
| 1   | A     | 206 | ASN  |
| 2   | B     | 39  | ASN  |
| 2   | B     | 68  | ASN  |
| 2   | B     | 87  | ASN  |
| 2   | B     | 94  | GLN  |
| 2   | B     | 122 | GLN  |
| 2   | B     | 154 | ASN  |
| 2   | B     | 239 | HIS  |
| 3   | C     | 22  | GLN  |
| 3   | C     | 153 | HIS  |
| 3   | C     | 220 | ASN  |
| 4   | D     | 91  | HIS  |
| 4   | D     | 106 | GLN  |
| 4   | D     | 174 | GLN  |
| 4   | D     | 196 | GLN  |
| 4   | D     | 213 | GLN  |
| 5   | E     | 1   | ASN  |
| 5   | E     | 2   | GLN  |
| 5   | E     | 5   | ASN  |
| 5   | E     | 40  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 172 | HIS  |
| 6   | F     | 201 | HIS  |
| 7   | G     | 67  | HIS  |
| 7   | G     | 89  | GLN  |
| 7   | G     | 91  | GLN  |
| 7   | G     | 126 | GLN  |
| 7   | G     | 237 | HIS  |
| 8   | H     | 22  | ASN  |
| 8   | H     | 66  | HIS  |
| 8   | H     | 106 | ASN  |
| 8   | H     | 143 | GLN  |
| 9   | I     | 6   | ASN  |
| 9   | I     | 39  | GLN  |
| 9   | I     | 80  | GLN  |
| 9   | I     | 144 | GLN  |
| 9   | I     | 168 | GLN  |
| 10  | J     | 8   | GLN  |
| 10  | J     | 27  | GLN  |
| 10  | J     | 61  | GLN  |
| 10  | J     | 101 | ASN  |
| 10  | J     | 132 | HIS  |
| 10  | J     | 174 | ASN  |
| 11  | K     | 10  | HIS  |
| 11  | K     | 117 | ASN  |
| 11  | K     | 124 | GLN  |
| 12  | L     | 8   | ASN  |
| 12  | L     | 79  | ASN  |
| 12  | L     | 108 | ASN  |
| 12  | L     | 131 | GLN  |
| 12  | L     | 146 | GLN  |
| 12  | L     | 151 | ASN  |
| 12  | L     | 157 | ASN  |
| 12  | L     | 159 | GLN  |
| 12  | L     | 160 | ASN  |
| 13  | M     | 46  | ASN  |
| 13  | M     | 104 | ASN  |
| 13  | M     | 108 | ASN  |
| 13  | M     | 157 | GLN  |
| 13  | M     | 208 | ASN  |
| 14  | N     | 28  | ASN  |
| 14  | N     | 81  | ASN  |
| 14  | N     | 157 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 87  | HIS  |
| 1   | O     | 94  | GLN  |
| 1   | O     | 111 | GLN  |
| 1   | O     | 139 | ASN  |
| 1   | O     | 147 | GLN  |
| 1   | O     | 165 | ASN  |
| 1   | O     | 178 | ASN  |
| 1   | O     | 206 | ASN  |
| 2   | P     | 39  | ASN  |
| 2   | P     | 68  | ASN  |
| 2   | P     | 94  | GLN  |
| 2   | P     | 122 | GLN  |
| 2   | P     | 154 | ASN  |
| 2   | P     | 239 | HIS  |
| 3   | Q     | 22  | GLN  |
| 3   | Q     | 220 | ASN  |
| 4   | R     | 91  | HIS  |
| 4   | R     | 106 | GLN  |
| 4   | R     | 110 | ASN  |
| 4   | R     | 174 | GLN  |
| 4   | R     | 196 | GLN  |
| 4   | R     | 203 | ASN  |
| 4   | R     | 213 | GLN  |
| 5   | S     | 1   | ASN  |
| 5   | S     | 2   | GLN  |
| 5   | S     | 5   | ASN  |
| 5   | S     | 40  | HIS  |
| 5   | S     | 163 | GLN  |
| 6   | T     | 201 | HIS  |
| 7   | U     | 89  | GLN  |
| 7   | U     | 91  | GLN  |
| 7   | U     | 126 | GLN  |
| 7   | U     | 237 | HIS  |
| 8   | V     | 22  | ASN  |
| 8   | V     | 66  | HIS  |
| 8   | V     | 106 | ASN  |
| 8   | V     | 143 | GLN  |
| 9   | W     | 6   | ASN  |
| 9   | W     | 39  | GLN  |
| 9   | W     | 64  | GLN  |
| 9   | W     | 80  | GLN  |
| 9   | W     | 144 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | W     | 168 | GLN  |
| 9   | W     | 187 | HIS  |
| 10  | X     | 8   | GLN  |
| 10  | X     | 27  | GLN  |
| 10  | X     | 61  | GLN  |
| 10  | X     | 132 | HIS  |
| 10  | X     | 174 | ASN  |
| 11  | Y     | 10  | HIS  |
| 11  | Y     | 38  | ASN  |
| 11  | Y     | 117 | ASN  |
| 11  | Y     | 124 | GLN  |
| 11  | Y     | 165 | HIS  |
| 12  | Z     | 8   | ASN  |
| 12  | Z     | 79  | ASN  |
| 12  | Z     | 108 | ASN  |
| 12  | Z     | 131 | GLN  |
| 12  | Z     | 146 | GLN  |
| 12  | Z     | 151 | ASN  |
| 12  | Z     | 159 | GLN  |
| 13  | a     | 46  | ASN  |
| 13  | a     | 104 | ASN  |
| 13  | a     | 108 | ASN  |
| 13  | a     | 157 | GLN  |
| 13  | a     | 208 | ASN  |
| 14  | b     | 28  | ASN  |
| 14  | b     | 66  | HIS  |
| 14  | b     | 81  | ASN  |
| 14  | b     | 97  | HIS  |
| 14  | b     | 157 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 66 ligands modelled in this entry, 60 are monoatomic - leaving 6 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 17  | 04C  | N     | 201 | 14   | 44,44,44     | 1.30 | 4 (9%)   | 54,58,58    | 1.16 | 5 (9%)   |
| 17  | 04C  | H     | 301 | 8    | 44,44,44     | 1.20 | 3 (6%)   | 54,58,58    | 0.98 | 3 (5%)   |
| 17  | 04C  | b     | 201 | 14   | 44,44,44     | 1.34 | 4 (9%)   | 54,58,58    | 1.13 | 6 (11%)  |
| 17  | 04C  | Y     | 301 | 11   | 44,44,44     | 1.30 | 2 (4%)   | 54,58,58    | 1.35 | 6 (11%)  |
| 17  | 04C  | K     | 301 | 11   | 44,44,44     | 1.26 | 3 (6%)   | 54,58,58    | 0.98 | 2 (3%)   |
| 17  | 04C  | V     | 301 | 8    | 44,44,44     | 1.25 | 3 (6%)   | 54,58,58    | 1.02 | 5 (9%)   |

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   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 17  | 04C  | N     | 201 | 14   | -       | 11/44/52/52 | 0/3/3/3 |
| 17  | 04C  | H     | 301 | 8    | -       | 20/44/52/52 | 0/3/3/3 |
| 17  | 04C  | b     | 201 | 14   | -       | 10/44/52/52 | 0/3/3/3 |
| 17  | 04C  | Y     | 301 | 11   | -       | 13/44/52/52 | 0/3/3/3 |
| 17  | 04C  | K     | 301 | 11   | -       | 12/44/52/52 | 0/3/3/3 |
| 17  | 04C  | V     | 301 | 8    | -       | 15/44/52/52 | 0/3/3/3 |

All (19) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 17  | N     | 201 | 04C  | C10-C9  | 3.57 | 1.59        | 1.53     |
| 17  | K     | 301 | 04C  | C10-C9  | 3.36 | 1.59        | 1.53     |
| 17  | K     | 301 | 04C  | C12-C10 | 3.25 | 1.56        | 1.52     |
| 17  | b     | 201 | 04C  | C10-C9  | 3.23 | 1.59        | 1.53     |
| 17  | b     | 201 | 04C  | C12-C10 | 3.21 | 1.56        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 17  | Y     | 301 | 04C  | C10-C9  | 3.16 | 1.58        | 1.53     |
| 17  | V     | 301 | 04C  | C10-C9  | 2.96 | 1.58        | 1.53     |
| 17  | Y     | 301 | 04C  | C12-C10 | 2.94 | 1.56        | 1.52     |
| 17  | H     | 301 | 04C  | C12-C10 | 2.91 | 1.56        | 1.52     |
| 17  | b     | 201 | 04C  | C7-C6   | 2.80 | 1.57        | 1.51     |
| 17  | V     | 301 | 04C  | C12-C10 | 2.79 | 1.55        | 1.52     |
| 17  | H     | 301 | 04C  | C10-C9  | 2.74 | 1.58        | 1.53     |
| 17  | N     | 201 | 04C  | C12-C10 | 2.69 | 1.55        | 1.52     |
| 17  | N     | 201 | 04C  | C7-C6   | 2.48 | 1.57        | 1.51     |
| 17  | V     | 301 | 04C  | C9-C8   | 2.36 | 1.57        | 1.53     |
| 17  | b     | 201 | 04C  | C9-C8   | 2.25 | 1.57        | 1.53     |
| 17  | N     | 201 | 04C  | C9-C8   | 2.11 | 1.57        | 1.53     |
| 17  | K     | 301 | 04C  | C9-C8   | 2.09 | 1.57        | 1.53     |
| 17  | H     | 301 | 04C  | C42-C43 | 2.08 | 1.42        | 1.38     |

All (27) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 17  | Y     | 301 | 04C  | C32-N31-C36 | 4.81  | 119.20      | 108.84   |
| 17  | b     | 201 | 04C  | C11-C10-C12 | -4.33 | 104.25      | 109.76   |
| 17  | K     | 301 | 04C  | C11-C10-C12 | -4.27 | 104.33      | 109.76   |
| 17  | Y     | 301 | 04C  | C33-C32-N31 | 4.25  | 116.58      | 110.12   |
| 17  | N     | 201 | 04C  | C11-C10-C12 | -3.98 | 104.70      | 109.76   |
| 17  | Y     | 301 | 04C  | C35-C36-N31 | 3.91  | 116.06      | 110.12   |
| 17  | N     | 201 | 04C  | C6-C7-C8    | 3.52  | 119.37      | 113.40   |
| 17  | H     | 301 | 04C  | C11-C10-C12 | -3.31 | 105.55      | 109.76   |
| 17  | V     | 301 | 04C  | C11-C10-C12 | -3.18 | 105.71      | 109.76   |
| 17  | Y     | 301 | 04C  | C11-C10-C12 | -2.75 | 106.25      | 109.76   |
| 17  | H     | 301 | 04C  | C7-C8-N22   | -2.74 | 106.19      | 110.08   |
| 17  | N     | 201 | 04C  | C40-C24-N25 | -2.65 | 105.33      | 110.83   |
| 17  | Y     | 301 | 04C  | C6-C7-C8    | 2.64  | 117.88      | 113.40   |
| 17  | V     | 301 | 04C  | C7-C8-N22   | -2.64 | 106.33      | 110.08   |
| 17  | Y     | 301 | 04C  | C7-C8-N22   | -2.43 | 106.63      | 110.08   |
| 17  | b     | 201 | 04C  | C6-C7-C8    | 2.40  | 117.47      | 113.40   |
| 17  | b     | 201 | 04C  | C40-C24-N25 | -2.36 | 105.94      | 110.83   |
| 17  | H     | 301 | 04C  | C32-N31-C36 | 2.24  | 113.66      | 108.84   |
| 17  | b     | 201 | 04C  | C30-N31-C32 | 2.20  | 114.57      | 111.14   |
| 17  | V     | 301 | 04C  | C6-C7-C8    | 2.20  | 117.13      | 113.40   |
| 17  | K     | 301 | 04C  | C32-N31-C36 | 2.17  | 113.51      | 108.84   |
| 17  | V     | 301 | 04C  | C30-N31-C36 | 2.12  | 114.45      | 111.14   |
| 17  | N     | 201 | 04C  | C7-C8-N22   | -2.12 | 107.07      | 110.08   |
| 17  | N     | 201 | 04C  | C32-N31-C36 | 2.10  | 113.37      | 108.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 17  | b     | 201 | 04C  | C30-N31-C36 | 2.04  | 114.32      | 111.14   |
| 17  | V     | 301 | 04C  | O37-C29-C30 | -2.03 | 117.46      | 121.02   |
| 17  | b     | 201 | 04C  | C7-C8-N22   | -2.03 | 107.20      | 110.08   |

There are no chirality outliers.

All (81) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 17  | H     | 301 | 04C  | C6-C7-C8-N22    |
| 17  | H     | 301 | 04C  | C6-C7-C8-C9     |
| 17  | H     | 301 | 04C  | C9-C10-C12-O13  |
| 17  | H     | 301 | 04C  | C11-C10-C12-O13 |
| 17  | K     | 301 | 04C  | C30-C29-N28-C27 |
| 17  | K     | 301 | 04C  | C6-C7-C8-N22    |
| 17  | K     | 301 | 04C  | C6-C7-C8-C9     |
| 17  | N     | 201 | 04C  | C9-C10-C12-O13  |
| 17  | N     | 201 | 04C  | C11-C10-C12-O13 |
| 17  | V     | 301 | 04C  | C6-C7-C8-C9     |
| 17  | Y     | 301 | 04C  | C6-C7-C8-N22    |
| 17  | Y     | 301 | 04C  | C6-C7-C8-C9     |
| 17  | Y     | 301 | 04C  | C11-C10-C9-C8   |
| 17  | Y     | 301 | 04C  | C12-C10-C9-C8   |
| 17  | b     | 201 | 04C  | C9-C10-C12-O13  |
| 17  | b     | 201 | 04C  | C11-C10-C12-O13 |
| 17  | K     | 301 | 04C  | O37-C29-N28-C27 |
| 17  | H     | 301 | 04C  | C47-C44-O45-C46 |
| 17  | H     | 301 | 04C  | C43-C44-O45-C46 |
| 17  | N     | 201 | 04C  | C47-C44-O45-C46 |
| 17  | N     | 201 | 04C  | C43-C44-O45-C46 |
| 17  | Y     | 301 | 04C  | C47-C44-O45-C46 |
| 17  | Y     | 301 | 04C  | C43-C44-O45-C46 |
| 17  | K     | 301 | 04C  | C43-C44-O45-C46 |
| 17  | K     | 301 | 04C  | C47-C44-O45-C46 |
| 17  | V     | 301 | 04C  | C47-C44-O45-C46 |
| 17  | V     | 301 | 04C  | C43-C44-O45-C46 |
| 17  | b     | 201 | 04C  | C47-C44-O45-C46 |
| 17  | b     | 201 | 04C  | C43-C44-O45-C46 |
| 17  | b     | 201 | 04C  | C23-C24-C40-C41 |
| 17  | b     | 201 | 04C  | N25-C24-C40-C41 |
| 17  | H     | 301 | 04C  | N25-C24-C40-C41 |
| 17  | V     | 301 | 04C  | N25-C24-C40-C41 |
| 17  | V     | 301 | 04C  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 17  | K     | 301 | 04C  | C23-C24-C40-C41 |
| 17  | V     | 301 | 04C  | C1-C6-C7-C8     |
| 17  | Y     | 301 | 04C  | C5-C6-C7-C8     |
| 17  | K     | 301 | 04C  | N25-C24-C40-C41 |
| 17  | H     | 301 | 04C  | C23-C24-C40-C41 |
| 17  | K     | 301 | 04C  | C1-C6-C7-C8     |
| 17  | K     | 301 | 04C  | C5-C6-C7-C8     |
| 17  | Y     | 301 | 04C  | C1-C6-C7-C8     |
| 17  | H     | 301 | 04C  | C11-C10-C9-C8   |
| 17  | V     | 301 | 04C  | C11-C10-C9-C8   |
| 17  | V     | 301 | 04C  | C6-C7-C8-N22    |
| 17  | H     | 301 | 04C  | O37-C29-C30-N31 |
| 17  | H     | 301 | 04C  | C11-C10-C9-O21  |
| 17  | V     | 301 | 04C  | C11-C10-C9-O21  |
| 17  | Y     | 301 | 04C  | C11-C10-C9-O21  |
| 17  | Y     | 301 | 04C  | C12-C10-C9-O21  |
| 17  | H     | 301 | 04C  | C1-C6-C7-C8     |
| 17  | V     | 301 | 04C  | C23-C24-C40-C41 |
| 17  | V     | 301 | 04C  | O37-C29-C30-N31 |
| 17  | H     | 301 | 04C  | C5-C6-C7-C8     |
| 17  | H     | 301 | 04C  | N28-C29-C30-N31 |
| 17  | V     | 301 | 04C  | N28-C29-C30-N31 |
| 17  | N     | 201 | 04C  | C1-C6-C7-C8     |
| 17  | N     | 201 | 04C  | C5-C6-C7-C8     |
| 17  | b     | 201 | 04C  | C5-C6-C7-C8     |
| 17  | b     | 201 | 04C  | C1-C6-C7-C8     |
| 17  | V     | 301 | 04C  | C29-C30-N31-C32 |
| 17  | b     | 201 | 04C  | C11-C10-C9-C8   |
| 17  | H     | 301 | 04C  | O49-C23-N22-C8  |
| 17  | H     | 301 | 04C  | C29-C30-N31-C32 |
| 17  | N     | 201 | 04C  | C29-C30-N31-C36 |
| 17  | N     | 201 | 04C  | C29-C30-N31-C32 |
| 17  | V     | 301 | 04C  | C29-C30-N31-C36 |
| 17  | H     | 301 | 04C  | C29-C30-N31-C36 |
| 17  | Y     | 301 | 04C  | C29-C30-N31-C32 |
| 17  | H     | 301 | 04C  | O39-C26-N25-C24 |
| 17  | N     | 201 | 04C  | N25-C24-C40-C41 |
| 17  | b     | 201 | 04C  | C11-C10-C9-O21  |
| 17  | Y     | 301 | 04C  | O49-C23-N22-C8  |
| 17  | V     | 301 | 04C  | C12-C10-C9-C8   |
| 17  | N     | 201 | 04C  | N22-C23-C24-N25 |
| 17  | H     | 301 | 04C  | C23-C24-N25-C26 |

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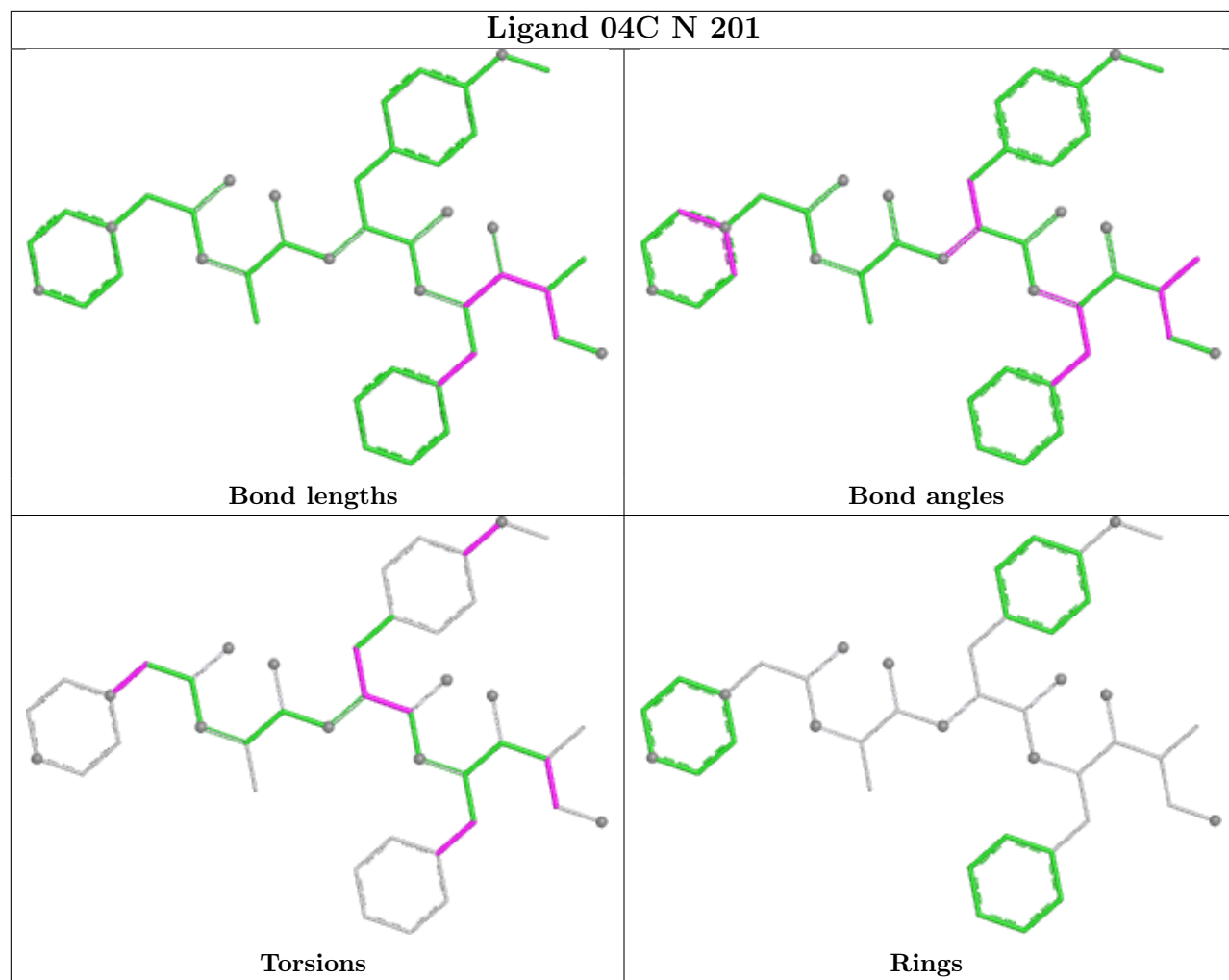
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 17  | Y     | 301 | 04C  | N25-C24-C40-C41 |
| 17  | K     | 301 | 04C  | C26-C27-N28-C29 |
| 17  | H     | 301 | 04C  | C27-C26-N25-C24 |
| 17  | K     | 301 | 04C  | O49-C23-N22-C8  |
| 17  | N     | 201 | 04C  | O49-C23-C24-N25 |

There are no ring outliers.

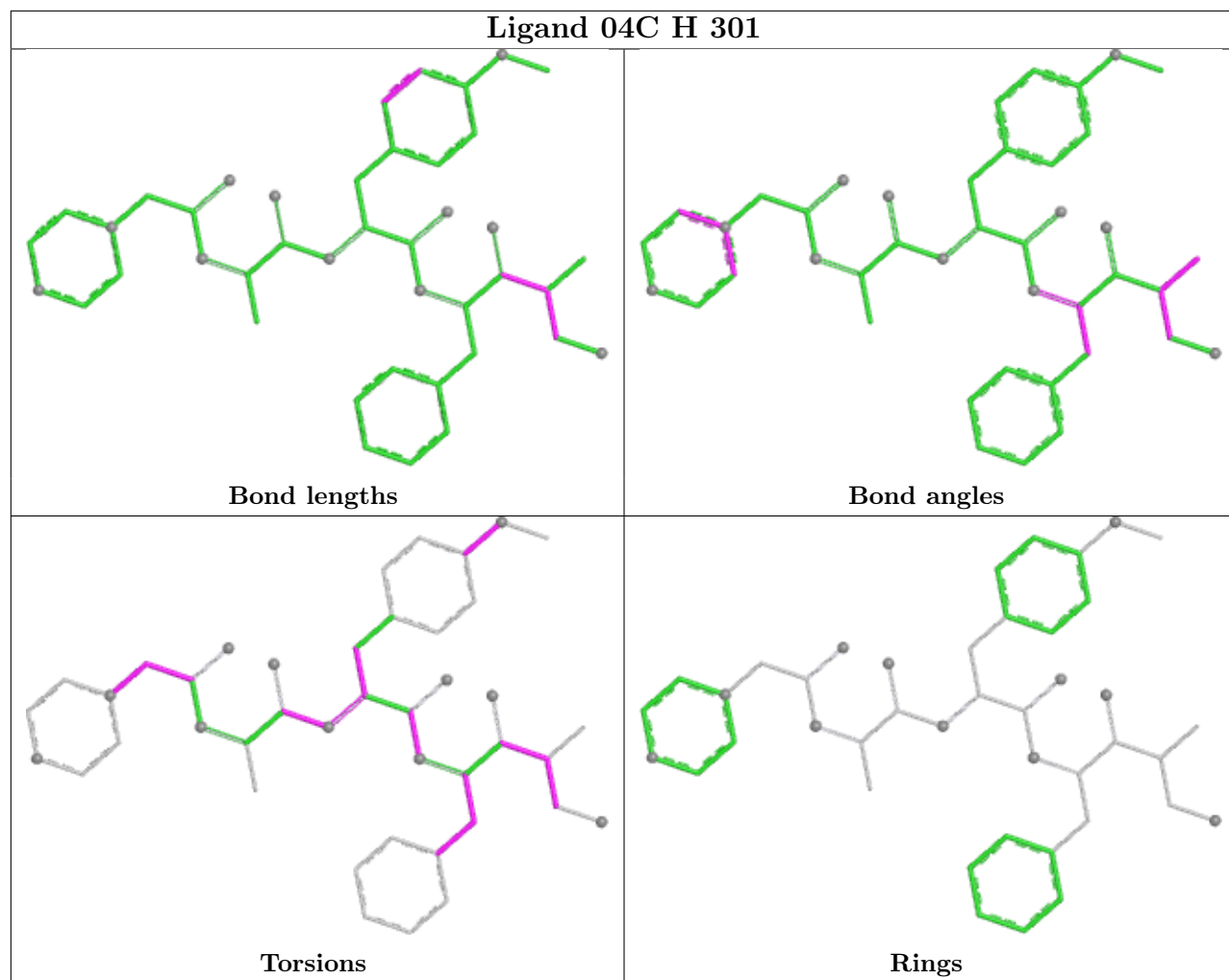
5 monomers are involved in 15 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 17  | N     | 201 | 04C  | 3       | 0            |
| 17  | b     | 201 | 04C  | 3       | 0            |
| 17  | Y     | 301 | 04C  | 4       | 0            |
| 17  | K     | 301 | 04C  | 4       | 0            |
| 17  | V     | 301 | 04C  | 1       | 0            |

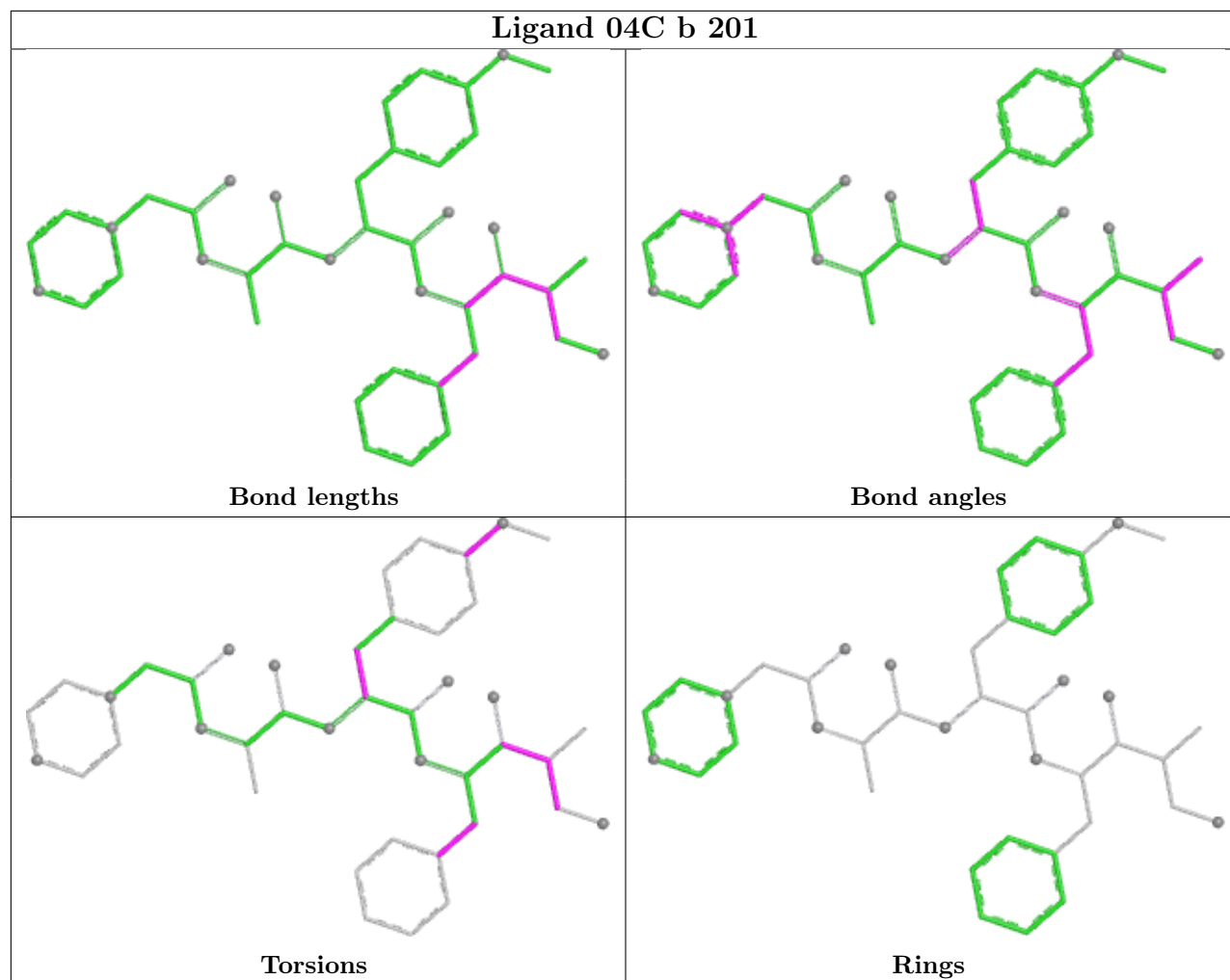
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



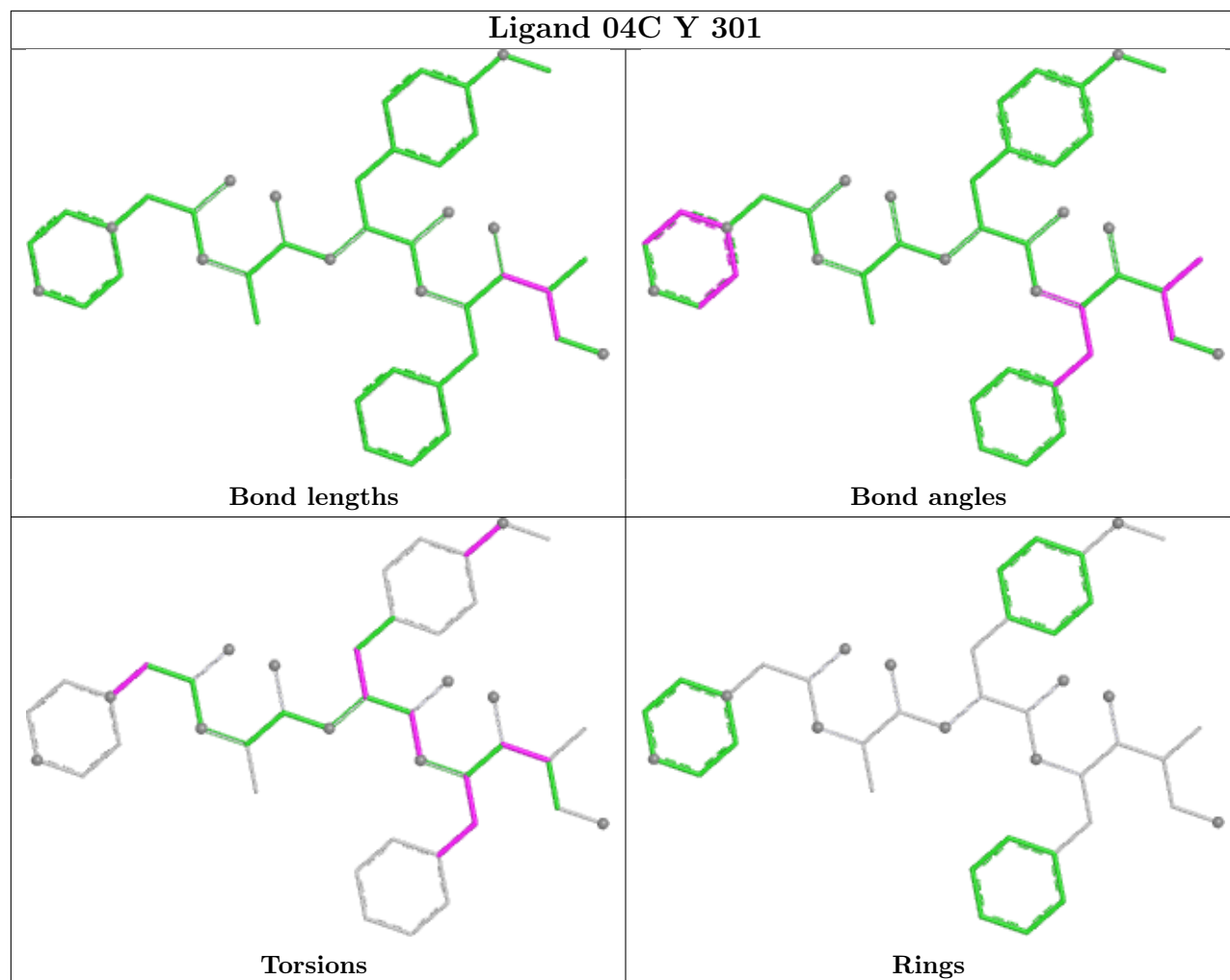
## Ligand 04C H 301



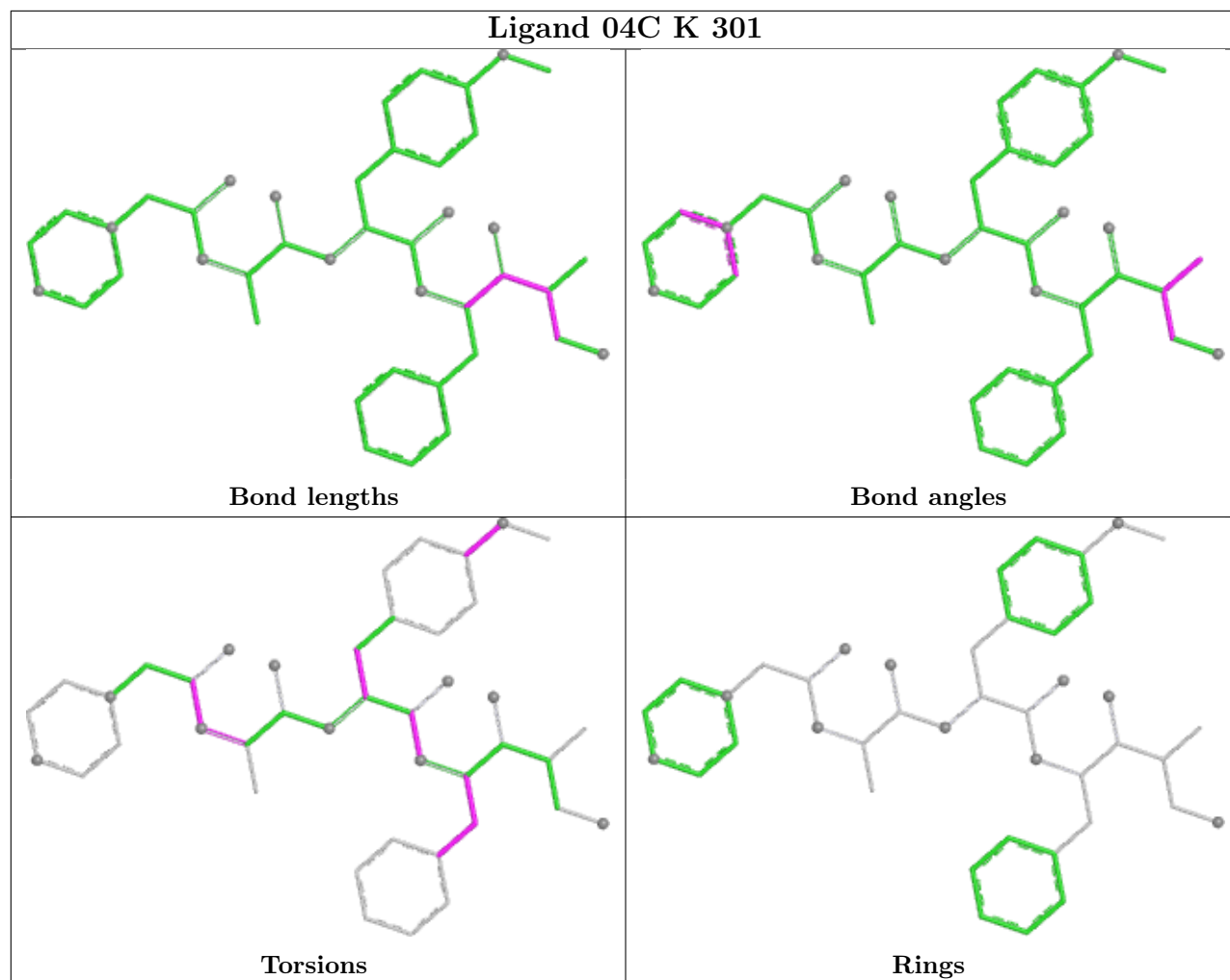
## Ligand 04C b 201

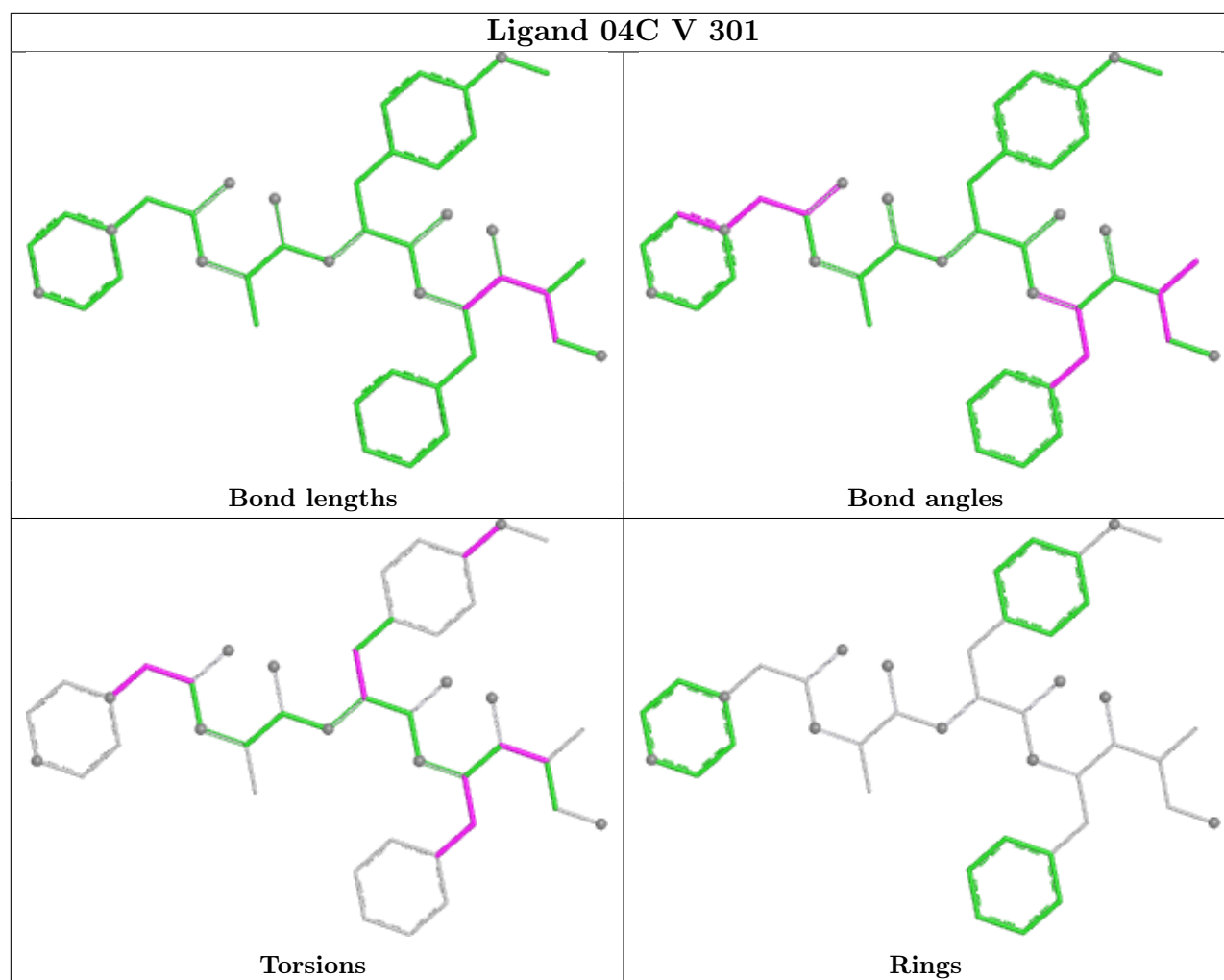


## Ligand 04C Y 301



## Ligand 04C K 301





## 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 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 230/234 (98%)  | 0.08   | 3 (1%) 75 67  | 44, 68, 95, 106       | 0     |
| 1   | O     | 230/234 (98%)  | -0.02  | 3 (1%) 75 67  | 35, 52, 86, 96        | 0     |
| 2   | B     | 248/261 (95%)  | 0.10   | 3 (1%) 76 69  | 45, 72, 121, 149      | 0     |
| 2   | P     | 248/261 (95%)  | -0.05  | 1 (0%) 88 85  | 32, 57, 99, 142       | 0     |
| 3   | C     | 238/248 (95%)  | 0.39   | 10 (4%) 40 32 | 51, 87, 150, 194      | 0     |
| 3   | Q     | 238/248 (95%)  | 0.25   | 2 (0%) 82 77  | 41, 74, 132, 174      | 0     |
| 4   | D     | 233/241 (96%)  | 0.38   | 5 (2%) 63 54  | 41, 91, 150, 200      | 0     |
| 4   | R     | 233/241 (96%)  | 0.26   | 2 (0%) 81 75  | 43, 83, 125, 154      | 0     |
| 5   | E     | 238/263 (90%)  | 0.02   | 0 100 100     | 34, 66, 107, 128      | 0     |
| 5   | S     | 238/263 (90%)  | -0.01  | 1 (0%) 88 85  | 35, 61, 102, 122      | 0     |
| 6   | F     | 244/255 (95%)  | 0.11   | 7 (2%) 53 45  | 37, 67, 103, 117      | 0     |
| 6   | T     | 244/255 (95%)  | -0.00  | 3 (1%) 76 69  | 34, 57, 93, 111       | 0     |
| 7   | G     | 243/246 (98%)  | 0.14   | 2 (0%) 82 77  | 47, 70, 108, 129      | 0     |
| 7   | U     | 243/246 (98%)  | 0.01   | 1 (0%) 88 85  | 32, 57, 99, 117       | 0     |
| 8   | H     | 219/234 (93%)  | -0.17  | 1 (0%) 87 83  | 11, 50, 94, 125       | 0     |
| 8   | V     | 219/234 (93%)  | -0.23  | 3 (1%) 73 65  | 4, 41, 78, 103        | 0     |
| 9   | I     | 204/205 (99%)  | -0.04  | 1 (0%) 87 83  | 33, 55, 82, 101       | 0     |
| 9   | W     | 204/205 (99%)  | -0.23  | 0 100 100     | 27, 42, 64, 82        | 0     |
| 10  | J     | 196/201 (97%)  | -0.21  | 0 100 100     | 38, 50, 72, 83        | 0     |
| 10  | X     | 196/201 (97%)  | -0.24  | 0 100 100     | 32, 48, 67, 83        | 0     |
| 11  | K     | 201/204 (98%)  | -0.09  | 3 (1%) 72 64  | 9, 47, 72, 87         | 0     |
| 11  | Y     | 201/204 (98%)  | 0.17   | 4 (1%) 65 56  | 5, 57, 82, 94         | 0     |
| 12  | L     | 213/213 (100%) | -0.20  | 0 100 100     | 29, 42, 64, 86        | 0     |
| 12  | Z     | 213/213 (100%) | -0.16  | 0 100 100     | 41, 49, 67, 96        | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13  | M     | 216/219 (98%)   | -0.26  | 0 100 100     | 29, 38, 61, 82        | 0     |
| 13  | a     | 216/219 (98%)   | -0.23  | 0 100 100     | 36, 44, 61, 82        | 0     |
| 14  | N     | 199/199 (100%)  | -0.19  | 1 (0%) 87 83  | 4, 43, 61, 72         | 0     |
| 14  | b     | 199/199 (100%)  | -0.14  | 0 100 100     | 3, 41, 61, 70         | 0     |
| All | All   | 6244/6446 (96%) | -0.01  | 56 (0%) 81 75 | 3, 56, 111, 200       | 0     |

All (56) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 8   | H     | 199 | ALA  | 4.9  |
| 8   | V     | 200 | GLY  | 4.7  |
| 6   | F     | 3   | ILE  | 4.5  |
| 3   | Q     | 45  | GLU  | 4.3  |
| 8   | V     | 199 | ALA  | 3.8  |
| 4   | D     | 233 | ILE  | 3.8  |
| 6   | F     | 4   | GLY  | 3.3  |
| 3   | C     | 45  | GLU  | 3.3  |
| 3   | C     | 233 | LYS  | 3.2  |
| 1   | A     | 178 | ASN  | 3.1  |
| 6   | F     | 5   | THR  | 3.1  |
| 4   | D     | 123 | GLY  | 3.1  |
| 2   | B     | 244 | ALA  | 3.0  |
| 7   | G     | 242 | ALA  | 3.0  |
| 2   | B     | 237 | LYS  | 2.9  |
| 2   | B     | 246 | ALA  | 2.8  |
| 3   | C     | 58  | VAL  | 2.7  |
| 1   | A     | 1   | ALA  | 2.7  |
| 4   | R     | 233 | ILE  | 2.7  |
| 3   | C     | 49  | VAL  | 2.6  |
| 11  | K     | 73  | ARG  | 2.6  |
| 2   | P     | 244 | ALA  | 2.6  |
| 11  | Y     | 73  | ARG  | 2.6  |
| 6   | T     | 41  | CYS  | 2.6  |
| 3   | C     | 135 | PHE  | 2.5  |
| 6   | F     | 186 | CYS  | 2.5  |
| 3   | C     | 50  | ALA  | 2.5  |
| 1   | A     | 230 | ALA  | 2.5  |
| 11  | Y     | 131 | GLY  | 2.5  |
| 1   | O     | 177 | TYR  | 2.5  |
| 11  | Y     | 64  | ARG  | 2.4  |
| 5   | S     | 233 | LEU  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | O     | 178 | ASN  | 2.4  |
| 11  | K     | 38  | ASN  | 2.3  |
| 3   | C     | 137 | PHE  | 2.3  |
| 6   | T     | 219 | LEU  | 2.3  |
| 4   | R     | 122 | PRO  | 2.2  |
| 3   | C     | 231 | ILE  | 2.2  |
| 6   | F     | 6   | GLY  | 2.2  |
| 7   | U     | 1   | SER  | 2.2  |
| 3   | Q     | 46  | LYS  | 2.2  |
| 9   | I     | 116 | PHE  | 2.2  |
| 14  | N     | 199 | GLU  | 2.2  |
| 11  | Y     | 40  | TYR  | 2.2  |
| 1   | O     | 29  | ALA  | 2.1  |
| 8   | V     | 198 | ARG  | 2.1  |
| 4   | D     | 177 | TYR  | 2.1  |
| 6   | T     | 186 | CYS  | 2.1  |
| 6   | F     | 30  | VAL  | 2.1  |
| 3   | C     | 221 | PRO  | 2.1  |
| 3   | C     | 46  | LYS  | 2.0  |
| 7   | G     | 5   | SER  | 2.0  |
| 4   | D     | 220 | MET  | 2.0  |
| 4   | D     | 180 | SER  | 2.0  |
| 6   | F     | 96  | SER  | 2.0  |
| 11  | K     | 64  | ARG  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 15  | CL   | R     | 302 | 1/1   | 0.61 | 0.11 | 59,59,59,59                 | 0     |
| 16  | K    | B     | 301 | 1/1   | 0.61 | 0.17 | 55,55,55,55                 | 0     |
| 15  | CL   | V     | 305 | 1/1   | 0.70 | 0.09 | 44,44,44,44                 | 0     |
| 16  | K    | G     | 301 | 1/1   | 0.71 | 0.10 | 56,56,56,56                 | 0     |
| 16  | K    | L     | 303 | 1/1   | 0.75 | 0.39 | 31,31,31,31                 | 0     |
| 16  | K    | Z     | 302 | 1/1   | 0.79 | 0.07 | 47,47,47,47                 | 0     |
| 16  | K    | K     | 303 | 1/1   | 0.82 | 0.15 | 51,51,51,51                 | 0     |
| 15  | CL   | P     | 301 | 1/1   | 0.85 | 0.08 | 39,39,39,39                 | 0     |
| 15  | CL   | S     | 302 | 1/1   | 0.85 | 0.06 | 45,45,45,45                 | 0     |
| 15  | CL   | X     | 302 | 1/1   | 0.86 | 0.09 | 51,51,51,51                 | 0     |
| 15  | CL   | X     | 301 | 1/1   | 0.86 | 0.07 | 46,46,46,46                 | 0     |
| 17  | 04C  | Y     | 301 | 42/42 | 0.86 | 0.11 | 2,16,29,34                  | 0     |
| 16  | K    | Z     | 303 | 1/1   | 0.87 | 0.06 | 24,24,24,24                 | 0     |
| 16  | K    | Z     | 304 | 1/1   | 0.87 | 0.21 | 40,40,40,40                 | 0     |
| 16  | K    | S     | 303 | 1/1   | 0.87 | 0.24 | 50,50,50,50                 | 0     |
| 16  | K    | b     | 203 | 1/1   | 0.88 | 0.22 | 45,45,45,45                 | 0     |
| 15  | CL   | M     | 301 | 1/1   | 0.88 | 0.07 | 39,39,39,39                 | 0     |
| 15  | CL   | U     | 301 | 1/1   | 0.89 | 0.08 | 45,45,45,45                 | 0     |
| 17  | 04C  | K     | 301 | 42/42 | 0.89 | 0.10 | 7,14,28,32                  | 0     |
| 15  | CL   | X     | 303 | 1/1   | 0.89 | 0.10 | 72,72,72,72                 | 0     |
| 17  | 04C  | N     | 201 | 42/42 | 0.90 | 0.10 | 2,3,8,11                    | 0     |
| 15  | CL   | a     | 303 | 1/1   | 0.90 | 0.05 | 44,44,44,44                 | 0     |
| 17  | 04C  | H     | 301 | 42/42 | 0.91 | 0.09 | 6,13,19,20                  | 0     |
| 16  | K    | X     | 304 | 1/1   | 0.91 | 0.07 | 70,70,70,70                 | 0     |
| 16  | K    | I     | 302 | 1/1   | 0.92 | 0.37 | 41,41,41,41                 | 0     |
| 17  | 04C  | b     | 201 | 42/42 | 0.92 | 0.09 | 2,3,12,17                   | 0     |
| 15  | CL   | L     | 302 | 1/1   | 0.93 | 0.08 | 24,24,24,24                 | 0     |
| 16  | K    | a     | 305 | 1/1   | 0.93 | 0.30 | 37,37,37,37                 | 0     |
| 17  | 04C  | V     | 301 | 42/42 | 0.93 | 0.08 | 3,5,24,25                   | 0     |
| 15  | CL   | V     | 306 | 1/1   | 0.93 | 0.07 | 40,40,40,40                 | 0     |
| 15  | CL   | N     | 203 | 1/1   | 0.93 | 0.05 | 36,36,36,36                 | 0     |
| 15  | CL   | J     | 301 | 1/1   | 0.94 | 0.04 | 35,35,35,35                 | 0     |
| 15  | CL   | a     | 304 | 1/1   | 0.94 | 0.04 | 44,44,44,44                 | 0     |
| 15  | CL   | Q     | 301 | 1/1   | 0.95 | 0.05 | 39,39,39,39                 | 0     |
| 15  | CL   | A     | 303 | 1/1   | 0.95 | 0.04 | 45,45,45,45                 | 0     |
| 15  | CL   | M     | 304 | 1/1   | 0.95 | 0.04 | 48,48,48,48                 | 0     |
| 15  | CL   | a     | 301 | 1/1   | 0.95 | 0.03 | 33,33,33,33                 | 0     |
| 15  | CL   | M     | 303 | 1/1   | 0.96 | 0.04 | 25,25,25,25                 | 0     |
| 15  | CL   | R     | 303 | 1/1   | 0.96 | 0.05 | 45,45,45,45                 | 0     |
| 16  | K    | M     | 305 | 1/1   | 0.96 | 0.07 | 37,37,37,37                 | 0     |
| 15  | CL   | Q     | 302 | 1/1   | 0.96 | 0.04 | 37,37,37,37                 | 0     |
| 15  | CL   | O     | 302 | 1/1   | 0.97 | 0.05 | 44,44,44,44                 | 0     |
| 15  | CL   | A     | 302 | 1/1   | 0.97 | 0.04 | 32,32,32,32                 | 0     |

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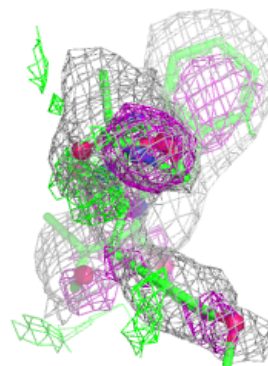
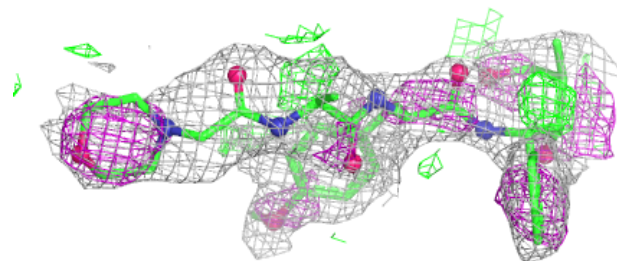
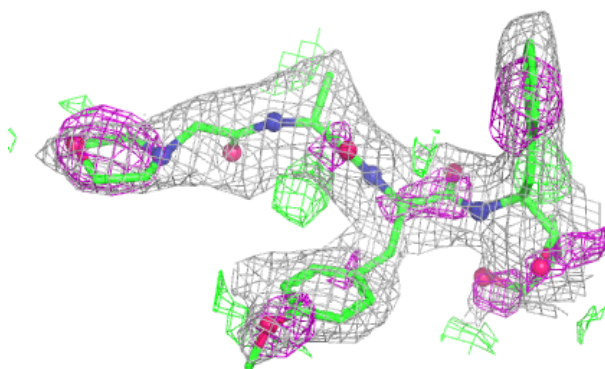
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 15  | CL   | D     | 301 | 1/1   | 0.97 | 0.03 | 35,35,35,35                 | 0     |
| 15  | CL   | E     | 301 | 1/1   | 0.97 | 0.07 | 42,42,42,42                 | 0     |
| 15  | CL   | Q     | 303 | 1/1   | 0.97 | 0.04 | 32,32,32,32                 | 0     |
| 15  | CL   | O     | 301 | 1/1   | 0.97 | 0.06 | 33,33,33,33                 | 0     |
| 15  | CL   | R     | 301 | 1/1   | 0.98 | 0.03 | 32,32,32,32                 | 0     |
| 15  | CL   | L     | 301 | 1/1   | 0.98 | 0.02 | 32,32,32,32                 | 0     |
| 15  | CL   | I     | 301 | 1/1   | 0.98 | 0.03 | 28,28,28,28                 | 0     |
| 15  | CL   | H     | 303 | 1/1   | 0.98 | 0.02 | 31,31,31,31                 | 0     |
| 15  | CL   | M     | 302 | 1/1   | 0.99 | 0.03 | 30,30,30,30                 | 0     |
| 15  | CL   | A     | 301 | 1/1   | 0.99 | 0.04 | 34,34,34,34                 | 0     |
| 15  | CL   | V     | 303 | 1/1   | 0.99 | 0.03 | 30,30,30,30                 | 0     |
| 15  | CL   | Z     | 301 | 1/1   | 0.99 | 0.06 | 26,26,26,26                 | 0     |
| 15  | CL   | V     | 304 | 1/1   | 0.99 | 0.04 | 33,33,33,33                 | 0     |
| 15  | CL   | a     | 302 | 1/1   | 0.99 | 0.03 | 29,29,29,29                 | 0     |
| 15  | CL   | Q     | 304 | 1/1   | 0.99 | 0.02 | 29,29,29,29                 | 0     |
| 15  | CL   | S     | 301 | 1/1   | 0.99 | 0.08 | 35,35,35,35                 | 0     |
| 15  | CL   | W     | 301 | 1/1   | 0.99 | 0.05 | 28,28,28,28                 | 0     |
| 18  | IOD  | H     | 302 | 1/1   | 0.99 | 0.10 | 49,49,49,49                 | 0     |
| 18  | IOD  | N     | 202 | 1/1   | 0.99 | 0.05 | 48,48,48,48                 | 0     |
| 18  | IOD  | V     | 302 | 1/1   | 0.99 | 0.18 | 17,17,17,17                 | 0     |
| 18  | IOD  | b     | 202 | 1/1   | 0.99 | 0.06 | 46,46,46,46                 | 0     |
| 18  | IOD  | Y     | 302 | 1/1   | 1.00 | 0.06 | 55,55,55,55                 | 0     |
| 18  | IOD  | K     | 302 | 1/1   | 1.00 | 0.07 | 53,53,53,53                 | 0     |

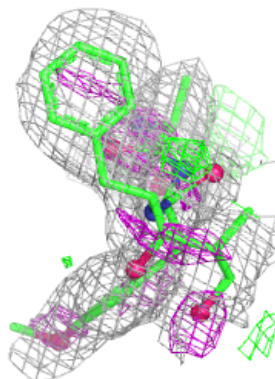
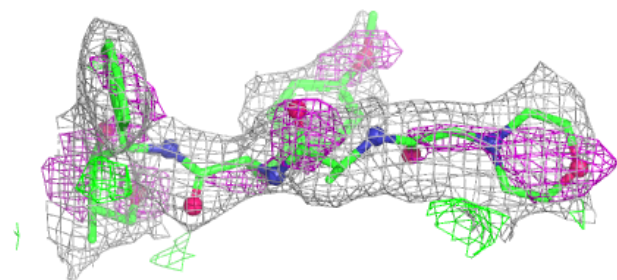
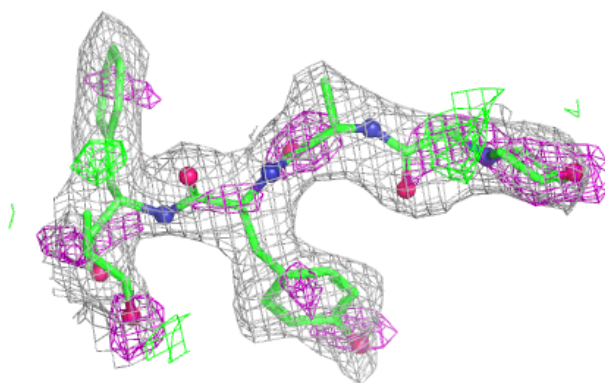
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around 04C Y 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 04C K 301:**

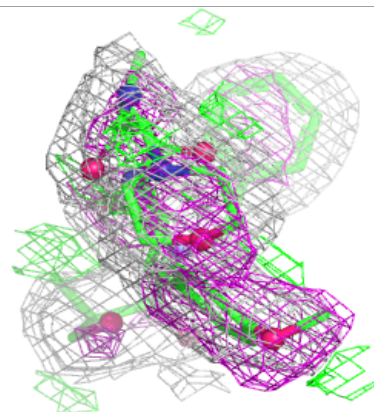
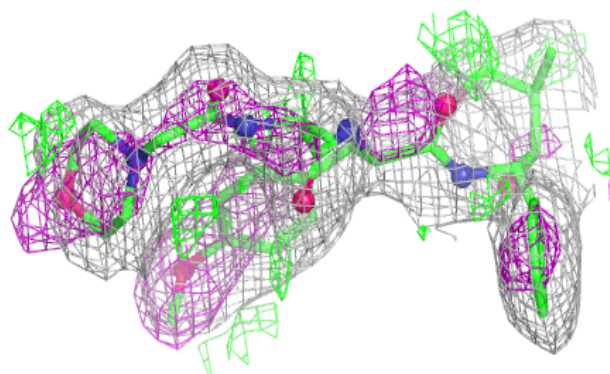
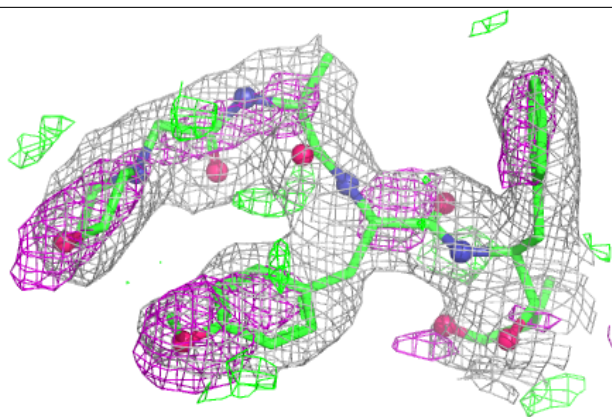
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



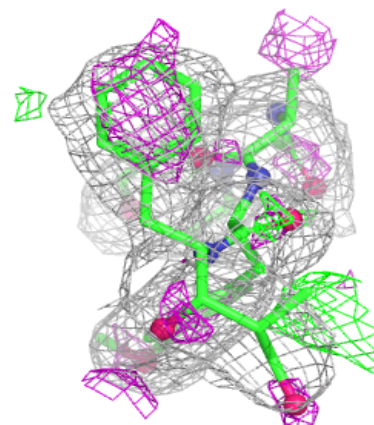
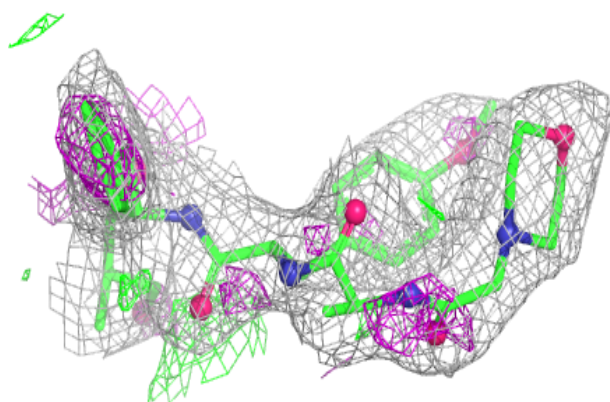
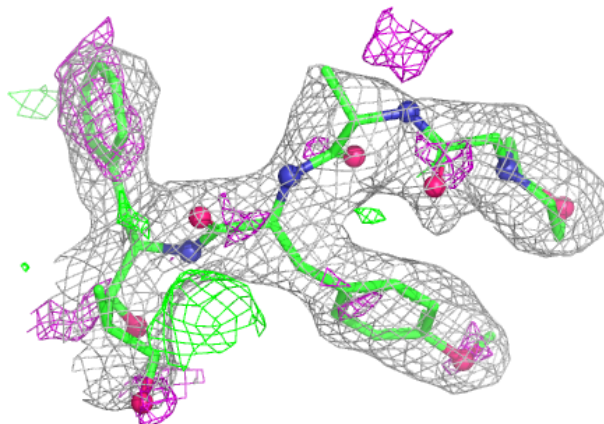


**Electron density around 04C N 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

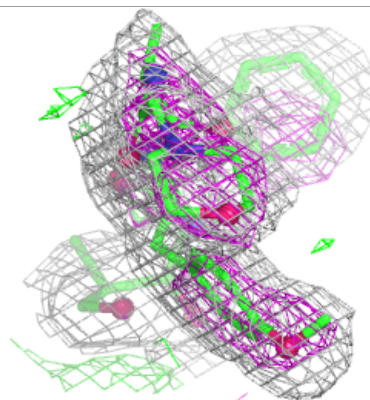
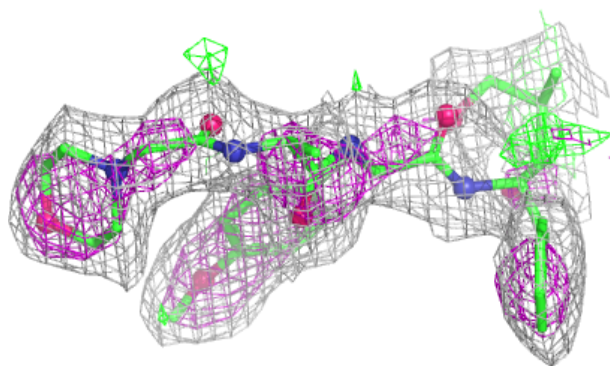
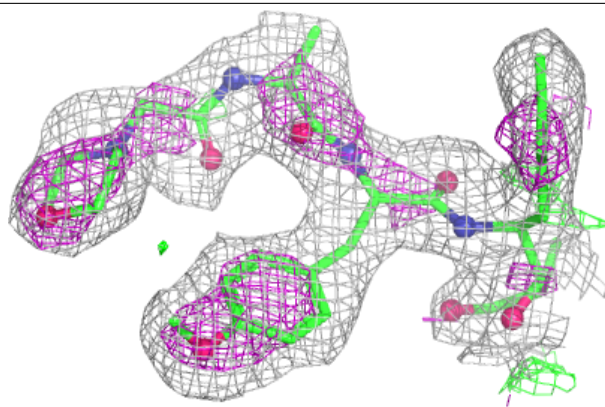
**Electron density around 04C H 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



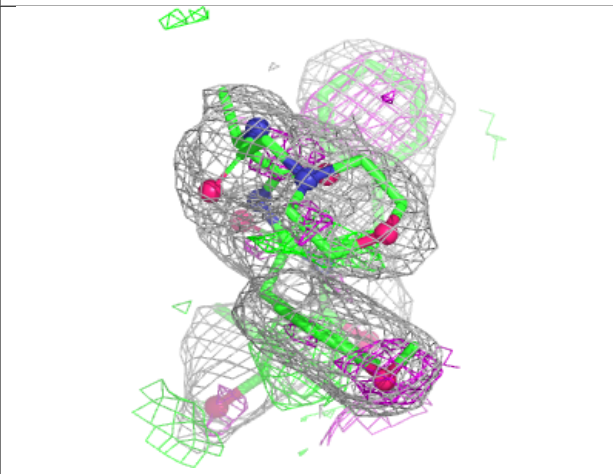
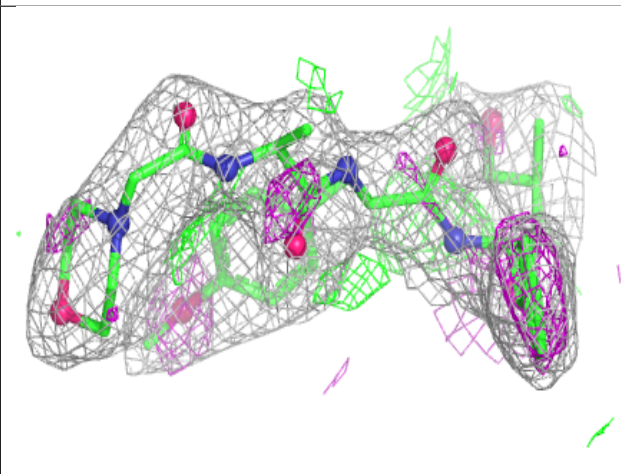
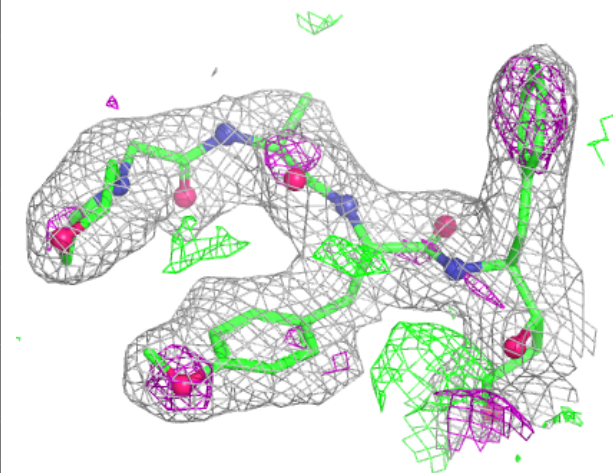
**Electron density around 04C b 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 04C V 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.