



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:07 PM UTC

PDB ID : 8OI1 / pdb\_00008oi1  
Title : Yeast 20S proteasome in complex with a photoswitchable cepafungin derivative (transCep4)  
Authors : Morstein, J.; Amatuni, A.; Schuster, A.; Kuttanlochner, W.; Ko, T.; Groll, M.; Adibekian, A.; Renata, H.; Trauner, D.H.  
Deposited on : 2023-03-21  
Resolution : 2.95 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:

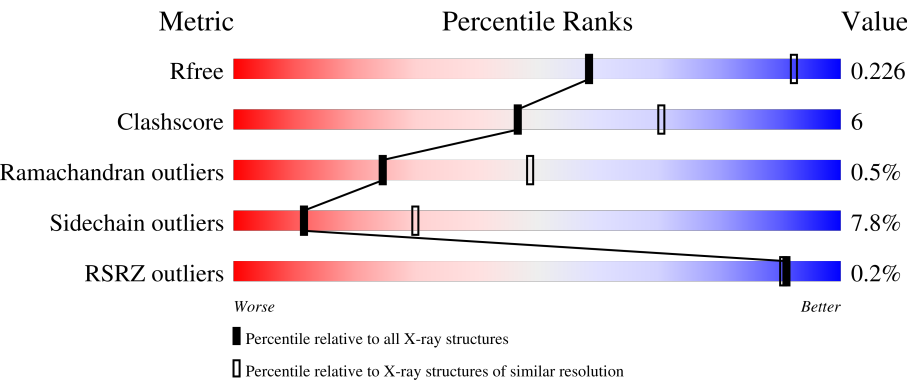
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| 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 2.95 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.



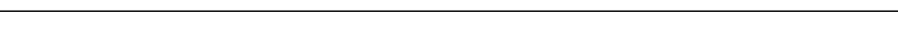
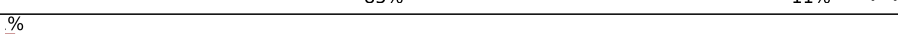
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| R <sub>free</sub>     | 180053                      | 1130 (2.98-2.94)                                      |
| Clashscore            | 190562                      | 1157 (2.98-2.94)                                      |
| Ramachandran outliers | 187476                      | 1101 (2.98-2.94)                                      |
| Sidechain outliers    | 187428                      | 1101 (2.98-2.94)                                      |
| RSRZ outliers         | 180081                      | 1130 (2.98-2.94)                                      |

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     | 250    | <div><div></div><div>88%11%.</div></div>     |
| 1   | O     | 250    | <div><div></div><div>85%14%.</div></div>     |
| 2   | B     | 258    | <div><div></div><div>73%19%. 5%</div></div>  |
| 2   | P     | 258    | <div><div></div><div>%76%18%. 5%</div></div> |

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| Mol | Chain | Length | Quality of chain                                                                                |
|-----|-------|--------|-------------------------------------------------------------------------------------------------|
| 3   | C     | 254    |  75% 17% 6%   |
| 3   | Q     | 254    |  78% 14% 6%   |
| 4   | D     | 260    |  70% 18% 10%  |
| 4   | R     | 260    |  69% 19% 10%  |
| 5   | E     | 234    |  82% 14% ..   |
| 5   | S     | 234    |  79% 17% ..   |
| 6   | F     | 288    |  72% 11% 16%  |
| 6   | T     | 288    |  69% 14% 16%  |
| 7   | G     | 252    |  79% 15% ..   |
| 7   | U     | 252    |  77% 16% ..   |
| 8   | H     | 232    |  80% 16% ..   |
| 8   | V     | 232    |  78% 18% ..   |
| 9   | I     | 205    |  83% 15% .  |
| 9   | W     | 205    |  82% 16% .  |
| 10  | J     | 198    |  85% 11% .. |
| 10  | X     | 198    |  86% 10% .. |
| 11  | K     | 212    |  79% 20% .  |
| 11  | Y     | 212    |  79% 20% .  |
| 12  | L     | 222    |  78% 20% .  |
| 12  | Z     | 222    |  76% 22% .  |
| 13  | M     | 246    |  79% 15% 5% |
| 13  | a     | 246    |  78% 15% 5% |
| 14  | N     | 196    |  82% 18% .  |
| 14  | b     | 196    |  82% 17% .  |

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49790 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     | 250      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1915  | 1219 | 315 | 377 | 4 |         |         |       |
| 1   | O     | 250      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1915  | 1219 | 315 | 377 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | B     | 244      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1904  | 1201 | 321 | 379 | 3 |         |         |       |
| 2   | P     | 244      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1904  | 1201 | 321 | 379 | 3 |         |         |       |

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | C     | 240      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1881  | 1176 | 329 | 372 | 4 |         |         |       |
| 3   | Q     | 240      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1881  | 1176 | 329 | 372 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | D     | 235      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1813  | 1136 | 304 | 366 | 7 |         |         |       |
| 4   | R     | 235      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1813  | 1136 | 304 | 366 | 7 |         |         |       |

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | E     | 231      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1773  | 1114 | 307 | 348 | 4 |         |         |       |
| 5   | S     | 231      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1773  | 1114 | 307 | 348 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 6   | F     | 243      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1892  | 1203 | 329 | 356 | 4 |         |         |       |
| 6   | T     | 243      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1892  | 1203 | 329 | 356 | 4 |         |         |       |

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 7   | G     | 241      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1907  | 1214 | 320 | 365 | 8 |         |         |       |
| 7   | U     | 241      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1907  | 1214 | 320 | 365 | 8 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 8   | H     | 226      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1082 | 298 | 332 | 7 |         |         |       |
| 8   | V     | 226      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1719  | 1082 | 298 | 332 | 7 |         |         |       |

- 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     |
|     |       |          | 1581  | 1010 | 258 | 305 | 8 |         |         |       |
| 9   | W     | 204      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1581  | 1010 | 258 | 305 | 8 |         |         |       |

- Molecule 10 is a protein called Proteasome subunit beta type-4.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | J     | 195      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1561  | 992 | 264 | 299 | 6 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | X     | 195      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1561  | 992 | 264 | 299 | 6 |         |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 11  | K     | 212      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1644  | 1045 | 280 | 312 | 7 |         |         |       |
| 11  | Y     | 212      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1644  | 1045 | 280 | 312 | 7 |         |         |       |

- Molecule 12 is a protein called Proteasome subunit beta type-6.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 12  | L     | 222      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1757  | 1115 | 303 | 335 | 4 |         |         |       |
| 12  | Z     | 222      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1757  | 1115 | 303 | 335 | 4 |         |         |       |

- Molecule 13 is a protein called Proteasome subunit beta type-7.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 13  | M     | 233      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1824  | 1154 | 312 | 351 | 7 |         |         |       |
| 13  | a     | 233      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1824  | 1154 | 312 | 351 | 7 |         |         |       |

- Molecule 14 is a protein called Proteasome subunit beta type-1.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14  | N     | 196      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1512  | 955 | 250 | 300 | 7 |         |         |       |
| 14  | b     | 196      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1512  | 955 | 250 | 300 | 7 |         |         |       |

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

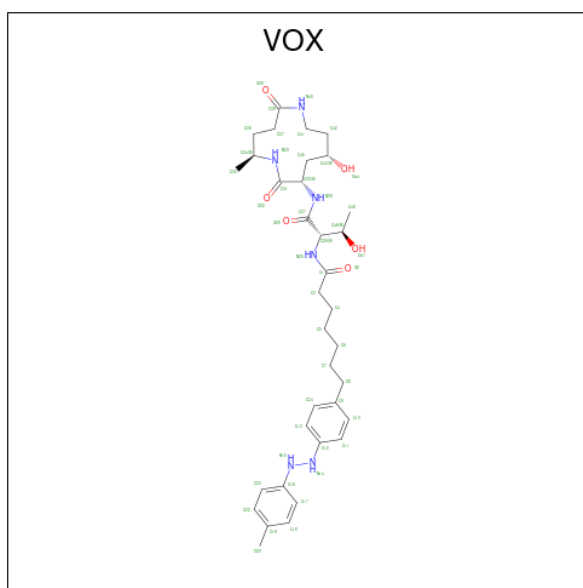
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 15  | G     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 15  | I     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 15  | J     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 15  | K     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 15  | N     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 15  | V     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 15  | Y     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 15  | Z     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 16 is {N}-[(2 {S},3 {R})-1-[(5 {S},8 {S},10 {S})-5-methyl-10-oxidanyl-2,7-bis(oxidanylidene)-1,6-diazacyclododec-8-yl]amino]-3-oxidanyl-1-oxidanylidene-butan-2-yl]-7-[4-[2-(4-methylphenyl)hydrazinyl]phenyl]heptanamide (CCD ID: VOX) (formula: C<sub>35</sub>H<sub>52</sub>N<sub>6</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).

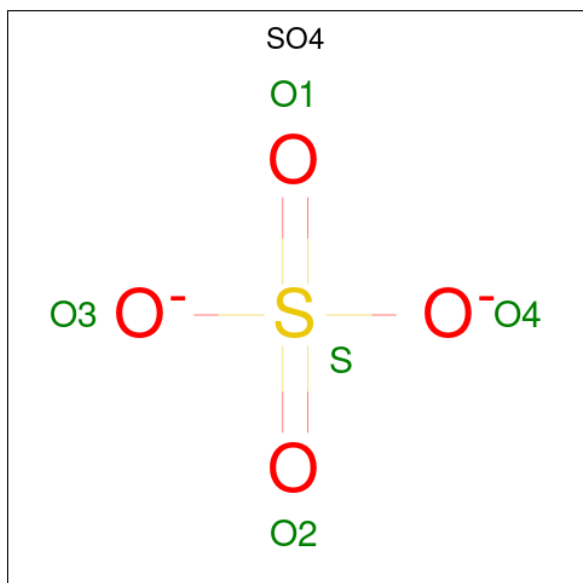


| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 16  | H     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 47    | 35 | 6 | 6 |         |         |
| 16  | K     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 47    | 35 | 6 | 6 |         |         |
| 16  | V     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 47    | 35 | 6 | 6 |         |         |
| 16  | Y     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 47    | 35 | 6 | 6 |         |         |

- Molecule 17 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 17  | N     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 17  | b     | 1        | Total Cl<br>1 1 | 0       | 0       |

- Molecule 18 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 18  | N     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 18  | b     | 1        | Total O S<br>5 4 1 | 0       | 0       |

- Molecule 19 is water.

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 19  | A     | 7        | Total O<br>7 7   | 0       | 0       |
| 19  | B     | 10       | Total O<br>10 10 | 0       | 0       |
| 19  | C     | 8        | Total O<br>8 8   | 0       | 0       |
| 19  | D     | 6        | Total O<br>6 6   | 0       | 0       |
| 19  | E     | 5        | Total O<br>5 5   | 0       | 0       |

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| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 19  | F     | 5        | Total O<br>5 5   | 0       | 0       |
| 19  | G     | 4        | Total O<br>4 4   | 0       | 0       |
| 19  | H     | 13       | Total O<br>13 13 | 0       | 0       |
| 19  | I     | 5        | Total O<br>5 5   | 0       | 0       |
| 19  | J     | 13       | Total O<br>13 13 | 0       | 0       |
| 19  | K     | 5        | Total O<br>5 5   | 0       | 0       |
| 19  | L     | 12       | Total O<br>12 12 | 0       | 0       |
| 19  | M     | 11       | Total O<br>11 11 | 0       | 0       |
| 19  | N     | 4        | Total O<br>4 4   | 0       | 0       |
| 19  | O     | 5        | Total O<br>5 5   | 0       | 0       |
| 19  | P     | 5        | Total O<br>5 5   | 0       | 0       |
| 19  | Q     | 8        | Total O<br>8 8   | 0       | 0       |
| 19  | R     | 1        | Total O<br>1 1   | 0       | 0       |
| 19  | S     | 3        | Total O<br>3 3   | 0       | 0       |
| 19  | T     | 10       | Total O<br>10 10 | 0       | 0       |
| 19  | U     | 8        | Total O<br>8 8   | 0       | 0       |
| 19  | V     | 14       | Total O<br>14 14 | 0       | 0       |
| 19  | W     | 5        | Total O<br>5 5   | 0       | 0       |
| 19  | X     | 11       | Total O<br>11 11 | 0       | 0       |
| 19  | Y     | 9        | Total O<br>9 9   | 0       | 0       |
| 19  | Z     | 10       | Total O<br>10 10 | 0       | 0       |

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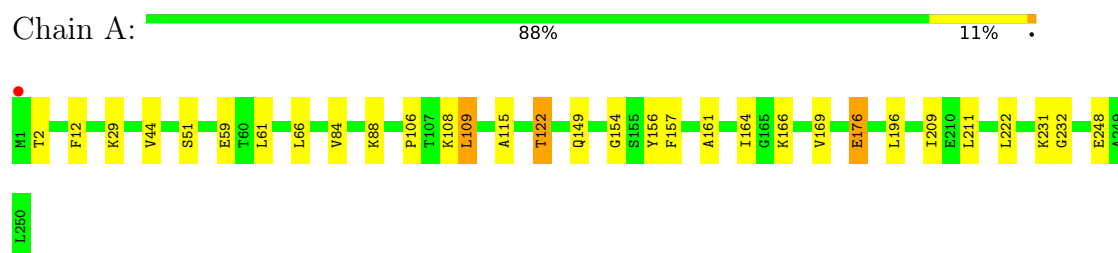
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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 19  | a     | 11       | Total | O  | 0       | 0       |
|     |       |          | 11    | 11 |         |         |
| 19  | b     | 5        | Total | O  | 0       | 0       |
|     |       |          | 5     | 5  |         |         |

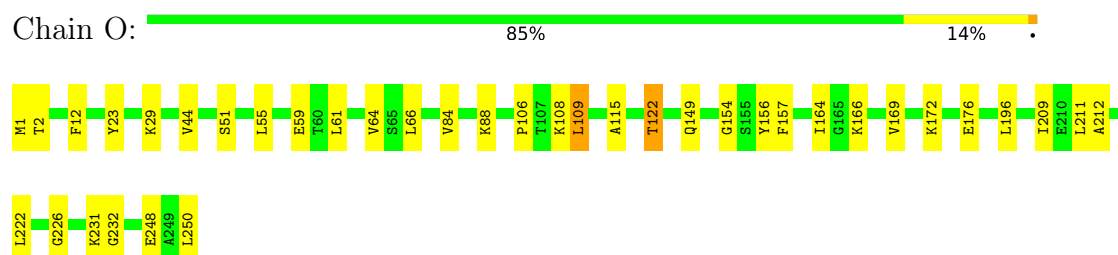
### 3 Residue-property plots

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

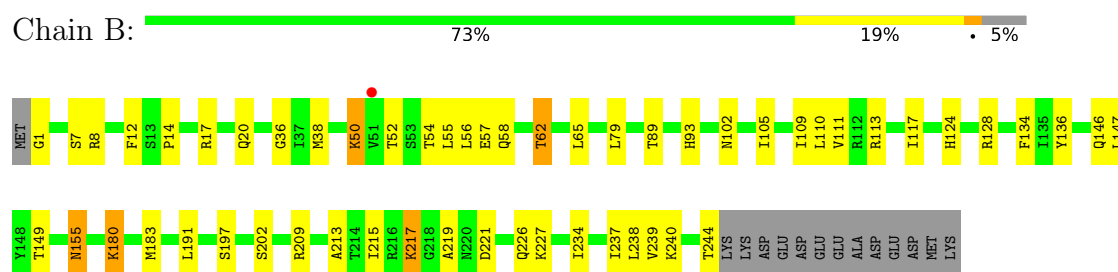
#### • Molecule 1: Proteasome subunit alpha type-2



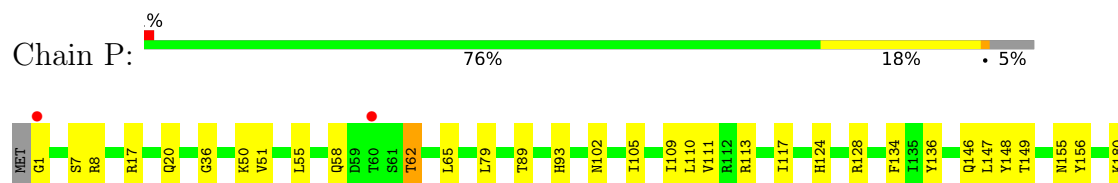
#### • Molecule 1: Proteasome subunit alpha type-2



#### • Molecule 2: Proteasome subunit alpha type-3

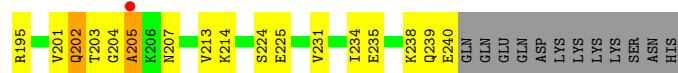
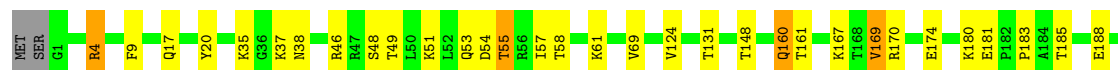
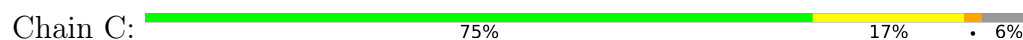


#### • Molecule 2: Proteasome subunit alpha type-3

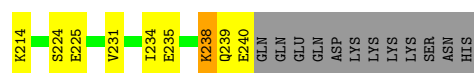
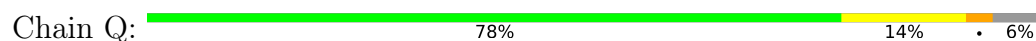




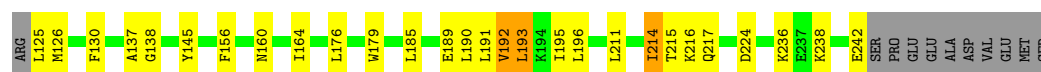
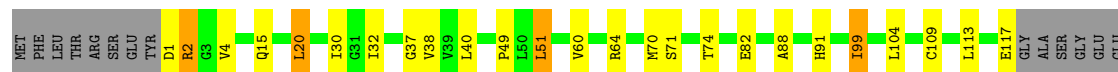
• Molecule 3: Proteasome subunit alpha type-4



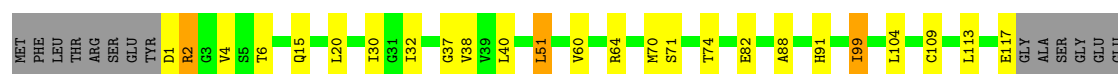
• Molecule 3: Proteasome subunit alpha type-4



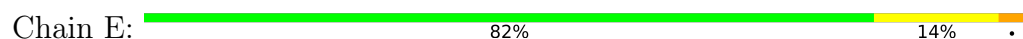
• Molecule 4: Proteasome subunit alpha type-5

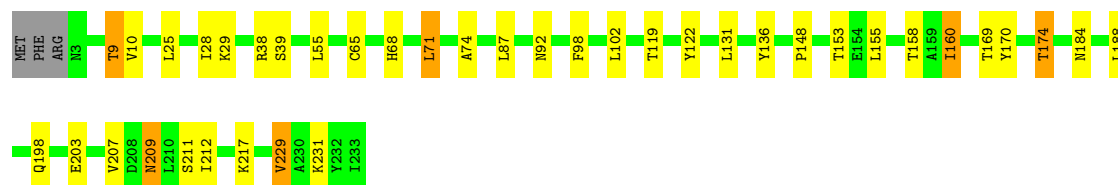


• Molecule 4: Proteasome subunit alpha type-5



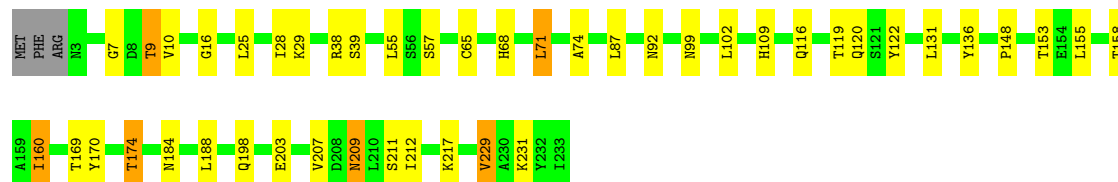
• Molecule 5: Proteasome subunit alpha type-6





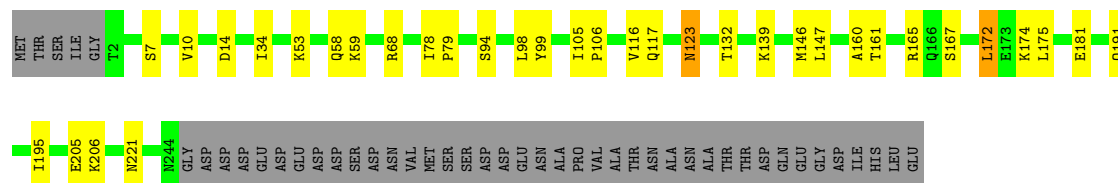
• Molecule 5: Proteasome subunit alpha type-6

Chain S: 79% 17% ..



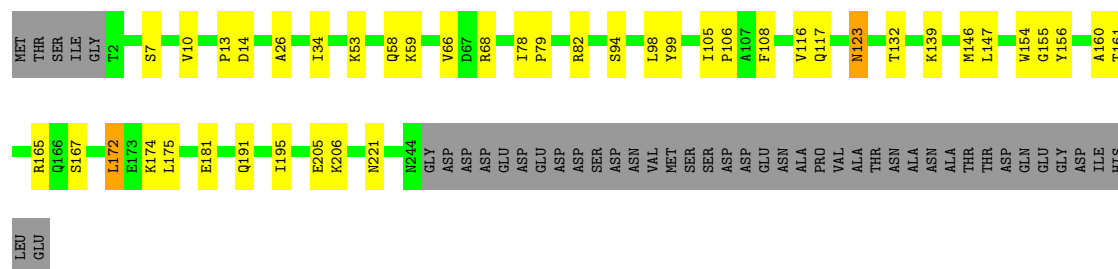
• Molecule 6: Probable proteasome subunit alpha type-7

Chain F: 72% 11% 16%



• Molecule 6: Probable proteasome subunit alpha type-7

Chain T: 69% 14% 16%



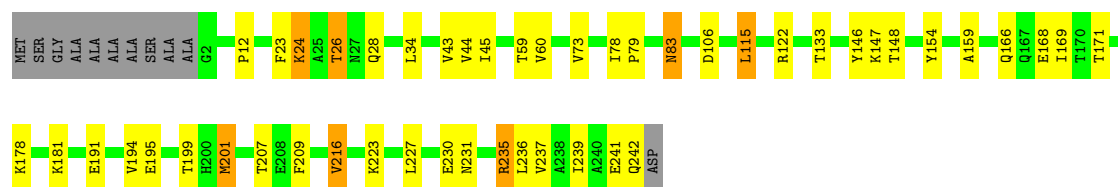
• Molecule 7: Proteasome subunit alpha type-1

Chain G: 79% 15% ..



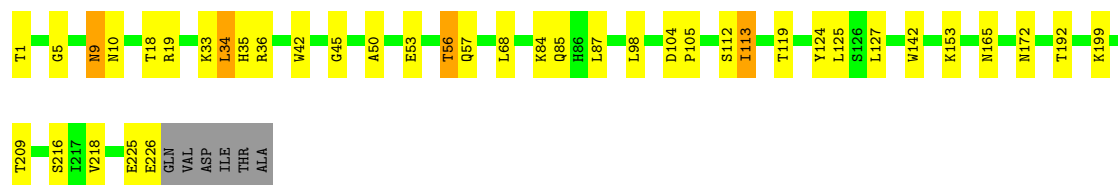
• Molecule 7: Proteasome subunit alpha type-1

Chain U:  77% 16%



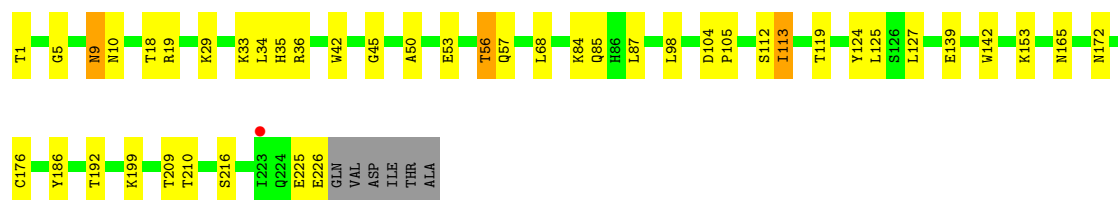
- Molecule 8: Proteasome subunit beta type-2

Chain H:  80% 16%



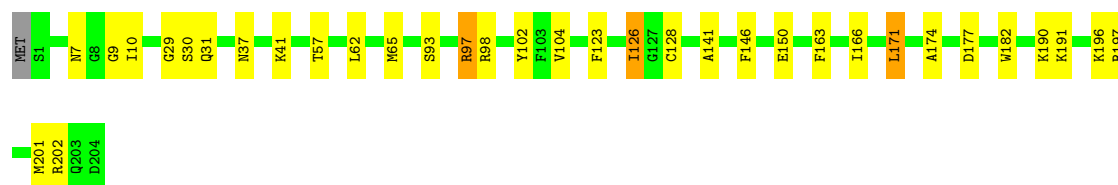
- Molecule 8: Proteasome subunit beta type-2

Chain V:  78% 18%



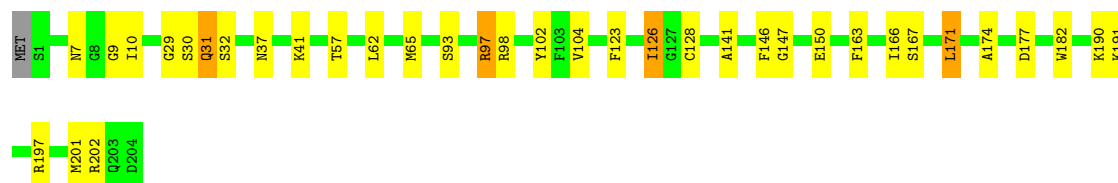
- Molecule 9: Proteasome subunit beta type-3

Chain I:  83% 15%



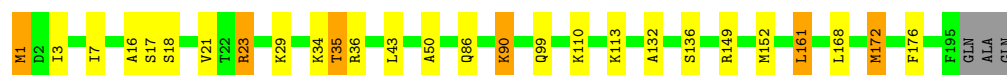
- Molecule 9: Proteasome subunit beta type-3

Chain W:  82% 16%



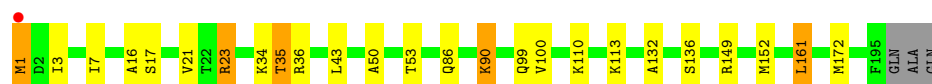
- Molecule 10: Proteasome subunit beta type-4

Chain J:  85% 11% . .



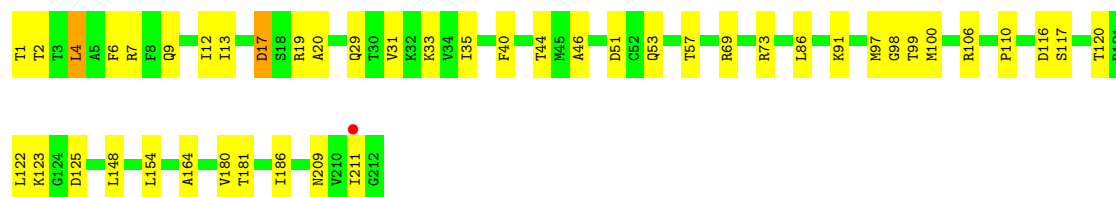
- Molecule 10: Proteasome subunit beta type-4

Chain X:  86% 10% . .



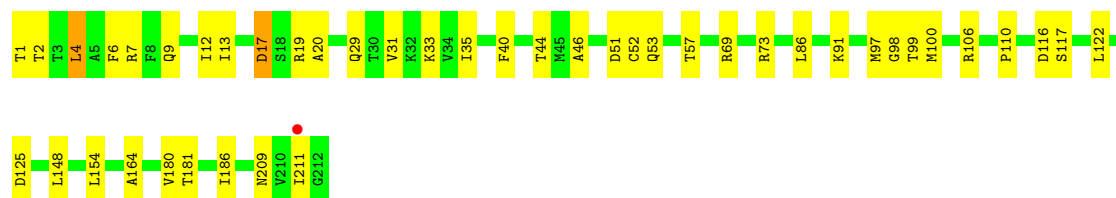
- Molecule 11: Proteasome subunit beta type-5

Chain K:  79% 20% .



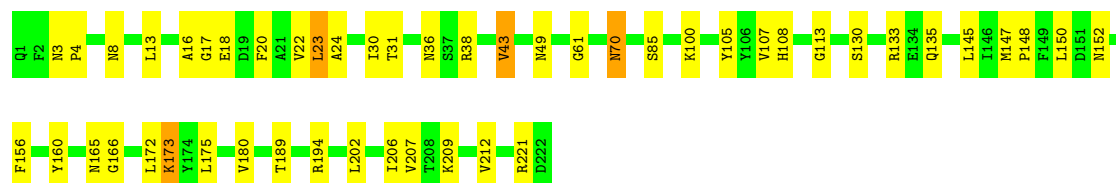
- Molecule 11: Proteasome subunit beta type-5

Chain Y:  79% 20% .



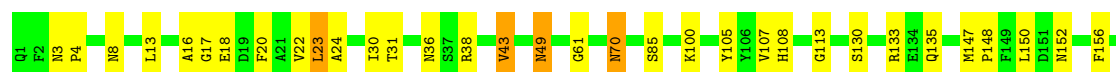
- Molecule 12: Proteasome subunit beta type-6

Chain L:  78% 20% .



- Molecule 12: Proteasome subunit beta type-6

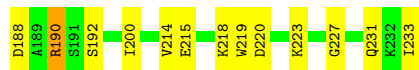
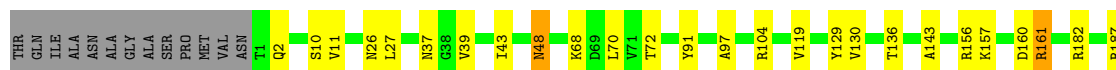
Chain Z:  76% 22% .





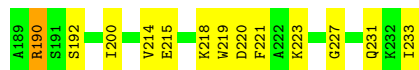
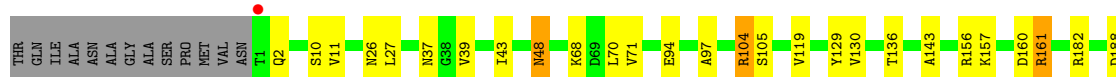
• Molecule 13: Proteasome subunit beta type-7

Chain M: 79% 15% 5%



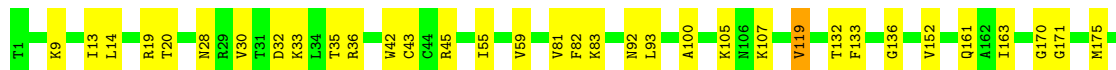
• Molecule 13: Proteasome subunit beta type-7

Chain a: 78% 15% 5%



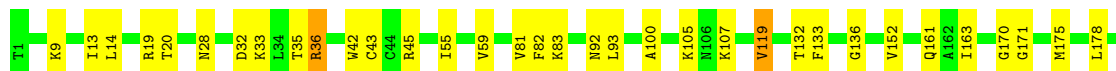
• Molecule 14: Proteasome subunit beta type-1

Chain N: 82% 18% 0%



• Molecule 14: Proteasome subunit beta type-1

Chain b: 82% 17% 0%



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 135.47Å 300.56Å 143.85Å<br>90.00° 113.10° 90.00°            | Depositor        |
| Resolution (Å)                                                          | 30.00 – 2.95<br>30.00 – 2.95                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 96.7 (30.00-2.95)<br>96.6 (30.00-2.95)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.09                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.34 (at 2.95Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.8.0258                                             | Depositor        |
| R, $R_{free}$                                                           | 0.174 , 0.224<br>(Not available) , 0.226                    | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 10696 reflections (5.00%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 76.4                                                        | Xtriage          |
| Anisotropy                                                              | 0.407                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 65.6                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.96                                                        | EDS              |
| Total number of atoms                                                   | 49790                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 93.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: CL, SO4, VOX, MG

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     | 1.02         | 0/1952         | 1.41        | 0/2642         |
| 1   | O     | 1.02         | 1/1952 (0.1%)  | 1.41        | 0/2642         |
| 2   | B     | 1.00         | 0/1934         | 1.42        | 0/2618         |
| 2   | P     | 1.00         | 0/1934         | 1.43        | 0/2618         |
| 3   | C     | 1.00         | 0/1910         | 1.46        | 0/2586         |
| 3   | Q     | 1.01         | 0/1910         | 1.46        | 0/2586         |
| 4   | D     | 1.01         | 0/1837         | 1.46        | 0/2475         |
| 4   | R     | 1.01         | 0/1837         | 1.47        | 0/2475         |
| 5   | E     | 1.01         | 0/1800         | 1.42        | 0/2433         |
| 5   | S     | 1.01         | 0/1800         | 1.43        | 0/2433         |
| 6   | F     | 0.99         | 0/1932         | 1.44        | 0/2609         |
| 6   | T     | 0.99         | 0/1932         | 1.44        | 0/2609         |
| 7   | G     | 0.99         | 0/1945         | 1.42        | 2/2634 (0.1%)  |
| 7   | U     | 0.99         | 0/1945         | 1.43        | 2/2634 (0.1%)  |
| 8   | H     | 1.02         | 0/1750         | 1.41        | 0/2373         |
| 8   | V     | 1.02         | 0/1750         | 1.41        | 0/2373         |
| 9   | I     | 1.00         | 1/1611 (0.1%)  | 1.41        | 0/2174         |
| 9   | W     | 1.00         | 1/1611 (0.1%)  | 1.41        | 0/2174         |
| 10  | J     | 0.98         | 0/1589         | 1.39        | 0/2142         |
| 10  | X     | 0.98         | 0/1589         | 1.37        | 0/2142         |
| 11  | K     | 1.00         | 0/1681         | 1.42        | 0/2274         |
| 11  | Y     | 1.00         | 0/1681         | 1.41        | 0/2274         |
| 12  | L     | 0.98         | 0/1795         | 1.36        | 0/2420         |
| 12  | Z     | 0.98         | 0/1795         | 1.36        | 0/2420         |
| 13  | M     | 0.99         | 0/1855         | 1.38        | 0/2514         |
| 13  | a     | 0.99         | 0/1855         | 1.38        | 0/2514         |
| 14  | N     | 0.99         | 0/1541         | 1.42        | 0/2087         |
| 14  | b     | 1.00         | 0/1541         | 1.42        | 0/2087         |
| All | All   | 1.00         | 3/50264 (0.0%) | 1.42        | 4/67962 (0.0%) |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | O     | 1   | MET  | SD-CE | 6.34 | 1.95        | 1.79     |
| 9   | I     | 57  | THR  | C-O   | 6.05 | 1.31        | 1.24     |
| 9   | W     | 57  | THR  | C-O   | 5.87 | 1.31        | 1.24     |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 7   | U     | 216 | VAL  | CA-C-N | 5.64 | 125.48      | 121.65   |
| 7   | U     | 216 | VAL  | C-N-CA | 5.64 | 125.48      | 121.65   |
| 7   | G     | 216 | VAL  | CA-C-N | 5.50 | 125.39      | 121.65   |
| 7   | G     | 216 | VAL  | C-N-CA | 5.50 | 125.39      | 121.65   |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1915  | 0        | 1929     | 20      | 0            |
| 1   | O     | 1915  | 0        | 1929     | 18      | 0            |
| 2   | B     | 1904  | 0        | 1904     | 40      | 0            |
| 2   | P     | 1904  | 0        | 1904     | 23      | 0            |
| 3   | C     | 1881  | 0        | 1895     | 23      | 0            |
| 3   | Q     | 1881  | 0        | 1895     | 17      | 0            |
| 4   | D     | 1813  | 0        | 1797     | 27      | 0            |
| 4   | R     | 1813  | 0        | 1797     | 29      | 0            |
| 5   | E     | 1773  | 0        | 1775     | 20      | 0            |
| 5   | S     | 1773  | 0        | 1775     | 25      | 0            |
| 6   | F     | 1892  | 0        | 1883     | 17      | 0            |
| 6   | T     | 1892  | 0        | 1883     | 25      | 0            |
| 7   | G     | 1907  | 0        | 1901     | 15      | 0            |
| 7   | U     | 1907  | 0        | 1901     | 21      | 0            |
| 8   | H     | 1719  | 0        | 1718     | 25      | 0            |
| 8   | V     | 1719  | 0        | 1718     | 30      | 0            |
| 9   | I     | 1581  | 0        | 1574     | 16      | 0            |
| 9   | W     | 1581  | 0        | 1574     | 20      | 0            |
| 10  | J     | 1561  | 0        | 1569     | 13      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 10  | X     | 1561  | 0        | 1569     | 10      | 0            |
| 11  | K     | 1644  | 0        | 1594     | 29      | 0            |
| 11  | Y     | 1644  | 0        | 1594     | 30      | 0            |
| 12  | L     | 1757  | 0        | 1711     | 29      | 0            |
| 12  | Z     | 1757  | 0        | 1711     | 33      | 0            |
| 13  | M     | 1824  | 0        | 1832     | 22      | 0            |
| 13  | a     | 1824  | 0        | 1832     | 23      | 0            |
| 14  | N     | 1512  | 0        | 1481     | 22      | 0            |
| 14  | b     | 1512  | 0        | 1481     | 20      | 0            |
| 15  | G     | 1     | 0        | 0        | 0       | 0            |
| 15  | I     | 2     | 0        | 0        | 0       | 0            |
| 15  | J     | 1     | 0        | 0        | 0       | 0            |
| 15  | K     | 2     | 0        | 0        | 0       | 0            |
| 15  | N     | 2     | 0        | 0        | 0       | 0            |
| 15  | V     | 1     | 0        | 0        | 0       | 0            |
| 15  | Y     | 1     | 0        | 0        | 0       | 0            |
| 15  | Z     | 1     | 0        | 0        | 0       | 0            |
| 16  | H     | 47    | 0        | 0        | 1       | 0            |
| 16  | K     | 47    | 0        | 0        | 0       | 0            |
| 16  | V     | 47    | 0        | 0        | 0       | 0            |
| 16  | Y     | 47    | 0        | 0        | 1       | 0            |
| 17  | N     | 1     | 0        | 0        | 0       | 0            |
| 17  | b     | 1     | 0        | 0        | 0       | 0            |
| 18  | N     | 5     | 0        | 0        | 0       | 0            |
| 18  | b     | 5     | 0        | 0        | 0       | 0            |
| 19  | A     | 7     | 0        | 0        | 0       | 0            |
| 19  | B     | 10    | 0        | 0        | 0       | 0            |
| 19  | C     | 8     | 0        | 0        | 0       | 0            |
| 19  | D     | 6     | 0        | 0        | 0       | 0            |
| 19  | E     | 5     | 0        | 0        | 0       | 0            |
| 19  | F     | 5     | 0        | 0        | 0       | 0            |
| 19  | G     | 4     | 0        | 0        | 0       | 0            |
| 19  | H     | 13    | 0        | 0        | 0       | 0            |
| 19  | I     | 5     | 0        | 0        | 0       | 0            |
| 19  | J     | 13    | 0        | 0        | 0       | 0            |
| 19  | K     | 5     | 0        | 0        | 0       | 0            |
| 19  | L     | 12    | 0        | 0        | 0       | 0            |
| 19  | M     | 11    | 0        | 0        | 0       | 0            |
| 19  | N     | 4     | 0        | 0        | 0       | 0            |
| 19  | O     | 5     | 0        | 0        | 0       | 0            |
| 19  | P     | 5     | 0        | 0        | 0       | 0            |
| 19  | Q     | 8     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 19  | R     | 1     | 0        | 0        | 0       | 0            |
| 19  | S     | 3     | 0        | 0        | 0       | 0            |
| 19  | T     | 10    | 0        | 0        | 0       | 0            |
| 19  | U     | 8     | 0        | 0        | 0       | 0            |
| 19  | V     | 14    | 0        | 0        | 0       | 0            |
| 19  | W     | 5     | 0        | 0        | 0       | 0            |
| 19  | X     | 11    | 0        | 0        | 0       | 0            |
| 19  | Y     | 9     | 0        | 0        | 0       | 0            |
| 19  | Z     | 10    | 0        | 0        | 0       | 0            |
| 19  | a     | 11    | 0        | 0        | 0       | 0            |
| 19  | b     | 5     | 0        | 0        | 0       | 0            |
| All | All   | 49790 | 0        | 49126    | 558     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (558) 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) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:50:LYS:HZ1   | 2:B:50:LYS:HA    | 1.34                     | 0.91              |
| 3:Q:160:GLN:HA   | 3:Q:160:GLN:HE21 | 1.36                     | 0.89              |
| 3:C:160:GLN:HE21 | 3:C:160:GLN:HA   | 1.36                     | 0.89              |
| 8:V:35:HIS:HB3   | 8:V:56:THR:HG21  | 1.53                     | 0.89              |
| 8:H:35:HIS:HB3   | 8:H:56:THR:HG21  | 1.55                     | 0.86              |
| 1:A:176:GLU:HG3  | 2:B:55:LEU:HD13  | 1.58                     | 0.83              |
| 12:Z:31:THR:HG23 | 12:Z:36:ASN:HD21 | 1.46                     | 0.81              |
| 8:H:98:LEU:HB2   | 8:H:113:ILE:CG2  | 2.11                     | 0.80              |
| 1:A:176:GLU:HG3  | 2:B:55:LEU:CD1   | 2.11                     | 0.80              |
| 8:V:98:LEU:HB2   | 8:V:113:ILE:CG2  | 2.11                     | 0.79              |
| 12:L:31:THR:HG23 | 12:L:36:ASN:HD21 | 1.49                     | 0.75              |
| 3:C:204:GLY:O    | 3:C:205:ALA:O    | 2.06                     | 0.74              |
| 2:B:8:ARG:HD2    | 3:C:4:ARG:NH2    | 2.04                     | 0.72              |
| 7:G:23:PHE:O     | 7:G:26:THR:HB    | 1.90                     | 0.72              |
| 2:B:50:LYS:HA    | 2:B:50:LYS:NZ    | 2.04                     | 0.72              |
| 4:R:99:ILE:HD11  | 4:R:104:LEU:HB2  | 1.72                     | 0.72              |
| 14:b:152:VAL:HA  | 14:b:175:MET:HE1 | 1.72                     | 0.72              |
| 3:Q:204:GLY:O    | 3:Q:205:ALA:O    | 2.07                     | 0.71              |
| 14:N:152:VAL:HA  | 14:N:175:MET:HE1 | 1.71                     | 0.71              |
| 2:B:52:THR:HG23  | 2:B:56:LEU:HD13  | 1.71                     | 0.71              |
| 4:D:99:ILE:HD11  | 4:D:104:LEU:HB2  | 1.72                     | 0.70              |
| 7:U:23:PHE:O     | 7:U:26:THR:HB    | 1.91                     | 0.70              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 14:N:14:LEU:HD11 | 14:N:100:ALA:HB3  | 1.72                     | 0.69              |
| 8:V:98:LEU:HB2   | 8:V:113:ILE:HG22  | 1.75                     | 0.69              |
| 6:F:68:ARG:NH1   | 13:M:72:THR:OG1   | 2.25                     | 0.69              |
| 14:b:14:LEU:HD11 | 14:b:100:ALA:HB3  | 1.73                     | 0.69              |
| 8:H:98:LEU:HB2   | 8:H:113:ILE:HG22  | 1.75                     | 0.68              |
| 8:V:84:LYS:HE2   | 8:V:119:THR:HG23  | 1.75                     | 0.68              |
| 8:H:113:ILE:HD12 | 8:H:119:THR:HG22  | 1.75                     | 0.67              |
| 8:H:84:LYS:HE2   | 8:H:119:THR:HG23  | 1.75                     | 0.67              |
| 8:V:113:ILE:HD12 | 8:V:119:THR:HG22  | 1.76                     | 0.67              |
| 1:A:176:GLU:HA   | 2:B:55:LEU:HD11   | 1.76                     | 0.66              |
| 8:H:142:TRP:O    | 13:a:218:LYS:HE2  | 1.97                     | 0.65              |
| 5:E:92:ASN:HD21  | 12:L:70:ASN:HD21  | 1.43                     | 0.65              |
| 5:S:92:ASN:HD21  | 12:Z:70:ASN:HD21  | 1.44                     | 0.64              |
| 6:F:146:MET:CE   | 6:F:161:THR:HB    | 2.28                     | 0.64              |
| 12:L:38:ARG:NH1  | 12:L:221:ARG:HB3  | 2.13                     | 0.63              |
| 6:T:146:MET:CE   | 6:T:161:THR:HB    | 2.28                     | 0.63              |
| 4:D:88:ALA:HA    | 4:D:99:ILE:HG21   | 1.80                     | 0.62              |
| 2:B:93:HIS:HB3   | 2:B:113:ARG:HH21  | 1.65                     | 0.62              |
| 2:P:93:HIS:HB3   | 2:P:113:ARG:HH21  | 1.64                     | 0.62              |
| 4:R:88:ALA:HA    | 4:R:99:ILE:HG21   | 1.80                     | 0.61              |
| 12:Z:8:ASN:HA    | 12:Z:30:ILE:O     | 2.01                     | 0.61              |
| 10:J:16:ALA:HB2  | 10:J:161:LEU:HD21 | 1.82                     | 0.61              |
| 11:K:20:ALA:HB2  | 11:K:31:VAL:HG21  | 1.83                     | 0.61              |
| 1:O:12:PHE:H     | 2:P:20:GLN:HE22   | 1.49                     | 0.61              |
| 10:X:16:ALA:HB2  | 10:X:161:LEU:HD21 | 1.81                     | 0.60              |
| 11:Y:20:ALA:HB2  | 11:Y:31:VAL:HG21  | 1.83                     | 0.59              |
| 6:F:146:MET:HE3  | 6:F:161:THR:HB    | 1.84                     | 0.59              |
| 11:Y:44:THR:HG21 | 11:Y:100:MET:HE2  | 1.84                     | 0.59              |
| 3:C:9:PHE:H      | 4:D:15:GLN:HE22   | 1.51                     | 0.59              |
| 14:b:35:THR:OG1  | 14:b:43:CYS:SG    | 2.61                     | 0.59              |
| 5:E:212:ILE:HD12 | 5:E:229:VAL:HG12  | 1.84                     | 0.59              |
| 12:L:113:GLY:HA2 | 12:L:207:VAL:HG11 | 1.85                     | 0.59              |
| 11:Y:51:ASP:HB3  | 11:Y:97:MET:HE2   | 1.84                     | 0.59              |
| 8:H:53:GLU:OE2   | 8:H:57:GLN:NE2    | 2.36                     | 0.59              |
| 11:K:53:GLN:O    | 11:K:57:THR:HG23  | 2.02                     | 0.59              |
| 12:L:8:ASN:HA    | 12:L:30:ILE:O     | 2.03                     | 0.59              |
| 14:N:35:THR:OG1  | 14:N:43:CYS:SG    | 2.61                     | 0.59              |
| 11:Y:19:ARG:O    | 11:Y:33:LYS:NZ    | 2.35                     | 0.59              |
| 8:V:53:GLU:OE2   | 8:V:57:GLN:NE2    | 2.35                     | 0.58              |
| 11:Y:4:LEU:C     | 11:Y:4:LEU:HD22   | 2.28                     | 0.58              |
| 4:D:51:LEU:HD12  | 4:D:51:LEU:C      | 2.27                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:K:44:THR:HG21  | 11:K:100:MET:HE2  | 1.85                     | 0.58              |
| 12:L:13:LEU:HD11  | 12:L:150:LEU:HD21 | 1.85                     | 0.58              |
| 11:K:51:ASP:HB3   | 11:K:97:MET:HE2   | 1.84                     | 0.58              |
| 5:S:212:ILE:HD12  | 5:S:229:VAL:HG12  | 1.84                     | 0.58              |
| 9:W:10:ILE:HG21   | 9:W:141:ALA:HB3   | 1.85                     | 0.58              |
| 12:Z:13:LEU:HD11  | 12:Z:150:LEU:HD21 | 1.86                     | 0.58              |
| 8:H:19:ARG:O      | 8:H:33:LYS:NZ     | 2.35                     | 0.58              |
| 1:O:122:THR:HG22  | 2:P:128:ARG:HH21  | 1.68                     | 0.58              |
| 4:R:51:LEU:C      | 4:R:51:LEU:HD12   | 2.28                     | 0.58              |
| 14:b:35:THR:HG21  | 14:b:45:ARG:HE    | 1.68                     | 0.58              |
| 10:J:149:ARG:O    | 10:J:152:MET:HG3  | 2.04                     | 0.58              |
| 13:M:156:ARG:HH11 | 8:V:165:ASN:HD22  | 1.51                     | 0.58              |
| 11:Y:53:GLN:O     | 11:Y:57:THR:HG23  | 2.03                     | 0.58              |
| 11:K:6:PHE:HA     | 11:K:125:ASP:O    | 2.03                     | 0.57              |
| 6:T:146:MET:HE3   | 6:T:161:THR:HB    | 1.84                     | 0.57              |
| 7:U:227:LEU:HB3   | 7:U:231:ASN:HB2   | 1.86                     | 0.57              |
| 12:Z:38:ARG:NH1   | 12:Z:221:ARG:HB3  | 2.19                     | 0.57              |
| 11:K:19:ARG:O     | 11:K:33:LYS:NZ    | 2.34                     | 0.57              |
| 5:S:71:LEU:HD22   | 5:S:71:LEU:C      | 2.29                     | 0.57              |
| 7:G:227:LEU:HB3   | 7:G:231:ASN:HB2   | 1.86                     | 0.57              |
| 9:I:10:ILE:HG21   | 9:I:141:ALA:HB3   | 1.86                     | 0.57              |
| 10:X:149:ARG:O    | 10:X:152:MET:HG3  | 2.03                     | 0.57              |
| 11:Y:6:PHE:HA     | 11:Y:125:ASP:O    | 2.04                     | 0.57              |
| 3:Q:9:PHE:H       | 4:R:15:GLN:HE22   | 1.52                     | 0.57              |
| 11:K:4:LEU:HD22   | 11:K:4:LEU:C      | 2.30                     | 0.57              |
| 12:Z:113:GLY:HA2  | 12:Z:207:VAL:HG11 | 1.86                     | 0.56              |
| 5:E:71:LEU:C      | 5:E:71:LEU:HD22   | 2.31                     | 0.56              |
| 6:F:34:ILE:HG22   | 6:F:160:ALA:HB2   | 1.88                     | 0.56              |
| 12:Z:181:ILE:HD13 | 12:Z:215:GLU:OE2  | 2.05                     | 0.56              |
| 1:O:55:LEU:HB3    | 7:U:159:ALA:O     | 2.05                     | 0.56              |
| 12:Z:49:ASN:HD21  | 12:Z:211:GLY:HA2  | 1.70                     | 0.56              |
| 6:T:34:ILE:HG22   | 6:T:160:ALA:HB2   | 1.88                     | 0.56              |
| 13:M:218:LYS:HE2  | 8:V:142:TRP:O     | 2.06                     | 0.56              |
| 14:N:19:ARG:O     | 14:N:33:LYS:NZ    | 2.37                     | 0.55              |
| 14:N:35:THR:HG21  | 14:N:45:ARG:HE    | 1.71                     | 0.55              |
| 4:D:160:ASN:HB3   | 4:D:179:TRP:CE2   | 2.42                     | 0.55              |
| 8:H:165:ASN:HD22  | 13:a:156:ARG:HH11 | 1.55                     | 0.55              |
| 11:K:44:THR:O     | 11:K:99:THR:OG1   | 2.24                     | 0.55              |
| 1:A:12:PHE:H      | 2:B:20:GLN:HE22   | 1.54                     | 0.55              |
| 11:K:7:ARG:NH1    | 11:K:110:PRO:O    | 2.37                     | 0.55              |
| 4:R:160:ASN:HB3   | 4:R:179:TRP:CE2   | 2.42                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:Y:7:ARG:NH1    | 11:Y:110:PRO:O    | 2.36                     | 0.54              |
| 8:H:18:THR:HG21   | 8:H:172:ASN:HB2   | 1.89                     | 0.54              |
| 9:I:9:GLY:HA3     | 9:I:41:LYS:HE2    | 1.90                     | 0.54              |
| 2:P:8:ARG:HD2     | 3:Q:4:ARG:NH2     | 2.23                     | 0.54              |
| 8:V:42:TRP:CG     | 8:V:176:CYS:HG    | 2.26                     | 0.54              |
| 8:V:112:SER:HB3   | 8:V:125:LEU:HD13  | 1.89                     | 0.54              |
| 12:L:13:LEU:CD1   | 12:L:150:LEU:HD21 | 2.38                     | 0.54              |
| 14:N:83:LYS:HG3   | 14:N:119:VAL:HG22 | 1.89                     | 0.54              |
| 2:P:93:HIS:HB3    | 2:P:113:ARG:NH2   | 2.23                     | 0.54              |
| 9:W:65:MET:HE1    | 9:W:93:SER:HB3    | 1.90                     | 0.54              |
| 5:E:155:LEU:HD13  | 5:E:158:THR:HB    | 1.89                     | 0.54              |
| 5:S:92:ASN:ND2    | 12:Z:70:ASN:HD21  | 2.05                     | 0.54              |
| 1:O:149:GLN:O     | 1:O:156:TYR:HA    | 2.08                     | 0.53              |
| 8:V:19:ARG:O      | 8:V:33:LYS:NZ     | 2.34                     | 0.53              |
| 9:I:65:MET:HE1    | 9:I:93:SER:HB3    | 1.89                     | 0.53              |
| 14:b:163:ILE:HG23 | 14:b:170:GLY:HA2  | 1.90                     | 0.53              |
| 13:M:97:ALA:HA    | 13:M:130:VAL:HG21 | 1.91                     | 0.53              |
| 3:Q:201:VAL:O     | 3:Q:202:GLN:HB3   | 2.08                     | 0.53              |
| 11:Y:40:PHE:CD1   | 11:Y:73:ARG:CZ    | 2.91                     | 0.53              |
| 10:X:1:MET:HB2    | 10:X:34:LYS:HE3   | 1.90                     | 0.53              |
| 4:R:82:GLU:OE2    | 11:Y:69:ARG:NH1   | 2.41                     | 0.53              |
| 1:A:149:GLN:O     | 1:A:156:TYR:HA    | 2.07                     | 0.53              |
| 5:E:92:ASN:ND2    | 12:L:70:ASN:HD21  | 2.06                     | 0.53              |
| 12:Z:13:LEU:CD1   | 12:Z:150:LEU:HD21 | 2.38                     | 0.53              |
| 13:a:97:ALA:HA    | 13:a:130:VAL:HG21 | 1.90                     | 0.53              |
| 2:B:146:GLN:HG2   | 3:C:57:ILE:HG21   | 1.91                     | 0.53              |
| 3:Q:195:ARG:HG2   | 3:Q:234:ILE:HG21  | 1.90                     | 0.53              |
| 8:V:18:THR:HG21   | 8:V:172:ASN:HB2   | 1.90                     | 0.53              |
| 11:Y:44:THR:O     | 11:Y:99:THR:OG1   | 2.23                     | 0.53              |
| 10:J:1:MET:HB2    | 10:J:34:LYS:HE3   | 1.90                     | 0.53              |
| 10:J:35:THR:HG23  | 10:J:43:LEU:HD11  | 1.91                     | 0.52              |
| 11:K:40:PHE:CD1   | 11:K:73:ARG:CZ    | 2.93                     | 0.52              |
| 14:N:163:ILE:HG23 | 14:N:170:GLY:HA2  | 1.89                     | 0.52              |
| 2:B:93:HIS:HB3    | 2:B:113:ARG:NH2   | 2.23                     | 0.52              |
| 3:C:195:ARG:HG2   | 3:C:234:ILE:HG21  | 1.90                     | 0.52              |
| 8:H:112:SER:HB3   | 8:H:125:LEU:HD13  | 1.90                     | 0.52              |
| 2:B:12:PHE:H      | 3:C:17:GLN:HE22   | 1.57                     | 0.52              |
| 5:E:68:HIS:HE1    | 5:E:102:LEU:O     | 1.92                     | 0.52              |
| 4:R:1:ASP:O       | 4:R:2:ARG:HB2     | 2.10                     | 0.52              |
| 7:U:83:ASN:C      | 7:U:83:ASN:HD22   | 2.18                     | 0.52              |
| 11:Y:46:ALA:HB3   | 11:Y:98:GLY:O     | 2.09                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:F:98:LEU:HD23  | 6:F:99:TYR:CZ     | 2.45                     | 0.52              |
| 10:J:50:ALA:O    | 11:K:91:LYS:NZ    | 2.42                     | 0.52              |
| 9:W:9:GLY:HA3    | 9:W:41:LYS:HE2    | 1.90                     | 0.52              |
| 1:A:176:GLU:CG   | 2:B:54:THR:OG1    | 2.58                     | 0.52              |
| 3:C:201:VAL:O    | 3:C:202:GLN:HB3   | 2.08                     | 0.52              |
| 14:b:83:LYS:HG3  | 14:b:119:VAL:HG22 | 1.89                     | 0.52              |
| 5:S:155:LEU:HD13 | 5:S:158:THR:HB    | 1.90                     | 0.52              |
| 2:P:134:PHE:O    | 2:P:149:THR:HA    | 2.10                     | 0.52              |
| 10:X:35:THR:HG23 | 10:X:43:LEU:HD11  | 1.92                     | 0.52              |
| 12:L:3:ASN:HD22  | 12:L:4:PRO:HD2    | 1.75                     | 0.52              |
| 3:Q:160:GLN:HE21 | 3:Q:160:GLN:CA    | 2.13                     | 0.52              |
| 12:Z:3:ASN:HD22  | 12:Z:4:PRO:HD2    | 1.75                     | 0.52              |
| 5:S:68:HIS:HE1   | 5:S:102:LEU:O     | 1.93                     | 0.51              |
| 2:B:134:PHE:O    | 2:B:149:THR:HA    | 2.10                     | 0.51              |
| 12:L:100:LYS:HD3 | 12:L:105:TYR:CE2  | 2.45                     | 0.51              |
| 2:P:1:GLY:HA3    | 5:S:122:TYR:CD1   | 2.46                     | 0.51              |
| 8:V:84:LYS:HA    | 8:V:113:ILE:HD11  | 1.93                     | 0.51              |
| 8:H:192:THR:O    | 8:H:192:THR:HG22  | 2.11                     | 0.51              |
| 5:S:170:TYR:HB2  | 5:S:198:GLN:HG3   | 1.93                     | 0.51              |
| 6:T:98:LEU:HD23  | 6:T:99:TYR:CZ     | 2.45                     | 0.51              |
| 2:B:50:LYS:HZ1   | 2:B:50:LYS:CA     | 2.16                     | 0.51              |
| 8:H:84:LYS:HA    | 8:H:113:ILE:HD11  | 1.92                     | 0.51              |
| 12:L:17:GLY:HA3  | 12:L:20:PHE:CE1   | 2.46                     | 0.51              |
| 11:K:46:ALA:HB3  | 11:K:98:GLY:O     | 2.11                     | 0.51              |
| 2:B:38:MET:HE1   | 3:C:54:ASP:OD2    | 2.11                     | 0.51              |
| 2:B:50:LYS:NZ    | 2:B:50:LYS:CA     | 2.73                     | 0.50              |
| 2:P:89:THR:HG21  | 2:P:117:ILE:CD1   | 2.41                     | 0.50              |
| 10:X:50:ALA:O    | 11:Y:91:LYS:NZ    | 2.43                     | 0.50              |
| 12:Z:16:ALA:O    | 12:Z:135:GLN:NE2  | 2.45                     | 0.50              |
| 1:O:222:LEU:HD13 | 1:O:232:GLY:HA2   | 1.93                     | 0.50              |
| 2:P:1:GLY:HA3    | 5:S:122:TYR:CE1   | 2.46                     | 0.50              |
| 2:P:124:HIS:HB3  | 3:Q:124:VAL:HG12  | 1.93                     | 0.50              |
| 4:R:91:HIS:CG    | 4:R:99:ILE:HB     | 2.46                     | 0.50              |
| 4:R:193:LEU:HD22 | 4:R:211:LEU:HD11  | 1.93                     | 0.50              |
| 13:a:161:ARG:HG3 | 13:a:161:ARG:HH11 | 1.77                     | 0.50              |
| 7:G:83:ASN:C     | 7:G:83:ASN:HD22   | 2.20                     | 0.50              |
| 13:M:233:ILE:OXT | 14:b:185:ARG:NE   | 2.32                     | 0.50              |
| 4:R:193:LEU:CD2  | 4:R:211:LEU:HD11  | 2.42                     | 0.50              |
| 4:D:1:ASP:O      | 4:D:2:ARG:HB2     | 2.11                     | 0.50              |
| 12:Z:100:LYS:HD3 | 12:Z:105:TYR:CE2  | 2.46                     | 0.50              |
| 14:N:171:GLY:HA2 | 13:a:219:TRP:CH2  | 2.46                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:R:37:GLY:HA2   | 4:R:145:TYR:CE1   | 2.46                     | 0.50              |
| 12:L:100:LYS:HD3 | 12:L:105:TYR:CZ   | 2.47                     | 0.50              |
| 8:V:192:THR:HG22 | 8:V:192:THR:O     | 2.12                     | 0.50              |
| 1:A:222:LEU:HD13 | 1:A:232:GLY:HA2   | 1.93                     | 0.49              |
| 4:D:37:GLY:HA2   | 4:D:145:TYR:CE1   | 2.47                     | 0.49              |
| 5:E:209:ASN:C    | 5:E:209:ASN:ND2   | 2.67                     | 0.49              |
| 12:Z:185:ARG:NH1 | 12:Z:217:TYR:CE1  | 2.80                     | 0.49              |
| 2:B:89:THR:HG21  | 2:B:117:ILE:CD1   | 2.42                     | 0.49              |
| 5:E:170:TYR:HB2  | 5:E:198:GLN:HG3   | 1.93                     | 0.49              |
| 6:T:13:PRO:O     | 7:U:24:LYS:HD2    | 2.12                     | 0.49              |
| 4:D:91:HIS:CG    | 4:D:99:ILE:HB     | 2.48                     | 0.49              |
| 5:S:92:ASN:HD21  | 12:Z:70:ASN:ND2   | 2.10                     | 0.49              |
| 5:S:209:ASN:C    | 5:S:209:ASN:ND2   | 2.69                     | 0.49              |
| 4:D:193:LEU:CD2  | 4:D:211:LEU:HD11  | 2.42                     | 0.49              |
| 11:Y:33:LYS:HE2  | 16:Y:301:VOX:C35  | 2.42                     | 0.49              |
| 12:Z:100:LYS:HD3 | 12:Z:105:TYR:CZ   | 2.48                     | 0.49              |
| 9:W:98:ARG:O     | 9:W:126:ILE:HD11  | 2.13                     | 0.49              |
| 12:Z:17:GLY:HA3  | 12:Z:20:PHE:CE1   | 2.47                     | 0.49              |
| 2:B:14:PRO:HA    | 3:C:20:TYR:CD1    | 2.48                     | 0.49              |
| 9:I:98:ARG:O     | 9:I:126:ILE:HD11  | 2.12                     | 0.49              |
| 14:b:19:ARG:O    | 14:b:33:LYS:NZ    | 2.35                     | 0.49              |
| 4:D:193:LEU:HD22 | 4:D:211:LEU:HD11  | 1.94                     | 0.49              |
| 6:T:155:GLY:HA3  | 7:U:59:THR:HG21   | 1.95                     | 0.49              |
| 6:T:191:GLN:O    | 6:T:195:ILE:HG13  | 2.12                     | 0.49              |
| 6:F:172:LEU:HD13 | 6:F:195:ILE:HD13  | 1.95                     | 0.48              |
| 12:L:16:ALA:O    | 12:L:135:GLN:NE2  | 2.46                     | 0.48              |
| 14:N:13:ILE:HG21 | 14:N:175:MET:HE2  | 1.95                     | 0.48              |
| 6:F:191:GLN:O    | 6:F:195:ILE:HG13  | 2.13                     | 0.48              |
| 6:T:68:ARG:NH1   | 13:a:71:VAL:CG1   | 2.76                     | 0.48              |
| 6:T:172:LEU:HD13 | 6:T:195:ILE:HD13  | 1.94                     | 0.48              |
| 10:X:21:VAL:HG11 | 11:Y:122:LEU:HD11 | 1.95                     | 0.48              |
| 7:G:73:VAL:HG12  | 7:G:133:THR:HB    | 1.94                     | 0.48              |
| 5:E:65:CYS:SG    | 5:E:71:LEU:HD12   | 2.53                     | 0.48              |
| 7:G:78:ILE:N     | 7:G:79:PRO:CD     | 2.77                     | 0.48              |
| 2:P:215:ILE:HG12 | 2:P:226:GLN:HG3   | 1.95                     | 0.48              |
| 10:X:23:ARG:NH1  | 11:Y:116:ASP:OD1  | 2.46                     | 0.48              |
| 12:Z:173:LYS:HA  | 12:Z:173:LYS:HE3  | 1.95                     | 0.48              |
| 2:B:215:ILE:HG12 | 2:B:226:GLN:HG3   | 1.95                     | 0.48              |
| 12:L:173:LYS:HE3 | 12:L:173:LYS:HA   | 1.95                     | 0.48              |
| 13:a:27:LEU:HB2  | 13:a:192:SER:HB3  | 1.96                     | 0.48              |
| 12:L:160:TYR:CD2 | 12:L:166:GLY:HA2  | 2.49                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 13:M:219:TRP:CH2 | 14:b:171:GLY:HA2  | 2.48                     | 0.48              |
| 10:J:21:VAL:HG11 | 11:K:122:LEU:HD11 | 1.95                     | 0.48              |
| 11:Y:35:ILE:CD1  | 11:Y:53:GLN:HA    | 2.43                     | 0.48              |
| 3:C:161:THR:HG21 | 3:C:169:VAL:HG22  | 1.95                     | 0.48              |
| 8:V:210:THR:HG21 | 9:W:167:SER:HB3   | 1.95                     | 0.47              |
| 12:Z:160:TYR:CD2 | 12:Z:166:GLY:HA2  | 2.49                     | 0.47              |
| 1:A:66:LEU:C     | 1:A:66:LEU:HD23   | 2.39                     | 0.47              |
| 1:A:122:THR:HG22 | 2:B:128:ARG:HH21  | 1.79                     | 0.47              |
| 10:J:23:ARG:NH1  | 11:K:116:ASP:OD1  | 2.46                     | 0.47              |
| 7:U:78:ILE:N     | 7:U:79:PRO:CD     | 2.76                     | 0.47              |
| 11:K:35:ILE:CD1  | 11:K:53:GLN:HA    | 2.44                     | 0.47              |
| 13:M:27:LEU:HB2  | 13:M:192:SER:HB3  | 1.95                     | 0.47              |
| 13:M:161:ARG:HG3 | 13:M:161:ARG:HH11 | 1.79                     | 0.47              |
| 14:b:13:ILE:HG21 | 14:b:175:MET:HE2  | 1.96                     | 0.47              |
| 8:V:87:LEU:HD12  | 8:V:113:ILE:HG12  | 1.96                     | 0.47              |
| 8:V:36:ARG:HG3   | 8:V:42:TRP:CE2    | 2.50                     | 0.47              |
| 13:a:48:ASN:H    | 13:a:48:ASN:HD22  | 1.61                     | 0.47              |
| 1:A:61:LEU:C     | 1:A:61:LEU:HD23   | 2.40                     | 0.47              |
| 2:B:124:HIS:HB3  | 3:C:124:VAL:HG12  | 1.96                     | 0.47              |
| 5:E:74:ALA:HB3   | 5:E:160:ILE:HD12  | 1.96                     | 0.47              |
| 1:O:61:LEU:HD23  | 1:O:61:LEU:C      | 2.39                     | 0.47              |
| 2:B:105:ILE:HD11 | 2:B:109:ILE:HG22  | 1.96                     | 0.47              |
| 7:G:191:GLU:O    | 7:G:235:ARG:HD3   | 2.15                     | 0.47              |
| 1:O:66:LEU:HD23  | 1:O:66:LEU:C      | 2.39                     | 0.47              |
| 3:Q:161:THR:HG21 | 3:Q:169:VAL:HG22  | 1.96                     | 0.47              |
| 5:S:74:ALA:HB3   | 5:S:160:ILE:HD12  | 1.96                     | 0.47              |
| 5:S:136:TYR:CE1  | 5:S:217:LYS:HA    | 2.49                     | 0.47              |
| 7:U:73:VAL:HG12  | 7:U:133:THR:HB    | 1.95                     | 0.47              |
| 7:U:191:GLU:O    | 7:U:235:ARG:HD3   | 2.15                     | 0.47              |
| 11:Y:19:ARG:HH21 | 11:Y:29:GLN:HE22  | 1.63                     | 0.47              |
| 14:b:59:VAL:HG22 | 14:b:81:VAL:HG12  | 1.97                     | 0.47              |
| 1:A:176:GLU:HG3  | 2:B:55:LEU:HD11   | 1.93                     | 0.47              |
| 8:V:84:LYS:HG3   | 8:V:85:GLN:N      | 2.30                     | 0.47              |
| 12:Z:23:LEU:HD13 | 12:Z:43:VAL:HG13  | 1.97                     | 0.47              |
| 5:E:136:TYR:CE1  | 5:E:217:LYS:HA    | 2.49                     | 0.47              |
| 6:F:146:MET:HE1  | 6:F:161:THR:HB    | 1.97                     | 0.47              |
| 8:H:84:LYS:HG3   | 8:H:85:GLN:N      | 2.30                     | 0.47              |
| 3:Q:185:THR:OG1  | 3:Q:188:GLU:HB2   | 2.14                     | 0.47              |
| 8:H:36:ARG:HG3   | 8:H:42:TRP:CE2    | 2.50                     | 0.47              |
| 8:H:50:ALA:HB2   | 9:I:128:CYS:HB2   | 1.95                     | 0.47              |
| 8:H:104:ASP:HB2  | 8:H:105:PRO:HD2   | 1.97                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 12:L:221:ARG:NH2 | 13:M:160:ASP:O    | 2.47                     | 0.47              |
| 4:R:32:ILE:HD12  | 4:R:192:VAL:HG23  | 1.96                     | 0.47              |
| 4:R:158:ARG:HB3  | 5:S:57:SER:HB3    | 1.97                     | 0.47              |
| 7:U:83:ASN:C     | 7:U:83:ASN:ND2    | 2.73                     | 0.47              |
| 11:K:86:LEU:C    | 11:K:86:LEU:HD13  | 2.40                     | 0.46              |
| 4:R:109:CYS:SG   | 4:R:156:PHE:HB3   | 2.55                     | 0.46              |
| 14:N:59:VAL:HG22 | 14:N:81:VAL:HG12  | 1.96                     | 0.46              |
| 2:P:105:ILE:HD11 | 2:P:109:ILE:HG22  | 1.96                     | 0.46              |
| 14:b:32:ASP:OD2  | 14:b:185:ARG:NH2  | 2.48                     | 0.46              |
| 13:M:182:ARG:HG3 | 13:M:214:VAL:HG13 | 1.98                     | 0.46              |
| 2:P:111:VAL:HG22 | 2:P:136:TYR:CG    | 2.51                     | 0.46              |
| 2:P:225:TYR:CD2  | 8:V:225:GLU:HA    | 2.50                     | 0.46              |
| 6:T:123:ASN:C    | 6:T:123:ASN:HD22  | 2.24                     | 0.46              |
| 8:H:5:GLY:O      | 8:H:124:TYR:HA    | 2.16                     | 0.46              |
| 2:B:111:VAL:HG22 | 2:B:136:TYR:CG    | 2.51                     | 0.46              |
| 4:D:38:VAL:HG11  | 4:D:137:ALA:HB1   | 1.98                     | 0.46              |
| 6:F:105:ILE:N    | 6:F:106:PRO:CD    | 2.78                     | 0.46              |
| 5:S:99:ASN:HB2   | 13:a:94:GLU:HG2   | 1.96                     | 0.46              |
| 6:T:105:ILE:N    | 6:T:106:PRO:CD    | 2.78                     | 0.46              |
| 12:L:22:VAL:HG12 | 12:L:206:ILE:HG13 | 1.97                     | 0.46              |
| 3:Q:204:GLY:HA3  | 3:Q:231:VAL:HG11  | 1.98                     | 0.46              |
| 11:Y:35:ILE:HD13 | 11:Y:53:GLN:HA    | 1.98                     | 0.46              |
| 11:Y:86:LEU:C    | 11:Y:86:LEU:HD13  | 2.41                     | 0.46              |
| 12:Z:22:VAL:HG12 | 12:Z:206:ILE:HG13 | 1.98                     | 0.46              |
| 9:I:171:LEU:HD11 | 9:I:201:MET:HB3   | 1.98                     | 0.46              |
| 14:N:132:THR:O   | 14:b:133:PHE:HA   | 2.16                     | 0.46              |
| 13:M:48:ASN:H    | 13:M:48:ASN:HD22  | 1.62                     | 0.46              |
| 12:Z:221:ARG:NH2 | 13:a:160:ASP:O    | 2.49                     | 0.46              |
| 13:a:227:GLY:HA3 | 13:a:231:GLN:HB3  | 1.98                     | 0.46              |
| 2:P:225:TYR:CE2  | 8:V:225:GLU:HG3   | 2.52                     | 0.45              |
| 4:R:191:LEU:O    | 4:R:195:ILE:HG13  | 2.17                     | 0.45              |
| 8:V:104:ASP:HB2  | 8:V:105:PRO:HD2   | 1.98                     | 0.45              |
| 9:W:171:LEU:HD11 | 9:W:201:MET:HB3   | 1.98                     | 0.45              |
| 4:D:32:ILE:HD12  | 4:D:192:VAL:HG23  | 1.97                     | 0.45              |
| 4:D:191:LEU:O    | 4:D:195:ILE:HG13  | 2.16                     | 0.45              |
| 5:S:65:CYS:SG    | 5:S:71:LEU:HD12   | 2.56                     | 0.45              |
| 8:H:87:LEU:HD12  | 8:H:113:ILE:HG12  | 1.96                     | 0.45              |
| 9:W:97:ARG:HD2   | 9:W:102:TYR:CZ    | 2.52                     | 0.45              |
| 2:B:213:ALA:HA   | 2:B:227:LYS:O     | 2.17                     | 0.45              |
| 2:B:36:GLY:C     | 2:B:147:LEU:HD11  | 2.42                     | 0.45              |
| 4:R:30:ILE:HD12  | 4:R:196:LEU:HG    | 1.99                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:E:92:ASN:HD21  | 12:L:70:ASN:ND2   | 2.12                     | 0.45              |
| 13:a:182:ARG:HG3 | 13:a:214:VAL:HG13 | 1.98                     | 0.45              |
| 5:E:170:TYR:O    | 5:E:174:THR:OG1   | 2.35                     | 0.45              |
| 1:O:106:PRO:HG2  | 1:O:109:LEU:HB2   | 1.99                     | 0.45              |
| 6:T:146:MET:HE1  | 6:T:161:THR:HB    | 1.98                     | 0.45              |
| 1:A:161:ALA:O    | 2:B:55:LEU:HB3    | 2.16                     | 0.45              |
| 3:C:185:THR:OG1  | 3:C:188:GLU:HB2   | 2.15                     | 0.45              |
| 12:L:145:LEU:O   | 9:W:147:GLY:HA3   | 2.16                     | 0.45              |
| 4:D:104:LEU:C    | 4:D:104:LEU:HD13  | 2.42                     | 0.45              |
| 5:E:9:THR:HG21   | 5:E:119:THR:HA    | 1.99                     | 0.45              |
| 5:E:71:LEU:HD23  | 5:E:131:LEU:HD22  | 1.99                     | 0.45              |
| 6:F:116:VAL:HG21 | 6:F:147:LEU:HD21  | 1.98                     | 0.45              |
| 5:S:170:TYR:O    | 5:S:174:THR:OG1   | 2.35                     | 0.45              |
| 4:D:109:CYS:SG   | 4:D:156:PHE:HB3   | 2.57                     | 0.45              |
| 7:G:83:ASN:C     | 7:G:83:ASN:ND2    | 2.75                     | 0.45              |
| 9:I:7:ASN:HA     | 9:I:29:GLY:O      | 2.16                     | 0.45              |
| 3:Q:160:GLN:HA   | 3:Q:160:GLN:NE2   | 2.18                     | 0.45              |
| 4:R:38:VAL:HG11  | 4:R:137:ALA:HB1   | 1.98                     | 0.45              |
| 11:Y:100:MET:HE2 | 11:Y:100:MET:HB2  | 1.88                     | 0.45              |
| 13:a:129:TYR:O   | 13:a:136:THR:HA   | 2.17                     | 0.45              |
| 7:G:73:VAL:CG1   | 7:G:133:THR:HB    | 2.47                     | 0.44              |
| 8:V:5:GLY:O      | 8:V:124:TYR:HA    | 2.17                     | 0.44              |
| 12:L:175:LEU:HB2 | 12:L:180:VAL:HG23 | 2.00                     | 0.44              |
| 13:M:227:GLY:HA3 | 13:M:231:GLN:HB3  | 1.98                     | 0.44              |
| 5:S:71:LEU:HD23  | 5:S:131:LEU:HD22  | 1.99                     | 0.44              |
| 14:N:32:ASP:OD2  | 14:N:185:ARG:NH2  | 2.50                     | 0.44              |
| 4:R:104:LEU:HD13 | 4:R:104:LEU:C     | 2.43                     | 0.44              |
| 9:W:7:ASN:HA     | 9:W:29:GLY:O      | 2.17                     | 0.44              |
| 12:Z:175:LEU:HB2 | 12:Z:180:VAL:HG23 | 1.99                     | 0.44              |
| 7:U:34:LEU:HD12  | 7:U:169:ILE:CG2   | 2.48                     | 0.44              |
| 9:W:163:PHE:CE1  | 9:W:197:ARG:HD2   | 2.53                     | 0.44              |
| 9:I:163:PHE:CE1  | 9:I:197:ARG:HD2   | 2.52                     | 0.44              |
| 1:O:23:TYR:CD1   | 7:U:12:PRO:HA     | 2.52                     | 0.44              |
| 4:R:160:ASN:HB3  | 4:R:179:TRP:CZ2   | 2.53                     | 0.44              |
| 12:Z:147:MET:N   | 12:Z:148:PRO:HD2  | 2.32                     | 0.44              |
| 9:I:141:ALA:HB2  | 9:I:177:ASP:HB2   | 2.00                     | 0.44              |
| 11:K:35:ILE:HD13 | 11:K:53:GLN:HA    | 1.98                     | 0.44              |
| 4:D:30:ILE:HD12  | 4:D:196:LEU:HG    | 2.00                     | 0.44              |
| 4:D:160:ASN:HB3  | 4:D:179:TRP:CZ2   | 2.53                     | 0.44              |
| 7:G:45:ILE:HG22  | 7:G:216:VAL:HG22  | 1.99                     | 0.44              |
| 8:H:218:VAL:CG2  | 9:I:196:LYS:HB2   | 2.48                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 12:L:23:LEU:HD13  | 12:L:43:VAL:HG13 | 1.98                     | 0.44              |
| 6:T:116:VAL:HG21  | 6:T:147:LEU:HD21 | 1.98                     | 0.44              |
| 6:T:154:TRP:CZ3   | 7:U:60:VAL:HA    | 2.53                     | 0.44              |
| 11:Y:2:THR:HG21   | 11:Y:164:ALA:CB  | 2.48                     | 0.44              |
| 2:B:14:PRO:HA     | 3:C:20:TYR:CE1   | 2.52                     | 0.44              |
| 2:B:234:ILE:O     | 2:B:238:LEU:HB2  | 2.18                     | 0.44              |
| 7:U:45:ILE:HG22   | 7:U:216:VAL:HG22 | 2.00                     | 0.44              |
| 9:W:141:ALA:HB2   | 9:W:177:ASP:HB2  | 2.00                     | 0.44              |
| 2:B:56:LEU:HD23   | 2:B:57:GLU:N     | 2.32                     | 0.43              |
| 8:H:34:LEU:HD12   | 8:H:34:LEU:HA    | 1.86                     | 0.43              |
| 9:I:97:ARG:HD2    | 9:I:102:TYR:CZ   | 2.53                     | 0.43              |
| 14:N:133:PHE:HA   | 14:b:132:THR:O   | 2.18                     | 0.43              |
| 2:B:217:LYS:HE3   | 2:B:217:LYS:HA   | 2.00                     | 0.43              |
| 3:C:160:GLN:HE21  | 3:C:160:GLN:CA   | 2.13                     | 0.43              |
| 3:C:204:GLY:HA3   | 3:C:231:VAL:HG11 | 1.98                     | 0.43              |
| 7:G:34:LEU:HD12   | 7:G:169:ILE:CG2  | 2.48                     | 0.43              |
| 4:R:214:ILE:O     | 4:R:214:ILE:HG13 | 2.17                     | 0.43              |
| 6:T:7:SER:HB3     | 6:T:10:VAL:HG21  | 2.00                     | 0.43              |
| 7:U:43:VAL:HG11   | 7:U:194:VAL:HA   | 2.01                     | 0.43              |
| 2:P:36:GLY:C      | 2:P:147:LEU:HD11 | 2.43                     | 0.43              |
| 5:S:9:THR:HG21    | 5:S:119:THR:HA   | 1.99                     | 0.43              |
| 6:T:7:SER:HB3     | 6:T:10:VAL:CG2   | 2.49                     | 0.43              |
| 7:U:115:LEU:HD12  | 7:U:115:LEU:HA   | 1.89                     | 0.43              |
| 10:J:29:LYS:HE3   | 11:K:123:LYS:O   | 2.19                     | 0.43              |
| 11:Y:44:THR:HG1   | 11:Y:100:MET:H   | 1.67                     | 0.43              |
| 4:D:70:MET:HG3    | 4:D:74:THR:HG22  | 2.01                     | 0.43              |
| 6:F:175:LEU:HD11  | 6:F:191:GLN:HE21 | 1.84                     | 0.43              |
| 11:K:19:ARG:HH21  | 11:K:29:GLN:HE22 | 1.66                     | 0.43              |
| 2:P:217:LYS:HE3   | 2:P:217:LYS:HA   | 2.00                     | 0.43              |
| 12:L:147:MET:N    | 12:L:148:PRO:HD2 | 2.33                     | 0.43              |
| 14:N:36:ARG:HG3   | 14:N:42:TRP:CE2  | 2.54                     | 0.43              |
| 2:P:234:ILE:O     | 2:P:238:LEU:HB2  | 2.18                     | 0.43              |
| 8:V:225:GLU:HG2   | 8:V:226:GLU:N    | 2.34                     | 0.43              |
| 9:W:146:PHE:O     | 9:W:150:GLU:HB2  | 2.19                     | 0.43              |
| 10:X:53:THR:HA    | 10:X:100:VAL:CG2 | 2.49                     | 0.43              |
| 2:B:238:LEU:HD12  | 2:B:238:LEU:HA   | 1.91                     | 0.43              |
| 4:D:138:GLY:HA2   | 4:D:214:ILE:HG12 | 2.00                     | 0.43              |
| 9:I:146:PHE:O     | 9:I:150:GLU:HB2  | 2.19                     | 0.43              |
| 11:K:12:ILE:HB    | 11:K:180:VAL:HB  | 2.01                     | 0.43              |
| 14:N:161:GLN:HE21 | 14:b:136:GLY:HA2 | 1.84                     | 0.43              |
| 1:O:226:GLY:HA3   | 8:V:186:TYR:O    | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:F:7:SER:HB3     | 6:F:10:VAL:HG21   | 2.00                     | 0.43              |
| 9:I:141:ALA:HB2   | 9:I:177:ASP:CB    | 2.48                     | 0.43              |
| 11:K:13:ILE:HD12  | 11:K:154:LEU:HA   | 2.01                     | 0.43              |
| 4:R:70:MET:HG3    | 4:R:74:THR:HG22   | 2.01                     | 0.43              |
| 1:A:106:PRO:HG2   | 1:A:109:LEU:HB2   | 2.00                     | 0.43              |
| 3:C:131:THR:OG1   | 3:C:148:THR:OG1   | 2.31                     | 0.43              |
| 5:E:38:ARG:HD2    | 5:E:39:SER:O      | 2.19                     | 0.43              |
| 12:L:61:GLY:CA    | 12:L:107:VAL:HG11 | 2.49                     | 0.43              |
| 13:M:11:VAL:O     | 13:M:143:ALA:HA   | 2.19                     | 0.43              |
| 13:M:119:VAL:HG23 | 13:M:200:ILE:HG22 | 2.01                     | 0.43              |
| 14:N:20:THR:HG22  | 14:N:28:ASN:HB3   | 2.00                     | 0.43              |
| 4:R:6:THR:HG21    | 5:S:7:GLY:O       | 2.19                     | 0.43              |
| 5:S:109:HIS:HB3   | 6:T:82:ARG:NH2    | 2.34                     | 0.43              |
| 6:T:78:ILE:HB     | 6:T:79:PRO:HD3    | 2.00                     | 0.43              |
| 7:U:73:VAL:CG1    | 7:U:133:THR:HB    | 2.48                     | 0.43              |
| 4:D:20:LEU:HD12   | 4:D:20:LEU:HA     | 1.92                     | 0.43              |
| 7:G:43:VAL:HG11   | 7:G:194:VAL:HA    | 2.00                     | 0.43              |
| 14:N:185:ARG:NE   | 13:a:233:ILE:OXT  | 2.34                     | 0.43              |
| 12:Z:61:GLY:CA    | 12:Z:107:VAL:HG11 | 2.49                     | 0.43              |
| 12:Z:152:ASN:O    | 12:Z:156:PHE:HA   | 2.19                     | 0.43              |
| 13:a:68:LYS:HE3   | 13:a:68:LYS:HA    | 2.01                     | 0.43              |
| 14:b:59:VAL:HG11  | 14:b:82:PHE:CE2   | 2.54                     | 0.43              |
| 4:D:214:ILE:O     | 4:D:214:ILE:HG13  | 2.19                     | 0.42              |
| 5:E:209:ASN:C     | 5:E:209:ASN:HD22  | 2.27                     | 0.42              |
| 13:M:187:ARG:NH1  | 8:V:139:GLU:OE1   | 2.50                     | 0.42              |
| 14:N:30:VAL:HG11  | 13:a:221:PHE:CE2  | 2.54                     | 0.42              |
| 11:K:2:THR:HG21   | 11:K:164:ALA:CB   | 2.49                     | 0.42              |
| 12:L:152:ASN:O    | 12:L:156:PHE:HA   | 2.19                     | 0.42              |
| 13:M:129:TYR:O    | 13:M:136:THR:HA   | 2.19                     | 0.42              |
| 5:S:38:ARG:HD2    | 5:S:39:SER:O      | 2.19                     | 0.42              |
| 7:U:195:GLU:HG3   | 7:U:235:ARG:HG3   | 2.01                     | 0.42              |
| 12:Z:61:GLY:HA2   | 12:Z:107:VAL:HG11 | 2.01                     | 0.42              |
| 14:b:20:THR:HG22  | 14:b:28:ASN:HB3   | 2.01                     | 0.42              |
| 1:A:122:THR:CG2   | 2:B:128:ARG:HH21  | 2.32                     | 0.42              |
| 3:C:205:ALA:C     | 3:C:207:ASN:H     | 2.27                     | 0.42              |
| 7:G:195:GLU:HG3   | 7:G:235:ARG:HG3   | 2.01                     | 0.42              |
| 8:H:225:GLU:HG2   | 8:H:226:GLU:N     | 2.34                     | 0.42              |
| 9:I:10:ILE:HD11   | 9:I:174:ALA:HB2   | 2.01                     | 0.42              |
| 10:J:132:ALA:HB1  | 10:J:136:SER:HB2  | 2.01                     | 0.42              |
| 2:P:213:ALA:HA    | 2:P:227:LYS:O     | 2.18                     | 0.42              |
| 6:T:34:ILE:HG22   | 6:T:160:ALA:CB    | 2.49                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:T:68:ARG:HH12  | 13:a:71:VAL:HG11  | 1.85                     | 0.42              |
| 6:F:7:SER:HB3    | 6:F:10:VAL:CG2    | 2.49                     | 0.42              |
| 1:O:115:ALA:HB1  | 1:O:154:GLY:O     | 2.19                     | 0.42              |
| 1:O:122:THR:CG2  | 2:P:128:ARG:HH21  | 2.31                     | 0.42              |
| 6:T:59:LYS:HE2   | 6:T:59:LYS:HA     | 2.00                     | 0.42              |
| 13:a:188:ASP:C   | 13:a:190:ARG:H    | 2.27                     | 0.42              |
| 4:D:126:MET:HE1  | 4:D:130:PHE:CE2   | 2.55                     | 0.42              |
| 6:F:123:ASN:C    | 6:F:123:ASN:HD22  | 2.27                     | 0.42              |
| 13:M:68:LYS:HE3  | 13:M:68:LYS:HA    | 2.02                     | 0.42              |
| 2:P:110:LEU:C    | 2:P:110:LEU:HD23  | 2.45                     | 0.42              |
| 4:R:185:LEU:O    | 4:R:189:GLU:HG3   | 2.20                     | 0.42              |
| 11:Y:13:ILE:HD12 | 11:Y:154:LEU:HA   | 2.01                     | 0.42              |
| 3:C:160:GLN:HA   | 3:C:160:GLN:NE2   | 2.18                     | 0.42              |
| 13:M:188:ASP:C   | 13:M:190:ARG:H    | 2.27                     | 0.42              |
| 3:Q:205:ALA:C    | 3:Q:207:ASN:H     | 2.27                     | 0.42              |
| 5:S:116:GLN:OE1  | 5:S:120:GLN:NE2   | 2.52                     | 0.42              |
| 8:V:18:THR:HG23  | 8:V:172:ASN:O     | 2.20                     | 0.42              |
| 1:A:115:ALA:HB1  | 1:A:154:GLY:O     | 2.19                     | 0.42              |
| 3:C:174:GLU:HG2  | 4:D:49:PRO:HG2    | 2.02                     | 0.42              |
| 6:F:34:ILE:HG22  | 6:F:160:ALA:CB    | 2.49                     | 0.42              |
| 3:Q:160:GLN:HE22 | 3:Q:170:ARG:HE    | 1.68                     | 0.42              |
| 1:A:176:GLU:CD   | 2:B:54:THR:HG1    | 2.22                     | 0.42              |
| 11:K:17:ASP:CG   | 11:K:33:LYS:HZ2   | 2.27                     | 0.42              |
| 5:S:28:ILE:HD11  | 5:S:148:PRO:CD    | 2.50                     | 0.42              |
| 9:W:10:ILE:HD11  | 9:W:174:ALA:HB2   | 2.01                     | 0.42              |
| 9:I:62:LEU:HD21  | 9:I:102:TYR:CD2   | 2.54                     | 0.42              |
| 14:N:136:GLY:HA2 | 14:b:161:GLN:HE21 | 1.84                     | 0.42              |
| 7:U:201:MET:HG2  | 7:U:209:PHE:CE2   | 2.55                     | 0.42              |
| 11:Y:12:ILE:HB   | 11:Y:180:VAL:HB   | 2.01                     | 0.42              |
| 1:A:109:LEU:HD22 | 1:A:109:LEU:HA    | 1.93                     | 0.42              |
| 6:F:78:ILE:HB    | 6:F:79:PRO:HD3    | 2.01                     | 0.42              |
| 1:O:196:LEU:HD23 | 1:O:209:ILE:HD12  | 2.02                     | 0.42              |
| 11:Y:53:GLN:OE1  | 12:Z:130:SER:HA   | 2.19                     | 0.42              |
| 2:B:155:ASN:HD22 | 2:B:155:ASN:HA    | 1.66                     | 0.41              |
| 4:D:185:LEU:O    | 4:D:189:GLU:HG3   | 2.20                     | 0.41              |
| 11:K:53:GLN:OE1  | 12:L:130:SER:HA   | 2.20                     | 0.41              |
| 13:M:26:ASN:HA   | 13:M:39:VAL:O     | 2.20                     | 0.41              |
| 4:R:138:GLY:HA2  | 4:R:214:ILE:HG12  | 2.01                     | 0.41              |
| 8:V:9:ASN:HD22   | 8:V:10:ASN:N      | 2.17                     | 0.41              |
| 11:Y:4:LEU:C     | 11:Y:4:LEU:CD2    | 2.93                     | 0.41              |
| 1:A:84:VAL:O     | 1:A:88:LYS:HG3    | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:110:LEU:HD23  | 2:B:110:LEU:C     | 2.45                     | 0.41              |
| 2:B:180:LYS:HD2   | 2:B:183:MET:HE3   | 2.02                     | 0.41              |
| 6:F:59:LYS:HE2    | 6:F:59:LYS:HA     | 2.01                     | 0.41              |
| 8:H:113:ILE:HD12  | 8:H:119:THR:CG2   | 2.47                     | 0.41              |
| 11:K:44:THR:HG1   | 11:K:100:MET:H    | 1.67                     | 0.41              |
| 12:L:24:ALA:HB1   | 12:L:202:LEU:HD11 | 2.02                     | 0.41              |
| 14:b:36:ARG:HG3   | 14:b:42:TRP:CE2   | 2.54                     | 0.41              |
| 3:C:160:GLN:HE22  | 3:C:170:ARG:HE    | 1.68                     | 0.41              |
| 6:T:66:VAL:HG11   | 6:T:108:PHE:CE1   | 2.55                     | 0.41              |
| 6:T:146:MET:HB3   | 6:T:156:TYR:CE1   | 2.55                     | 0.41              |
| 12:Z:38:ARG:HD2   | 12:Z:221:ARG:NH2  | 2.35                     | 0.41              |
| 1:A:196:LEU:HD23  | 1:A:209:ILE:HD12  | 2.02                     | 0.41              |
| 13:M:27:LEU:HD23  | 13:M:190:ARG:O    | 2.20                     | 0.41              |
| 14:N:59:VAL:HG11  | 14:N:82:PHE:CE2   | 2.56                     | 0.41              |
| 10:X:132:ALA:HB1  | 10:X:136:SER:HB2  | 2.02                     | 0.41              |
| 12:Z:147:MET:N    | 12:Z:148:PRO:CD   | 2.83                     | 0.41              |
| 13:a:26:ASN:HA    | 13:a:39:VAL:O     | 2.20                     | 0.41              |
| 4:D:82:GLU:OE2    | 11:K:69:ARG:NH1   | 2.54                     | 0.41              |
| 10:J:50:ALA:HB1   | 11:K:120:THR:OG1  | 2.20                     | 0.41              |
| 11:K:97:MET:HB3   | 11:K:117:SER:HB3  | 2.03                     | 0.41              |
| 12:L:61:GLY:HA2   | 12:L:107:VAL:HG11 | 2.01                     | 0.41              |
| 2:P:146:GLN:HB3   | 2:P:148:TYR:CE2   | 2.56                     | 0.41              |
| 9:W:62:LEU:CD1    | 9:W:104:VAL:HG21  | 2.50                     | 0.41              |
| 9:W:141:ALA:HB2   | 9:W:177:ASP:CB    | 2.49                     | 0.41              |
| 10:X:86:GLN:O     | 10:X:90:LYS:HB2   | 2.21                     | 0.41              |
| 11:Y:52:CYS:SG    | 11:Y:97:MET:HG3   | 2.60                     | 0.41              |
| 12:Z:24:ALA:HB1   | 12:Z:202:LEU:HD11 | 2.03                     | 0.41              |
| 3:C:46:ARG:HH22   | 3:C:55:THR:HG21   | 1.86                     | 0.41              |
| 7:G:201:MET:HG2   | 7:G:209:PHE:CE2   | 2.55                     | 0.41              |
| 14:N:14:LEU:HD11  | 14:N:100:ALA:CB   | 2.45                     | 0.41              |
| 13:a:119:VAL:HG23 | 13:a:200:ILE:HG22 | 2.01                     | 0.41              |
| 8:H:9:ASN:HD22    | 8:H:10:ASN:N      | 2.18                     | 0.41              |
| 1:O:64:VAL:HG11   | 1:O:212:ALA:HB3   | 2.02                     | 0.41              |
| 6:T:175:LEU:HD11  | 6:T:191:GLN:HE21  | 1.85                     | 0.41              |
| 9:W:62:LEU:HD21   | 9:W:102:TYR:CD2   | 2.55                     | 0.41              |
| 3:C:204:GLY:C     | 3:C:205:ALA:O     | 2.63                     | 0.41              |
| 13:M:220:ASP:O    | 13:M:223:LYS:HG2  | 2.20                     | 0.41              |
| 1:O:64:VAL:HG11   | 1:O:212:ALA:CB    | 2.51                     | 0.41              |
| 1:O:250:LEU:HD13  | 1:O:250:LEU:C     | 2.46                     | 0.41              |
| 3:Q:204:GLY:C     | 3:Q:205:ALA:O     | 2.64                     | 0.41              |
| 4:R:32:ILE:CD1    | 4:R:192:VAL:HG23  | 2.51                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:U:106:ASP:HB3   | 7:U:146:TYR:CZ    | 2.56                     | 0.41              |
| 2:B:202:SER:OG    | 2:B:209:ARG:NH2   | 2.54                     | 0.41              |
| 5:E:98:PHE:O      | 13:M:91:TYR:HA    | 2.21                     | 0.41              |
| 8:H:45:GLY:HA2    | 8:H:98:LEU:HD23   | 2.03                     | 0.41              |
| 10:J:168:LEU:O    | 10:J:172:MET:HB2  | 2.20                     | 0.41              |
| 11:K:4:LEU:C      | 11:K:4:LEU:CD2    | 2.94                     | 0.41              |
| 14:N:55:ILE:HD11  | 14:N:93:LEU:HD13  | 2.02                     | 0.41              |
| 1:O:44:VAL:HG23   | 1:O:211:LEU:HD21  | 2.01                     | 0.41              |
| 1:O:84:VAL:O      | 1:O:88:LYS:HG3    | 2.21                     | 0.41              |
| 2:P:149:THR:O     | 2:P:156:TYR:HA    | 2.21                     | 0.41              |
| 4:R:71:SER:HB3    | 4:R:164:ILE:HD12  | 2.03                     | 0.41              |
| 9:W:126:ILE:HD12  | 9:W:126:ILE:HA    | 1.97                     | 0.41              |
| 12:L:194:ARG:CZ   | 8:V:29:LYS:HE2    | 2.50                     | 0.41              |
| 12:L:207:VAL:HG22 | 12:L:212:VAL:HG22 | 2.03                     | 0.41              |
| 4:R:126:MET:HE1   | 4:R:130:PHE:CE2   | 2.55                     | 0.41              |
| 7:G:106:ASP:HB3   | 7:G:146:TYR:CZ    | 2.56                     | 0.40              |
| 16:H:301:VOX:O2   | 16:H:301:VOX:C27  | 2.69                     | 0.40              |
| 9:I:62:LEU:CD1    | 9:I:104:VAL:HG21  | 2.52                     | 0.40              |
| 10:J:18:SER:HB2   | 10:J:176:PHE:HB2  | 2.03                     | 0.40              |
| 9:W:171:LEU:HD12  | 9:W:171:LEU:HA    | 1.93                     | 0.40              |
| 11:Y:17:ASP:CG    | 11:Y:33:LYS:HZ2   | 2.28                     | 0.40              |
| 12:Z:207:VAL:HG22 | 12:Z:212:VAL:HG22 | 2.03                     | 0.40              |
| 13:a:220:ASP:O    | 13:a:223:LYS:HG2  | 2.21                     | 0.40              |
| 4:D:113:LEU:HD23  | 4:D:113:LEU:HA    | 1.91                     | 0.40              |
| 3:Q:234:ILE:O     | 3:Q:238:LYS:HD2   | 2.22                     | 0.40              |
| 5:S:16:GLY:O      | 6:T:26:ALA:HB2    | 2.21                     | 0.40              |
| 9:W:31:GLN:HB3    | 9:W:32:SER:H      | 1.73                     | 0.40              |
| 13:a:104:ARG:HG3  | 13:a:105:SER:N    | 2.36                     | 0.40              |
| 1:A:44:VAL:HG23   | 1:A:211:LEU:HD21  | 2.01                     | 0.40              |
| 5:E:28:ILE:HD11   | 5:E:148:PRO:CD    | 2.50                     | 0.40              |
| 10:J:86:GLN:O     | 10:J:90:LYS:HB2   | 2.21                     | 0.40              |
| 2:B:1:GLY:HA3     | 5:E:122:TYR:CD1   | 2.55                     | 0.40              |
| 4:D:71:SER:HB3    | 4:D:164:ILE:HD12  | 2.04                     | 0.40              |
| 7:G:34:LEU:HD23   | 7:G:34:LEU:C      | 2.46                     | 0.40              |
| 3:Q:46:ARG:HH22   | 3:Q:55:THR:HG21   | 1.86                     | 0.40              |
| 8:V:45:GLY:HA2    | 8:V:98:LEU:HD23   | 2.03                     | 0.40              |
| 8:V:50:ALA:HB2    | 9:W:128:CYS:HB2   | 2.03                     | 0.40              |
| 13:a:11:VAL:O     | 13:a:143:ALA:HA   | 2.22                     | 0.40              |
| 14:b:55:ILE:HD11  | 14:b:93:LEU:HD13  | 2.02                     | 0.40              |
| 4:R:113:LEU:HD23  | 4:R:113:LEU:HA    | 1.91                     | 0.40              |
| 4:R:204:LEU:HD23  | 4:R:204:LEU:C     | 2.47                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 7:U:147:LYS:O   | 7:U:154:TYR:HA   | 2.22                     | 0.40              |
| 11:Y:97:MET:HB3 | 11:Y:117:SER:HB3 | 2.04                     | 0.40              |
| 12:Z:164:THR:O  | 12:Z:167:LYS:HD2 | 2.22                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 248/250 (99%) | 240 (97%) | 6 (2%)  | 2 (1%)   | 16          | 37  |
| 1   | O     | 248/250 (99%) | 240 (97%) | 6 (2%)  | 2 (1%)   | 16          | 37  |
| 2   | B     | 242/258 (94%) | 228 (94%) | 11 (4%) | 3 (1%)   | 10          | 28  |
| 2   | P     | 242/258 (94%) | 226 (93%) | 12 (5%) | 4 (2%)   | 7           | 20  |
| 3   | C     | 238/254 (94%) | 226 (95%) | 8 (3%)  | 4 (2%)   | 7           | 20  |
| 3   | Q     | 238/254 (94%) | 226 (95%) | 8 (3%)  | 4 (2%)   | 7           | 20  |
| 4   | D     | 231/260 (89%) | 221 (96%) | 9 (4%)  | 1 (0%)   | 30          | 53  |
| 4   | R     | 231/260 (89%) | 221 (96%) | 9 (4%)  | 1 (0%)   | 30          | 53  |
| 5   | E     | 229/234 (98%) | 217 (95%) | 12 (5%) | 0        | 100         | 100 |
| 5   | S     | 229/234 (98%) | 217 (95%) | 12 (5%) | 0        | 100         | 100 |
| 6   | F     | 241/288 (84%) | 229 (95%) | 11 (5%) | 1 (0%)   | 30          | 53  |
| 6   | T     | 241/288 (84%) | 229 (95%) | 11 (5%) | 1 (0%)   | 30          | 53  |
| 7   | G     | 239/252 (95%) | 232 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 7   | U     | 239/252 (95%) | 232 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 8   | H     | 224/232 (97%) | 219 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 8   | V     | 224/232 (97%) | 220 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 9   | I     | 202/205 (98%) | 192 (95%) | 10 (5%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 9   | W     | 202/205 (98%)   | 193 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 10  | J     | 193/198 (98%)   | 182 (94%)  | 11 (6%)  | 0        | 100         | 100 |
| 10  | X     | 193/198 (98%)   | 182 (94%)  | 11 (6%)  | 0        | 100         | 100 |
| 11  | K     | 210/212 (99%)   | 204 (97%)  | 4 (2%)   | 2 (1%)   | 12          | 32  |
| 11  | Y     | 210/212 (99%)   | 204 (97%)  | 4 (2%)   | 2 (1%)   | 12          | 32  |
| 12  | L     | 220/222 (99%)   | 213 (97%)  | 6 (3%)   | 1 (0%)   | 24          | 49  |
| 12  | Z     | 220/222 (99%)   | 213 (97%)  | 6 (3%)   | 1 (0%)   | 24          | 49  |
| 13  | M     | 231/246 (94%)   | 217 (94%)  | 14 (6%)  | 0        | 100         | 100 |
| 13  | a     | 231/246 (94%)   | 217 (94%)  | 14 (6%)  | 0        | 100         | 100 |
| 14  | N     | 194/196 (99%)   | 189 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 14  | b     | 194/196 (99%)   | 190 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| All | All   | 6284/6614 (95%) | 6019 (96%) | 236 (4%) | 29 (0%)  | 24          | 49  |

All (29) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 2   | THR  |
| 3   | C     | 205 | ALA  |
| 4   | D     | 2   | ARG  |
| 11  | K     | 209 | ASN  |
| 1   | O     | 2   | THR  |
| 2   | P     | 51  | VAL  |
| 3   | Q     | 205 | ALA  |
| 4   | R     | 2   | ARG  |
| 11  | Y     | 209 | ASN  |
| 1   | A     | 166 | LYS  |
| 3   | C     | 202 | GLN  |
| 1   | O     | 166 | LYS  |
| 3   | Q     | 202 | GLN  |
| 2   | B     | 62  | THR  |
| 2   | B     | 219 | ALA  |
| 2   | B     | 221 | ASP  |
| 11  | K     | 106 | ARG  |
| 2   | P     | 62  | THR  |
| 2   | P     | 219 | ALA  |
| 2   | P     | 221 | ASP  |
| 3   | Q     | 225 | GLU  |
| 11  | Y     | 106 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 225 | GLU  |
| 6   | F     | 205 | GLU  |
| 6   | T     | 205 | GLU  |
| 12  | Z     | 165 | ASN  |
| 3   | C     | 183 | PRO  |
| 12  | L     | 165 | ASN  |
| 3   | Q     | 183 | PRO  |

### 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     | 209/209 (100%) | 197 (94%) | 12 (6%)  | 18          | 42 |
| 1   | O     | 209/209 (100%) | 196 (94%) | 13 (6%)  | 16          | 39 |
| 2   | B     | 203/216 (94%)  | 186 (92%) | 17 (8%)  | 10          | 26 |
| 2   | P     | 203/216 (94%)  | 185 (91%) | 18 (9%)  | 9           | 24 |
| 3   | C     | 212/226 (94%)  | 187 (88%) | 25 (12%) | 5           | 15 |
| 3   | Q     | 212/226 (94%)  | 187 (88%) | 25 (12%) | 5           | 15 |
| 4   | D     | 194/215 (90%)  | 173 (89%) | 21 (11%) | 6           | 18 |
| 4   | R     | 194/215 (90%)  | 173 (89%) | 21 (11%) | 6           | 18 |
| 5   | E     | 190/193 (98%)  | 171 (90%) | 19 (10%) | 7           | 20 |
| 5   | S     | 190/193 (98%)  | 171 (90%) | 19 (10%) | 7           | 20 |
| 6   | F     | 201/239 (84%)  | 186 (92%) | 15 (8%)  | 12          | 31 |
| 6   | T     | 201/239 (84%)  | 186 (92%) | 15 (8%)  | 12          | 31 |
| 7   | G     | 206/210 (98%)  | 182 (88%) | 24 (12%) | 5           | 16 |
| 7   | U     | 206/210 (98%)  | 182 (88%) | 24 (12%) | 5           | 16 |
| 8   | H     | 185/190 (97%)  | 174 (94%) | 11 (6%)  | 18          | 41 |
| 8   | V     | 185/190 (97%)  | 174 (94%) | 11 (6%)  | 18          | 41 |
| 9   | I     | 172/173 (99%)  | 160 (93%) | 12 (7%)  | 14          | 34 |
| 9   | W     | 172/173 (99%)  | 160 (93%) | 12 (7%)  | 14          | 34 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 10  | J     | 173/175 (99%)   | 160 (92%)  | 13 (8%)  | 12          | 31 |
| 10  | X     | 173/175 (99%)   | 160 (92%)  | 13 (8%)  | 12          | 31 |
| 11  | K     | 169/169 (100%)  | 161 (95%)  | 8 (5%)   | 23          | 49 |
| 11  | Y     | 169/169 (100%)  | 161 (95%)  | 8 (5%)   | 23          | 49 |
| 12  | L     | 185/185 (100%)  | 173 (94%)  | 12 (6%)  | 15          | 37 |
| 12  | Z     | 185/185 (100%)  | 173 (94%)  | 12 (6%)  | 15          | 37 |
| 13  | M     | 199/208 (96%)   | 188 (94%)  | 11 (6%)  | 19          | 43 |
| 13  | a     | 199/208 (96%)   | 188 (94%)  | 11 (6%)  | 19          | 43 |
| 14  | N     | 162/162 (100%)  | 156 (96%)  | 6 (4%)   | 30          | 55 |
| 14  | b     | 162/162 (100%)  | 155 (96%)  | 7 (4%)   | 26          | 52 |
| All | All   | 5320/5540 (96%) | 4905 (92%) | 415 (8%) | 11          | 30 |

All (415) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 29  | LYS  |
| 1   | A     | 51  | SER  |
| 1   | A     | 59  | GLU  |
| 1   | A     | 108 | LYS  |
| 1   | A     | 109 | LEU  |
| 1   | A     | 122 | THR  |
| 1   | A     | 157 | PHE  |
| 1   | A     | 164 | ILE  |
| 1   | A     | 169 | VAL  |
| 1   | A     | 176 | GLU  |
| 1   | A     | 231 | LYS  |
| 1   | A     | 248 | GLU  |
| 2   | B     | 7   | SER  |
| 2   | B     | 17  | ARG  |
| 2   | B     | 50  | LYS  |
| 2   | B     | 58  | GLN  |
| 2   | B     | 62  | THR  |
| 2   | B     | 65  | LEU  |
| 2   | B     | 79  | LEU  |
| 2   | B     | 102 | ASN  |
| 2   | B     | 155 | ASN  |
| 2   | B     | 180 | LYS  |
| 2   | B     | 191 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 197 | SER  |
| 2   | B     | 217 | LYS  |
| 2   | B     | 237 | ILE  |
| 2   | B     | 239 | VAL  |
| 2   | B     | 240 | LYS  |
| 2   | B     | 244 | THR  |
| 3   | C     | 4   | ARG  |
| 3   | C     | 35  | LYS  |
| 3   | C     | 37  | LYS  |
| 3   | C     | 38  | ASN  |
| 3   | C     | 48  | SER  |
| 3   | C     | 49  | THR  |
| 3   | C     | 51  | LYS  |
| 3   | C     | 53  | GLN  |
| 3   | C     | 55  | THR  |
| 3   | C     | 58  | THR  |
| 3   | C     | 61  | LYS  |
| 3   | C     | 69  | VAL  |
| 3   | C     | 160 | GLN  |
| 3   | C     | 167 | LYS  |
| 3   | C     | 169 | VAL  |
| 3   | C     | 180 | LYS  |
| 3   | C     | 181 | GLU  |
| 3   | C     | 203 | THR  |
| 3   | C     | 213 | VAL  |
| 3   | C     | 214 | LYS  |
| 3   | C     | 224 | SER  |
| 3   | C     | 235 | GLU  |
| 3   | C     | 238 | LYS  |
| 3   | C     | 239 | GLN  |
| 3   | C     | 240 | GLU  |
| 4   | D     | 4   | VAL  |
| 4   | D     | 20  | LEU  |
| 4   | D     | 40  | LEU  |
| 4   | D     | 51  | LEU  |
| 4   | D     | 60  | VAL  |
| 4   | D     | 64  | ARG  |
| 4   | D     | 99  | ILE  |
| 4   | D     | 117 | GLU  |
| 4   | D     | 125 | LEU  |
| 4   | D     | 176 | LEU  |
| 4   | D     | 190 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 192 | VAL  |
| 4   | D     | 193 | LEU  |
| 4   | D     | 214 | ILE  |
| 4   | D     | 215 | THR  |
| 4   | D     | 216 | LYS  |
| 4   | D     | 217 | GLN  |
| 4   | D     | 224 | ASP  |
| 4   | D     | 236 | LYS  |
| 4   | D     | 238 | LYS  |
| 4   | D     | 242 | GLU  |
| 5   | E     | 9   | THR  |
| 5   | E     | 10  | VAL  |
| 5   | E     | 25  | LEU  |
| 5   | E     | 29  | LYS  |
| 5   | E     | 55  | LEU  |
| 5   | E     | 71  | LEU  |
| 5   | E     | 87  | LEU  |
| 5   | E     | 153 | THR  |
| 5   | E     | 160 | ILE  |
| 5   | E     | 169 | THR  |
| 5   | E     | 174 | THR  |
| 5   | E     | 184 | ASN  |
| 5   | E     | 188 | LEU  |
| 5   | E     | 203 | GLU  |
| 5   | E     | 207 | VAL  |
| 5   | E     | 209 | ASN  |
| 5   | E     | 211 | SER  |
| 5   | E     | 229 | VAL  |
| 5   | E     | 231 | LYS  |
| 6   | F     | 14  | ASP  |
| 6   | F     | 53  | LYS  |
| 6   | F     | 58  | GLN  |
| 6   | F     | 94  | SER  |
| 6   | F     | 117 | GLN  |
| 6   | F     | 123 | ASN  |
| 6   | F     | 132 | THR  |
| 6   | F     | 139 | LYS  |
| 6   | F     | 165 | ARG  |
| 6   | F     | 167 | SER  |
| 6   | F     | 172 | LEU  |
| 6   | F     | 174 | LYS  |
| 6   | F     | 181 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | F     | 206 | LYS  |
| 6   | F     | 221 | ASN  |
| 7   | G     | 24  | LYS  |
| 7   | G     | 26  | THR  |
| 7   | G     | 28  | GLN  |
| 7   | G     | 44  | VAL  |
| 7   | G     | 83  | ASN  |
| 7   | G     | 115 | LEU  |
| 7   | G     | 122 | ARG  |
| 7   | G     | 148 | THR  |
| 7   | G     | 166 | GLN  |
| 7   | G     | 168 | GLU  |
| 7   | G     | 171 | THR  |
| 7   | G     | 178 | LYS  |
| 7   | G     | 181 | LYS  |
| 7   | G     | 199 | THR  |
| 7   | G     | 201 | MET  |
| 7   | G     | 207 | THR  |
| 7   | G     | 223 | LYS  |
| 7   | G     | 230 | GLU  |
| 7   | G     | 235 | ARG  |
| 7   | G     | 236 | LEU  |
| 7   | G     | 237 | VAL  |
| 7   | G     | 239 | ILE  |
| 7   | G     | 241 | GLU  |
| 7   | G     | 242 | GLN  |
| 8   | H     | 1   | THR  |
| 8   | H     | 9   | ASN  |
| 8   | H     | 34  | LEU  |
| 8   | H     | 56  | THR  |
| 8   | H     | 68  | LEU  |
| 8   | H     | 113 | ILE  |
| 8   | H     | 127 | LEU  |
| 8   | H     | 153 | LYS  |
| 8   | H     | 199 | LYS  |
| 8   | H     | 209 | THR  |
| 8   | H     | 216 | SER  |
| 9   | I     | 30  | SER  |
| 9   | I     | 31  | GLN  |
| 9   | I     | 37  | ASN  |
| 9   | I     | 97  | ARG  |
| 9   | I     | 123 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | I     | 126 | ILE  |
| 9   | I     | 166 | ILE  |
| 9   | I     | 171 | LEU  |
| 9   | I     | 182 | TRP  |
| 9   | I     | 190 | LYS  |
| 9   | I     | 191 | LYS  |
| 9   | I     | 202 | ARG  |
| 10  | J     | 1   | MET  |
| 10  | J     | 3   | ILE  |
| 10  | J     | 7   | ILE  |
| 10  | J     | 17  | SER  |
| 10  | J     | 23  | ARG  |
| 10  | J     | 35  | THR  |
| 10  | J     | 36  | ARG  |
| 10  | J     | 90  | LYS  |
| 10  | J     | 99  | GLN  |
| 10  | J     | 110 | LYS  |
| 10  | J     | 113 | LYS  |
| 10  | J     | 161 | LEU  |
| 10  | J     | 172 | MET  |
| 11  | K     | 1   | THR  |
| 11  | K     | 4   | LEU  |
| 11  | K     | 9   | GLN  |
| 11  | K     | 17  | ASP  |
| 11  | K     | 148 | LEU  |
| 11  | K     | 181 | THR  |
| 11  | K     | 186 | ILE  |
| 11  | K     | 211 | ILE  |
| 12  | L     | 18  | GLU  |
| 12  | L     | 23  | LEU  |
| 12  | L     | 43  | VAL  |
| 12  | L     | 49  | ASN  |
| 12  | L     | 70  | ASN  |
| 12  | L     | 85  | SER  |
| 12  | L     | 108 | HIS  |
| 12  | L     | 133 | ARG  |
| 12  | L     | 172 | LEU  |
| 12  | L     | 173 | LYS  |
| 12  | L     | 189 | THR  |
| 12  | L     | 209 | LYS  |
| 13  | M     | 2   | GLN  |
| 13  | M     | 10  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | M     | 37  | ASN  |
| 13  | M     | 43  | ILE  |
| 13  | M     | 48  | ASN  |
| 13  | M     | 70  | LEU  |
| 13  | M     | 104 | ARG  |
| 13  | M     | 157 | LYS  |
| 13  | M     | 161 | ARG  |
| 13  | M     | 190 | ARG  |
| 13  | M     | 215 | GLU  |
| 14  | N     | 9   | LYS  |
| 14  | N     | 92  | ASN  |
| 14  | N     | 105 | LYS  |
| 14  | N     | 107 | LYS  |
| 14  | N     | 119 | VAL  |
| 14  | N     | 178 | LEU  |
| 1   | O     | 29  | LYS  |
| 1   | O     | 51  | SER  |
| 1   | O     | 59  | GLU  |
| 1   | O     | 108 | LYS  |
| 1   | O     | 109 | LEU  |
| 1   | O     | 122 | THR  |
| 1   | O     | 157 | PHE  |
| 1   | O     | 164 | ILE  |
| 1   | O     | 169 | VAL  |
| 1   | O     | 172 | LYS  |
| 1   | O     | 176 | GLU  |
| 1   | O     | 231 | LYS  |
| 1   | O     | 248 | GLU  |
| 2   | P     | 7   | SER  |
| 2   | P     | 17  | ARG  |
| 2   | P     | 50  | LYS  |
| 2   | P     | 55  | LEU  |
| 2   | P     | 58  | GLN  |
| 2   | P     | 62  | THR  |
| 2   | P     | 65  | LEU  |
| 2   | P     | 79  | LEU  |
| 2   | P     | 102 | ASN  |
| 2   | P     | 155 | ASN  |
| 2   | P     | 180 | LYS  |
| 2   | P     | 191 | LEU  |
| 2   | P     | 197 | SER  |
| 2   | P     | 217 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | P     | 237 | ILE  |
| 2   | P     | 239 | VAL  |
| 2   | P     | 240 | LYS  |
| 2   | P     | 244 | THR  |
| 3   | Q     | 4   | ARG  |
| 3   | Q     | 35  | LYS  |
| 3   | Q     | 37  | LYS  |
| 3   | Q     | 38  | ASN  |
| 3   | Q     | 48  | SER  |
| 3   | Q     | 49  | THR  |
| 3   | Q     | 51  | LYS  |
| 3   | Q     | 53  | GLN  |
| 3   | Q     | 55  | THR  |
| 3   | Q     | 58  | THR  |
| 3   | Q     | 61  | LYS  |
| 3   | Q     | 69  | VAL  |
| 3   | Q     | 160 | GLN  |
| 3   | Q     | 167 | LYS  |
| 3   | Q     | 169 | VAL  |
| 3   | Q     | 180 | LYS  |
| 3   | Q     | 181 | GLU  |
| 3   | Q     | 203 | THR  |
| 3   | Q     | 213 | VAL  |
| 3   | Q     | 214 | LYS  |
| 3   | Q     | 224 | SER  |
| 3   | Q     | 235 | GLU  |
| 3   | Q     | 238 | LYS  |
| 3   | Q     | 239 | GLN  |
| 3   | Q     | 240 | GLU  |
| 4   | R     | 4   | VAL  |
| 4   | R     | 20  | LEU  |
| 4   | R     | 40  | LEU  |
| 4   | R     | 51  | LEU  |
| 4   | R     | 60  | VAL  |
| 4   | R     | 64  | ARG  |
| 4   | R     | 99  | ILE  |
| 4   | R     | 117 | GLU  |
| 4   | R     | 125 | LEU  |
| 4   | R     | 176 | LEU  |
| 4   | R     | 190 | LEU  |
| 4   | R     | 192 | VAL  |
| 4   | R     | 193 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | R     | 214 | ILE  |
| 4   | R     | 215 | THR  |
| 4   | R     | 216 | LYS  |
| 4   | R     | 217 | GLN  |
| 4   | R     | 224 | ASP  |
| 4   | R     | 236 | LYS  |
| 4   | R     | 238 | LYS  |
| 4   | R     | 242 | GLU  |
| 5   | S     | 9   | THR  |
| 5   | S     | 10  | VAL  |
| 5   | S     | 25  | LEU  |
| 5   | S     | 29  | LYS  |
| 5   | S     | 55  | LEU  |
| 5   | S     | 71  | LEU  |
| 5   | S     | 87  | LEU  |
| 5   | S     | 153 | THR  |
| 5   | S     | 160 | ILE  |
| 5   | S     | 169 | THR  |
| 5   | S     | 174 | THR  |
| 5   | S     | 184 | ASN  |
| 5   | S     | 188 | LEU  |
| 5   | S     | 203 | GLU  |
| 5   | S     | 207 | VAL  |
| 5   | S     | 209 | ASN  |
| 5   | S     | 211 | SER  |
| 5   | S     | 229 | VAL  |
| 5   | S     | 231 | LYS  |
| 6   | T     | 14  | ASP  |
| 6   | T     | 53  | LYS  |
| 6   | T     | 58  | GLN  |
| 6   | T     | 94  | SER  |
| 6   | T     | 117 | GLN  |
| 6   | T     | 123 | ASN  |
| 6   | T     | 132 | THR  |
| 6   | T     | 139 | LYS  |
| 6   | T     | 165 | ARG  |
| 6   | T     | 167 | SER  |
| 6   | T     | 172 | LEU  |
| 6   | T     | 174 | LYS  |
| 6   | T     | 181 | GLU  |
| 6   | T     | 206 | LYS  |
| 6   | T     | 221 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | U     | 24  | LYS  |
| 7   | U     | 26  | THR  |
| 7   | U     | 28  | GLN  |
| 7   | U     | 44  | VAL  |
| 7   | U     | 83  | ASN  |
| 7   | U     | 115 | LEU  |
| 7   | U     | 122 | ARG  |
| 7   | U     | 148 | THR  |
| 7   | U     | 166 | GLN  |
| 7   | U     | 168 | GLU  |
| 7   | U     | 171 | THR  |
| 7   | U     | 178 | LYS  |
| 7   | U     | 181 | LYS  |
| 7   | U     | 199 | THR  |
| 7   | U     | 201 | MET  |
| 7   | U     | 207 | THR  |
| 7   | U     | 223 | LYS  |
| 7   | U     | 230 | GLU  |
| 7   | U     | 235 | ARG  |
| 7   | U     | 236 | LEU  |
| 7   | U     | 237 | VAL  |
| 7   | U     | 239 | ILE  |
| 7   | U     | 241 | GLU  |
| 7   | U     | 242 | GLN  |
| 8   | V     | 1   | THR  |
| 8   | V     | 9   | ASN  |
| 8   | V     | 34  | LEU  |
| 8   | V     | 56  | THR  |
| 8   | V     | 68  | LEU  |
| 8   | V     | 113 | ILE  |
| 8   | V     | 127 | LEU  |
| 8   | V     | 153 | LYS  |
| 8   | V     | 199 | LYS  |
| 8   | V     | 209 | THR  |
| 8   | V     | 216 | SER  |
| 9   | W     | 30  | SER  |
| 9   | W     | 31  | GLN  |
| 9   | W     | 37  | ASN  |
| 9   | W     | 97  | ARG  |
| 9   | W     | 123 | PHE  |
| 9   | W     | 126 | ILE  |
| 9   | W     | 166 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | W     | 171 | LEU  |
| 9   | W     | 182 | TRP  |
| 9   | W     | 190 | LYS  |
| 9   | W     | 191 | LYS  |
| 9   | W     | 202 | ARG  |
| 10  | X     | 1   | MET  |
| 10  | X     | 3   | ILE  |
| 10  | X     | 7   | ILE  |
| 10  | X     | 17  | SER  |
| 10  | X     | 23  | ARG  |
| 10  | X     | 35  | THR  |
| 10  | X     | 36  | ARG  |
| 10  | X     | 90  | LYS  |
| 10  | X     | 99  | GLN  |
| 10  | X     | 110 | LYS  |
| 10  | X     | 113 | LYS  |
| 10  | X     | 161 | LEU  |
| 10  | X     | 172 | MET  |
| 11  | Y     | 1   | THR  |
| 11  | Y     | 4   | LEU  |
| 11  | Y     | 9   | GLN  |
| 11  | Y     | 17  | ASP  |
| 11  | Y     | 148 | LEU  |
| 11  | Y     | 181 | THR  |
| 11  | Y     | 186 | ILE  |
| 11  | Y     | 211 | ILE  |
| 12  | Z     | 18  | GLU  |
| 12  | Z     | 23  | LEU  |
| 12  | Z     | 43  | VAL  |
| 12  | Z     | 49  | ASN  |
| 12  | Z     | 70  | ASN  |
| 12  | Z     | 85  | SER  |
| 12  | Z     | 108 | HIS  |
| 12  | Z     | 133 | ARG  |
| 12  | Z     | 172 | LEU  |
| 12  | Z     | 173 | LYS  |
| 12  | Z     | 189 | THR  |
| 12  | Z     | 209 | LYS  |
| 13  | a     | 2   | GLN  |
| 13  | a     | 10  | SER  |
| 13  | a     | 37  | ASN  |
| 13  | a     | 43  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | a     | 48  | ASN  |
| 13  | a     | 70  | LEU  |
| 13  | a     | 104 | ARG  |
| 13  | a     | 157 | LYS  |
| 13  | a     | 161 | ARG  |
| 13  | a     | 190 | ARG  |
| 13  | a     | 215 | GLU  |
| 14  | b     | 9   | LYS  |
| 14  | b     | 36  | ARG  |
| 14  | b     | 92  | ASN  |
| 14  | b     | 105 | LYS  |
| 14  | b     | 107 | LYS  |
| 14  | b     | 119 | VAL  |
| 14  | b     | 178 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (186) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 149 | GLN  |
| 2   | B     | 20  | GLN  |
| 2   | B     | 95  | GLN  |
| 2   | B     | 102 | ASN  |
| 2   | B     | 119 | GLN  |
| 2   | B     | 123 | GLN  |
| 2   | B     | 124 | HIS  |
| 2   | B     | 155 | ASN  |
| 3   | C     | 17  | GLN  |
| 3   | C     | 38  | ASN  |
| 3   | C     | 116 | GLN  |
| 3   | C     | 120 | GLN  |
| 3   | C     | 147 | GLN  |
| 3   | C     | 160 | GLN  |
| 3   | C     | 233 | GLN  |
| 3   | C     | 239 | GLN  |
| 4   | D     | 15  | GLN  |
| 4   | D     | 91  | HIS  |
| 4   | D     | 100 | ASN  |
| 4   | D     | 106 | GLN  |
| 4   | D     | 160 | ASN  |
| 4   | D     | 210 | GLN  |
| 4   | D     | 225 | ASN  |
| 5   | E     | 3   | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 4   | ASN  |
| 5   | E     | 68  | HIS  |
| 5   | E     | 99  | ASN  |
| 5   | E     | 116 | GLN  |
| 5   | E     | 118 | ASN  |
| 5   | E     | 120 | GLN  |
| 5   | E     | 151 | ASN  |
| 5   | E     | 209 | ASN  |
| 6   | F     | 58  | GLN  |
| 6   | F     | 86  | ASN  |
| 6   | F     | 117 | GLN  |
| 6   | F     | 140 | ASN  |
| 6   | F     | 191 | GLN  |
| 6   | F     | 203 | ASN  |
| 6   | F     | 240 | GLN  |
| 7   | G     | 6   | HIS  |
| 7   | G     | 30  | ASN  |
| 7   | G     | 83  | ASN  |
| 7   | G     | 114 | ASN  |
| 7   | G     | 117 | GLN  |
| 7   | G     | 121 | GLN  |
| 7   | G     | 166 | GLN  |
| 7   | G     | 175 | ASN  |
| 7   | G     | 184 | HIS  |
| 7   | G     | 186 | ASN  |
| 7   | G     | 242 | GLN  |
| 8   | H     | 9   | ASN  |
| 8   | H     | 30  | ASN  |
| 8   | H     | 66  | HIS  |
| 8   | H     | 165 | ASN  |
| 8   | H     | 172 | ASN  |
| 8   | H     | 189 | ASN  |
| 9   | I     | 37  | ASN  |
| 9   | I     | 63  | ASN  |
| 9   | I     | 71  | ASN  |
| 9   | I     | 88  | GLN  |
| 9   | I     | 203 | GLN  |
| 10  | J     | 37  | GLN  |
| 10  | J     | 55  | GLN  |
| 10  | J     | 63  | ASN  |
| 10  | J     | 146 | HIS  |
| 10  | J     | 147 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | J     | 191 | GLN  |
| 11  | K     | 29  | GLN  |
| 11  | K     | 85  | ASN  |
| 11  | K     | 133 | GLN  |
| 11  | K     | 176 | ASN  |
| 11  | K     | 190 | ASN  |
| 11  | K     | 208 | ASN  |
| 12  | L     | 3   | ASN  |
| 12  | L     | 29  | ASN  |
| 12  | L     | 36  | ASN  |
| 12  | L     | 49  | ASN  |
| 12  | L     | 70  | ASN  |
| 12  | L     | 76  | HIS  |
| 12  | L     | 80  | ASN  |
| 12  | L     | 152 | ASN  |
| 12  | L     | 153 | GLN  |
| 12  | L     | 165 | ASN  |
| 12  | L     | 197 | GLN  |
| 13  | M     | 18  | ASN  |
| 13  | M     | 48  | ASN  |
| 13  | M     | 102 | GLN  |
| 13  | M     | 108 | ASN  |
| 13  | M     | 194 | ASN  |
| 13  | M     | 203 | ASN  |
| 13  | M     | 211 | ASN  |
| 13  | M     | 213 | GLN  |
| 14  | N     | 38  | HIS  |
| 14  | N     | 141 | ASN  |
| 1   | O     | 149 | GLN  |
| 2   | P     | 20  | GLN  |
| 2   | P     | 95  | GLN  |
| 2   | P     | 119 | GLN  |
| 2   | P     | 123 | GLN  |
| 2   | P     | 124 | HIS  |
| 2   | P     | 155 | ASN  |
| 2   | P     | 220 | ASN  |
| 3   | Q     | 38  | ASN  |
| 3   | Q     | 116 | GLN  |
| 3   | Q     | 120 | GLN  |
| 3   | Q     | 147 | GLN  |
| 3   | Q     | 160 | GLN  |
| 3   | Q     | 233 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Q     | 239 | GLN  |
| 4   | R     | 15  | GLN  |
| 4   | R     | 91  | HIS  |
| 4   | R     | 100 | ASN  |
| 4   | R     | 146 | GLN  |
| 4   | R     | 160 | ASN  |
| 4   | R     | 210 | GLN  |
| 4   | R     | 225 | ASN  |
| 5   | S     | 3   | ASN  |
| 5   | S     | 4   | ASN  |
| 5   | S     | 68  | HIS  |
| 5   | S     | 99  | ASN  |
| 5   | S     | 116 | GLN  |
| 5   | S     | 118 | ASN  |
| 5   | S     | 120 | GLN  |
| 5   | S     | 151 | ASN  |
| 5   | S     | 209 | ASN  |
| 6   | T     | 58  | GLN  |
| 6   | T     | 86  | ASN  |
| 6   | T     | 117 | GLN  |
| 6   | T     | 123 | ASN  |
| 6   | T     | 140 | ASN  |
| 6   | T     | 191 | GLN  |
| 6   | T     | 203 | ASN  |
| 6   | T     | 240 | GLN  |
| 7   | U     | 30  | ASN  |
| 7   | U     | 83  | ASN  |
| 7   | U     | 114 | ASN  |
| 7   | U     | 117 | GLN  |
| 7   | U     | 121 | GLN  |
| 7   | U     | 166 | GLN  |
| 7   | U     | 175 | ASN  |
| 7   | U     | 184 | HIS  |
| 7   | U     | 186 | ASN  |
| 7   | U     | 242 | GLN  |
| 8   | V     | 9   | ASN  |
| 8   | V     | 30  | ASN  |
| 8   | V     | 165 | ASN  |
| 8   | V     | 172 | ASN  |
| 8   | V     | 189 | ASN  |
| 8   | V     | 200 | GLN  |
| 9   | W     | 37  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | W     | 63  | ASN  |
| 9   | W     | 71  | ASN  |
| 9   | W     | 88  | GLN  |
| 9   | W     | 203 | GLN  |
| 10  | X     | 37  | GLN  |
| 10  | X     | 55  | GLN  |
| 10  | X     | 63  | ASN  |
| 10  | X     | 86  | GLN  |
| 10  | X     | 191 | GLN  |
| 11  | Y     | 29  | GLN  |
| 11  | Y     | 85  | ASN  |
| 11  | Y     | 133 | GLN  |
| 11  | Y     | 176 | ASN  |
| 11  | Y     | 208 | ASN  |
| 12  | Z     | 3   | ASN  |
| 12  | Z     | 29  | ASN  |
| 12  | Z     | 36  | ASN  |
| 12  | Z     | 49  | ASN  |
| 12  | Z     | 70  | ASN  |
| 12  | Z     | 80  | ASN  |
| 12  | Z     | 152 | ASN  |
| 12  | Z     | 153 | GLN  |
| 12  | Z     | 155 | ASN  |
| 12  | Z     | 165 | ASN  |
| 12  | Z     | 197 | GLN  |
| 13  | a     | 18  | ASN  |
| 13  | a     | 48  | ASN  |
| 13  | a     | 102 | GLN  |
| 13  | a     | 108 | ASN  |
| 13  | a     | 194 | ASN  |
| 13  | a     | 203 | ASN  |
| 13  | a     | 211 | ASN  |
| 13  | a     | 213 | GLN  |
| 14  | b     | 38  | HIS  |
| 14  | b     | 69  | GLN  |
| 14  | b     | 161 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 13 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 | $\# Z  > 2$ |
| 16  | VOX  | H     | 301 | 8    | 49,49,49     | 1.95 | 8 (16%)     | 62,64,64    | 1.41 | 11 (17%)    |
| 16  | VOX  | V     | 301 | 8    | 49,49,49     | 2.04 | 7 (14%)     | 62,64,64    | 1.41 | 8 (12%)     |
| 16  | VOX  | Y     | 301 | 11   | 49,49,49     | 1.89 | 7 (14%)     | 62,64,64    | 1.30 | 7 (11%)     |
| 18  | SO4  | N     | 204 | -    | 4,4,4        | 0.32 | 0           | 6,6,6       | 0.07 | 0           |
| 18  | SO4  | b     | 202 | -    | 4,4,4        | 0.32 | 0           | 6,6,6       | 0.08 | 0           |
| 16  | VOX  | K     | 301 | 11   | 49,49,49     | 1.97 | 8 (16%)     | 62,64,64    | 1.16 | 8 (12%)     |

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   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 16  | VOX  | H     | 301 | 8    | -       | 10/53/53/53 | 0/2/3/3 |
| 16  | VOX  | Y     | 301 | 11   | -       | 9/53/53/53  | 0/2/3/3 |
| 16  | VOX  | K     | 301 | 11   | -       | 10/53/53/53 | 0/2/3/3 |
| 16  | VOX  | V     | 301 | 8    | -       | 13/53/53/53 | 0/2/3/3 |

All (30) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | Y     | 301 | VOX  | C37-C38 | -7.18 | 1.37        | 1.51     |
| 16  | H     | 301 | VOX  | C37-C38 | -6.89 | 1.37        | 1.51     |
| 16  | V     | 301 | VOX  | C37-C38 | -6.87 | 1.37        | 1.51     |
| 16  | K     | 301 | VOX  | C37-C38 | -6.77 | 1.37        | 1.51     |
| 16  | K     | 301 | VOX  | C30-C31 | -6.11 | 1.37        | 1.52     |
| 16  | V     | 301 | VOX  | C30-C31 | -6.02 | 1.37        | 1.52     |
| 16  | V     | 301 | VOX  | C8-C9   | -5.61 | 1.35        | 1.51     |
| 16  | H     | 301 | VOX  | C30-C31 | -5.50 | 1.39        | 1.52     |
| 16  | Y     | 301 | VOX  | C30-C31 | -5.39 | 1.39        | 1.52     |
| 16  | H     | 301 | VOX  | C8-C9   | -5.34 | 1.36        | 1.51     |
| 16  | Y     | 301 | VOX  | C8-C9   | -4.76 | 1.38        | 1.51     |
| 16  | K     | 301 | VOX  | C20-C19 | -4.55 | 1.37        | 1.51     |
| 16  | Y     | 301 | VOX  | C20-C19 | -4.51 | 1.37        | 1.51     |
| 16  | K     | 301 | VOX  | C36-C34 | -4.47 | 1.46        | 1.53     |
| 16  | V     | 301 | VOX  | C20-C19 | -4.42 | 1.38        | 1.51     |
| 16  | H     | 301 | VOX  | C20-C19 | -4.28 | 1.38        | 1.51     |
| 16  | K     | 301 | VOX  | C8-C9   | -4.06 | 1.40        | 1.51     |
| 16  | V     | 301 | VOX  | C36-C34 | -3.69 | 1.47        | 1.53     |
| 16  | H     | 301 | VOX  | C36-C34 | -3.63 | 1.47        | 1.53     |
| 16  | V     | 301 | VOX  | C12-N14 | -2.60 | 1.31        | 1.39     |
| 16  | H     | 301 | VOX  | C12-N14 | -2.59 | 1.31        | 1.39     |
| 16  | K     | 301 | VOX  | C42-C43 | -2.58 | 1.45        | 1.52     |
| 16  | V     | 301 | VOX  | C16-N15 | -2.49 | 1.31        | 1.39     |
| 16  | H     | 301 | VOX  | C46-C26 | -2.43 | 1.46        | 1.53     |
| 16  | Y     | 301 | VOX  | C16-N15 | -2.42 | 1.31        | 1.39     |
| 16  | K     | 301 | VOX  | C16-N15 | -2.27 | 1.32        | 1.39     |
| 16  | H     | 301 | VOX  | C16-N15 | -2.16 | 1.32        | 1.39     |
| 16  | Y     | 301 | VOX  | C12-N14 | -2.10 | 1.32        | 1.39     |
| 16  | Y     | 301 | VOX  | C31-N33 | 2.08  | 1.38        | 1.34     |
| 16  | K     | 301 | VOX  | C42-C41 | -2.02 | 1.45        | 1.52     |

All (34) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | K     | 301 | VOX  | C35-C34-C36 | -4.05 | 104.09      | 111.48   |
| 16  | H     | 301 | VOX  | C48-C46-C26 | -3.73 | 104.91      | 112.29   |
| 16  | Y     | 301 | VOX  | O32-C31-N33 | -3.68 | 116.38      | 122.96   |
| 16  | V     | 301 | VOX  | C35-C34-C36 | -3.58 | 104.96      | 111.48   |
| 16  | V     | 301 | VOX  | C16-N15-N14 | -3.36 | 110.14      | 119.14   |
| 16  | V     | 301 | VOX  | O32-C31-N33 | -3.34 | 116.98      | 122.96   |
| 16  | H     | 301 | VOX  | C46-C26-C27 | -3.13 | 104.49      | 111.32   |
| 16  | H     | 301 | VOX  | C37-C36-C34 | -3.02 | 109.30      | 114.04   |
| 16  | K     | 301 | VOX  | C37-C36-C34 | -2.89 | 109.50      | 114.04   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 16  | Y     | 301 | VOX  | C46-C26-N25 | -2.78 | 104.31      | 111.70   |
| 16  | H     | 301 | VOX  | O32-C31-N33 | -2.75 | 118.03      | 122.96   |
| 16  | Y     | 301 | VOX  | C37-C36-C34 | -2.73 | 109.75      | 114.04   |
| 16  | Y     | 301 | VOX  | C41-N40-C38 | -2.73 | 117.74      | 122.82   |
| 16  | H     | 301 | VOX  | C34-N33-C31 | -2.55 | 117.94      | 123.91   |
| 16  | V     | 301 | VOX  | C4-C3-C1    | -2.54 | 106.15      | 113.19   |
| 16  | H     | 301 | VOX  | C35-C34-C36 | -2.48 | 106.97      | 111.48   |
| 16  | K     | 301 | VOX  | C42-C41-N40 | -2.43 | 105.21      | 111.88   |
| 16  | H     | 301 | VOX  | C4-C3-C1    | -2.42 | 106.48      | 113.19   |
| 16  | K     | 301 | VOX  | O32-C31-N33 | -2.42 | 118.62      | 122.96   |
| 16  | Y     | 301 | VOX  | C36-C34-N33 | 2.30  | 114.38      | 110.42   |
| 16  | K     | 301 | VOX  | C48-C46-C26 | -2.29 | 107.77      | 112.29   |
| 16  | V     | 301 | VOX  | C37-C36-C34 | -2.25 | 110.51      | 114.04   |
| 16  | Y     | 301 | VOX  | C34-N33-C31 | -2.24 | 118.68      | 123.91   |
| 16  | Y     | 301 | VOX  | C35-C34-C36 | -2.23 | 107.42      | 111.48   |
| 16  | H     | 301 | VOX  | C24-C9-C10  | 2.22  | 121.53      | 118.23   |
| 16  | V     | 301 | VOX  | C23-C22-C19 | -2.12 | 118.93      | 121.37   |
| 16  | K     | 301 | VOX  | C45-C43-C42 | -2.11 | 107.96      | 112.42   |
| 16  | H     | 301 | VOX  | C16-N15-N14 | -2.09 | 113.54      | 119.14   |
| 16  | V     | 301 | VOX  | C34-N33-C31 | -2.08 | 119.05      | 123.91   |
| 16  | V     | 301 | VOX  | C48-C46-C26 | -2.08 | 108.18      | 112.29   |
| 16  | K     | 301 | VOX  | C46-C26-N25 | -2.07 | 106.19      | 111.70   |
| 16  | H     | 301 | VOX  | C7-C8-C9    | -2.07 | 105.95      | 113.67   |
| 16  | H     | 301 | VOX  | C23-C22-C19 | -2.06 | 119.00      | 121.37   |
| 16  | K     | 301 | VOX  | C46-C26-C27 | -2.05 | 106.84      | 111.32   |

There are no chirality outliers.

All (42) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 16  | H     | 301 | VOX  | C41-C42-C43-O44 |
| 16  | H     | 301 | VOX  | N29-C30-C45-C43 |
| 16  | K     | 301 | VOX  | C41-C42-C43-O44 |
| 16  | K     | 301 | VOX  | N29-C30-C45-C43 |
| 16  | V     | 301 | VOX  | C41-C42-C43-O44 |
| 16  | V     | 301 | VOX  | N29-C30-C45-C43 |
| 16  | Y     | 301 | VOX  | C41-C42-C43-O44 |
| 16  | Y     | 301 | VOX  | N29-C30-C45-C43 |
| 16  | K     | 301 | VOX  | C34-C36-C37-C38 |
| 16  | H     | 301 | VOX  | C31-C30-C45-C43 |
| 16  | V     | 301 | VOX  | C31-C30-C45-C43 |
| 16  | K     | 301 | VOX  | C31-C30-C45-C43 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 16  | K     | 301 | VOX  | C6-C7-C8-C9     |
| 16  | Y     | 301 | VOX  | C31-C30-C45-C43 |
| 16  | Y     | 301 | VOX  | C6-C7-C8-C9     |
| 16  | V     | 301 | VOX  | C17-C16-N15-N14 |
| 16  | Y     | 301 | VOX  | C1-C3-C4-C5     |
| 16  | K     | 301 | VOX  | C41-C42-C43-C45 |
| 16  | K     | 301 | VOX  | C3-C4-C5-C6     |
| 16  | Y     | 301 | VOX  | C5-C6-C7-C8     |
| 16  | V     | 301 | VOX  | C11-C12-N14-N15 |
| 16  | V     | 301 | VOX  | C23-C16-N15-N14 |
| 16  | V     | 301 | VOX  | C1-C3-C4-C5     |
| 16  | H     | 301 | VOX  | C34-C36-C37-C38 |
| 16  | V     | 301 | VOX  | C4-C5-C6-C7     |
| 16  | V     | 301 | VOX  | C41-C42-C43-C45 |
| 16  | V     | 301 | VOX  | C13-C12-N14-N15 |
| 16  | H     | 301 | VOX  | C5-C6-C7-C8     |
| 16  | Y     | 301 | VOX  | C41-C42-C43-C45 |
| 16  | H     | 301 | VOX  | C6-C7-C8-C9     |
| 16  | H     | 301 | VOX  | C4-C5-C6-C7     |
| 16  | K     | 301 | VOX  | C4-C5-C6-C7     |
| 16  | K     | 301 | VOX  | C5-C6-C7-C8     |
| 16  | H     | 301 | VOX  | C41-C42-C43-C45 |
| 16  | V     | 301 | VOX  | C34-C36-C37-C38 |
| 16  | Y     | 301 | VOX  | C3-C4-C5-C6     |
| 16  | K     | 301 | VOX  | O44-C43-C45-C30 |
| 16  | H     | 301 | VOX  | C27-C26-N25-C1  |
| 16  | V     | 301 | VOX  | C6-C7-C8-C9     |
| 16  | H     | 301 | VOX  | C3-C4-C5-C6     |
| 16  | Y     | 301 | VOX  | C34-C36-C37-C38 |
| 16  | V     | 301 | VOX  | C3-C4-C5-C6     |

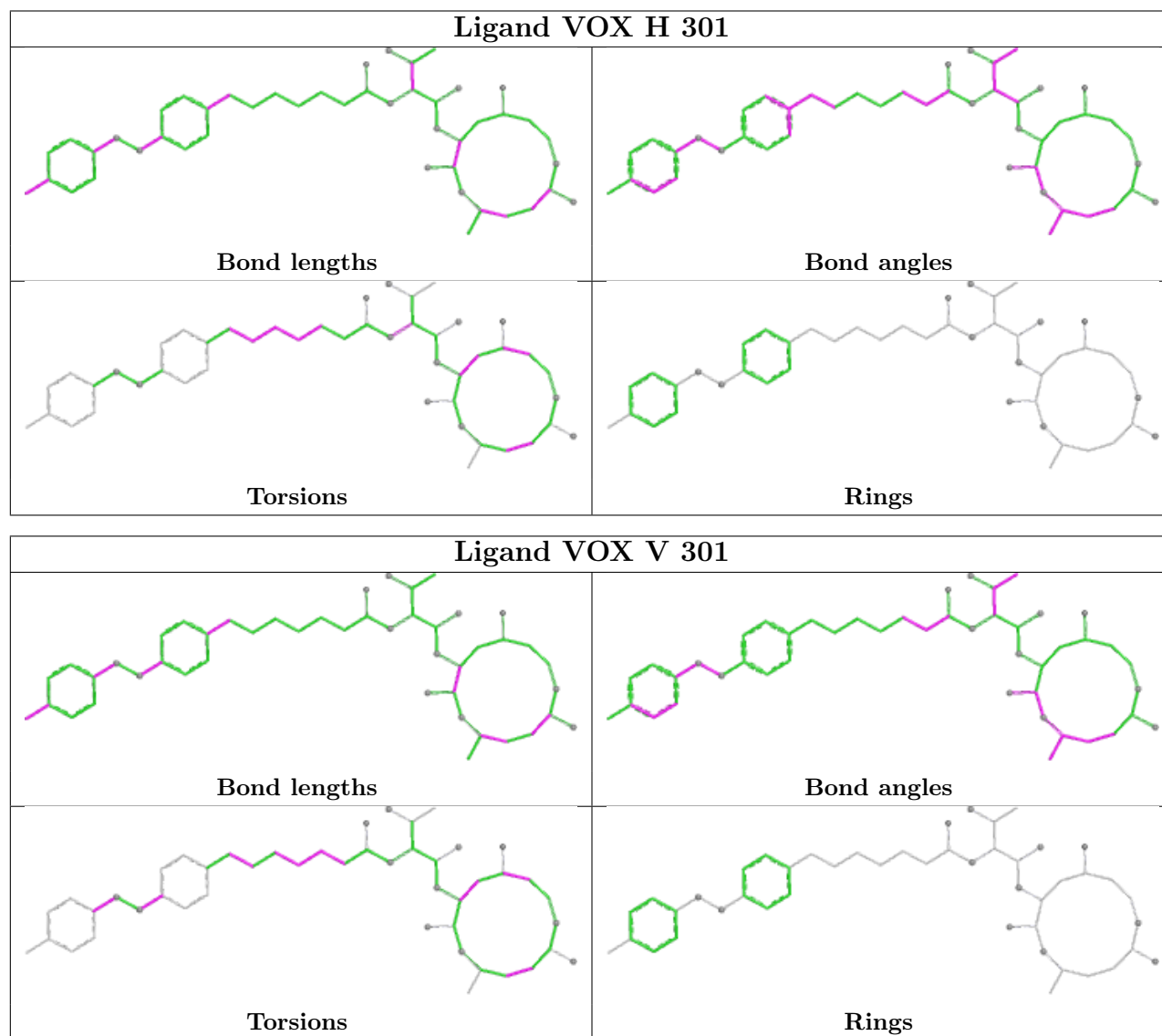
There are no ring outliers.

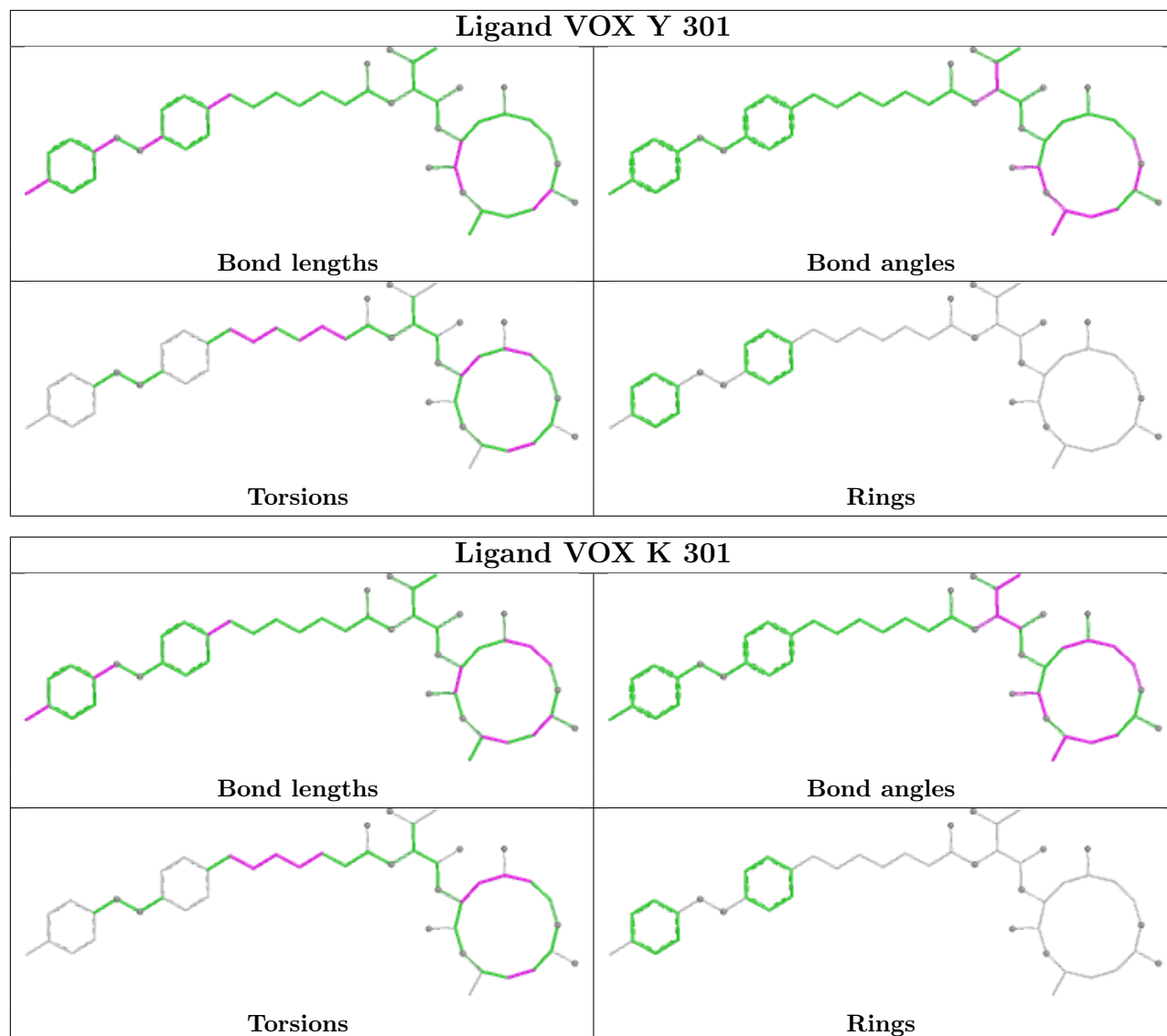
2 monomers are involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 16  | H     | 301 | VOX  | 1       | 0            |
| 16  | Y     | 301 | VOX  | 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.





## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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     | 250/250 (100%) | -0.57  | 1 (0%) 88 86 | 67, 85, 118, 174      | 0       |
| 1   | O     | 250/250 (100%) | -0.54  | 0 100 100    | 72, 92, 125, 174      | 0       |
| 2   | B     | 244/258 (94%)  | -0.33  | 1 (0%) 88 86 | 69, 93, 142, 174      | 0       |
| 2   | P     | 244/258 (94%)  | -0.38  | 2 (0%) 82 78 | 72, 95, 146, 179      | 0       |
| 3   | C     | 240/254 (94%)  | -0.38  | 1 (0%) 88 86 | 67, 95, 146, 166      | 0       |
| 3   | Q     | 240/254 (94%)  | -0.30  | 1 (0%) 88 86 | 74, 105, 161, 176     | 0       |
| 4   | D     | 235/260 (90%)  | -0.44  | 0 100 100    | 70, 94, 122, 156      | 0       |
| 4   | R     | 235/260 (90%)  | -0.46  | 0 100 100    | 71, 100, 135, 152     | 0       |
| 5   | E     | 231/234 (98%)  | -0.42  | 0 100 100    | 75, 99, 128, 158      | 0       |
| 5   | S     | 231/234 (98%)  | -0.36  | 0 100 100    | 78, 108, 145, 176     | 0       |
| 6   | F     | 243/288 (84%)  | -0.44  | 0 100 100    | 68, 92, 133, 166      | 0       |
| 6   | T     | 243/288 (84%)  | -0.46  | 0 100 100    | 73, 99, 139, 153      | 0       |
| 7   | G     | 241/252 (95%)  | -0.48  | 0 100 100    | 64, 87, 115, 157      | 0       |
| 7   | U     | 241/252 (95%)  | -0.53  | 0 100 100    | 68, 88, 119, 141      | 0       |
| 8   | H     | 226/232 (97%)  | -0.53  | 0 100 100    | 64, 81, 111, 173      | 0       |
| 8   | V     | 226/232 (97%)  | -0.47  | 1 (0%) 88 86 | 64, 83, 115, 181      | 0       |
| 9   | I     | 204/205 (99%)  | -0.52  | 0 100 100    | 64, 83, 109, 139      | 0       |
| 9   | W     | 204/205 (99%)  | -0.55  | 0 100 100    | 64, 82, 110, 139      | 0       |
| 10  | J     | 195/198 (98%)  | -0.53  | 0 100 100    | 65, 84, 111, 150      | 0       |
| 10  | X     | 195/198 (98%)  | -0.52  | 1 (0%) 87 83 | 68, 87, 110, 146      | 0       |
| 11  | K     | 212/212 (100%) | -0.51  | 1 (0%) 87 83 | 69, 87, 112, 131      | 0       |
| 11  | Y     | 212/212 (100%) | -0.52  | 1 (0%) 87 83 | 69, 88, 116, 132      | 0       |
| 12  | L     | 222/222 (100%) | -0.48  | 0 100 100    | 65, 83, 116, 138      | 0       |
| 12  | Z     | 222/222 (100%) | -0.52  | 0 100 100    | 65, 84, 119, 136      | 0       |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 13  | M     | 233/246 (94%)   | -0.52  | 0 100 100     | 66, 85, 108, 128      | 0     |
| 13  | a     | 233/246 (94%)   | -0.54  | 1 (0%) 88 86  | 64, 84, 105, 123      | 0     |
| 14  | N     | 196/196 (100%)  | -0.50  | 0 100 100     | 68, 80, 110, 125      | 0     |
| 14  | b     | 196/196 (100%)  | -0.49  | 0 100 100     | 66, 82, 111, 127      | 0     |
| All | All   | 6344/6614 (95%) | -0.47  | 11 (0%) 91 90 | 64, 89, 130, 181      | 0     |

All (11) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | Q     | 50  | LEU  | 3.7  |
| 10  | X     | 1   | MET  | 3.6  |
| 11  | K     | 211 | ILE  | 3.4  |
| 1   | A     | 1   | MET  | 3.1  |
| 11  | Y     | 211 | ILE  | 2.9  |
| 13  | a     | 1   | THR  | 2.7  |
| 2   | B     | 51  | VAL  | 2.3  |
| 3   | C     | 205 | ALA  | 2.3  |
| 2   | P     | 1   | GLY  | 2.2  |
| 2   | P     | 60  | THR  | 2.2  |
| 8   | V     | 223 | ILE  | 2.1  |

## 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(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 15  | MG   | I     | 302 | 1/1   | 0.82 | 0.19 | 117,117,117,117            | 0     |

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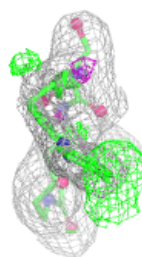
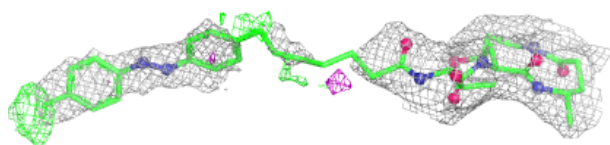
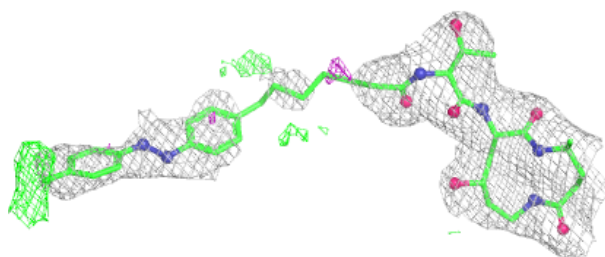
*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 18  | SO4  | N     | 204 | 5/5   | 0.91 | 0.21 | 110,111,116,121             | 0     |
| 18  | SO4  | b     | 202 | 5/5   | 0.91 | 0.15 | 138,138,144,150             | 0     |
| 15  | MG   | K     | 303 | 1/1   | 0.92 | 0.15 | 92,92,92,92                 | 0     |
| 16  | VOX  | K     | 301 | 47/47 | 0.93 | 0.11 | 65,80,122,125               | 0     |
| 16  | VOX  | V     | 301 | 47/47 | 0.93 | 0.10 | 66,80,109,118               | 0     |
| 16  | VOX  | H     | 301 | 47/47 | 0.94 | 0.10 | 70,82,119,121               | 0     |
| 16  | VOX  | Y     | 301 | 47/47 | 0.94 | 0.10 | 70,81,113,116               | 0     |
| 17  | CL   | b     | 201 | 1/1   | 0.95 | 0.11 | 90,90,90,90                 | 0     |
| 15  | MG   | I     | 301 | 1/1   | 0.95 | 0.19 | 92,92,92,92                 | 0     |
| 15  | MG   | N     | 202 | 1/1   | 0.95 | 0.04 | 76,76,76,76                 | 0     |
| 15  | MG   | Z     | 301 | 1/1   | 0.96 | 0.05 | 86,86,86,86                 | 0     |
| 15  | MG   | K     | 302 | 1/1   | 0.96 | 0.06 | 88,88,88,88                 | 0     |
| 15  | MG   | Y     | 302 | 1/1   | 0.97 | 0.05 | 84,84,84,84                 | 0     |
| 15  | MG   | G     | 301 | 1/1   | 0.97 | 0.07 | 89,89,89,89                 | 0     |
| 15  | MG   | V     | 302 | 1/1   | 0.97 | 0.09 | 104,104,104,104             | 0     |
| 17  | CL   | N     | 203 | 1/1   | 0.98 | 0.07 | 92,92,92,92                 | 0     |
| 15  | MG   | J     | 201 | 1/1   | 0.98 | 0.10 | 61,61,61,61                 | 0     |
| 15  | MG   | N     | 201 | 1/1   | 0.99 | 0.07 | 72,72,72,72                 | 0     |

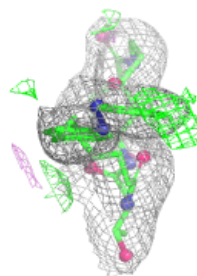
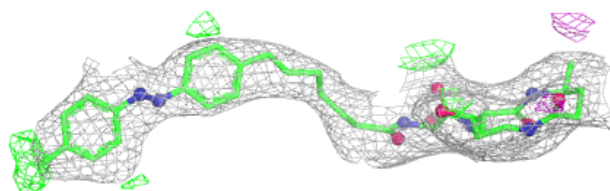
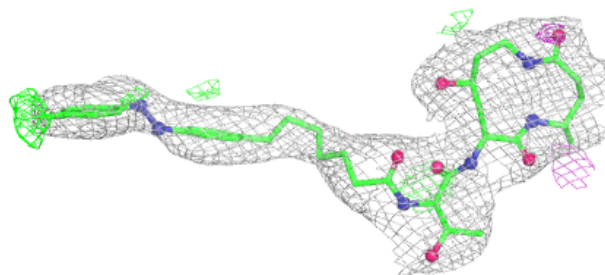
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around VOX 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)

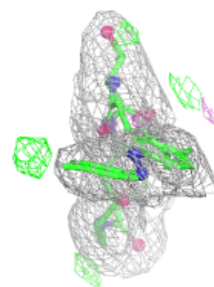
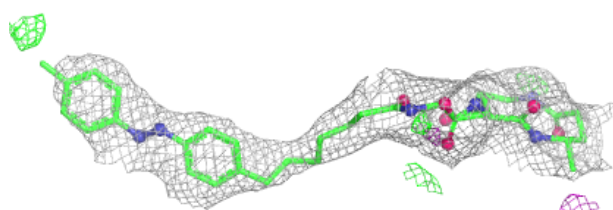
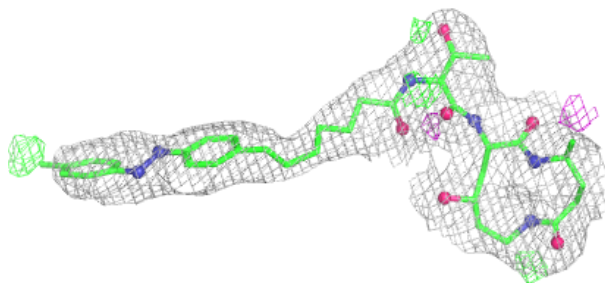
**Electron density around VOX V 301:**

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

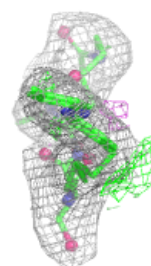
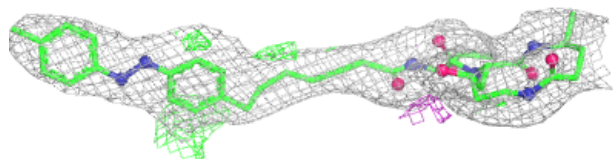
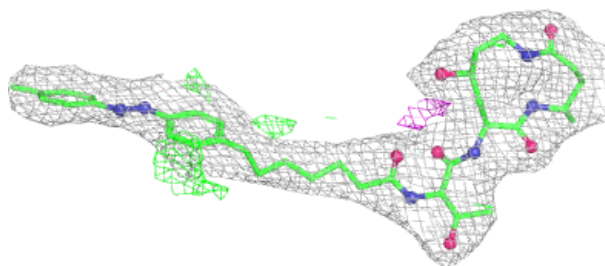


**Electron density around VOX H 301:**

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

**Electron density around VOX 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)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.